

DRAFT - WORK IN PROGRESS

Where Theoretical Physics Comes From

Trevor Scheopner
trevor@scheopner.com

Please send any errors you notice or feedback for improvement to the author.

©2025 Trevor Scheopner.
All Rights Reserved.

If you got something out of this book and want to support me:



<https://ko-fi.com/trevorscheopner>

June 26, 2025

Contents

What is the point?	viii

I Classical Physics	1

1 Analytical Mechanics	3

1.1 Physics is Dynamics	3
1.2 Physics as a Science	7
1.3 Writing Transformations	12
1.3.1 The Generator of a Transformation	12
1.3.2 The Lie Bracket	15
1.3.3 The Phase Space	16
1.4 Hamilton's Equations	18
1.5 Functional Differentiation	22
1.5.1 Motivating the Definition	22
1.5.2 Relationship with Partial Differentiation	23
1.5.3 The Euler-Lagrange Formula	25
1.6 The Existence of an Invariant Action	29
1.7 The Lagrangian	32
1.8 The Non-uniqueness of the Action	37
1.9 Canonical Transformations	41
1.9.1 Time Reversal	43
1.9.2 Preservation of the Poisson Bracket	44
1.9.3 Common Subsets of Transformations	50
1.10 Noether's Theorem (Version 1)	55
1.11 Lie Algebras and Lie Groups	60
1.12 (2 nd Pass) Incorporating Higher Derivatives	65
1.13 (2 nd Pass) The Hamilton-Jacobi Equation	68
1.14 (2 nd Pass) Adiabatic Invariants and Integrable Systems	70
1.15 (2 nd Pass) The Theorem of Normal Modes	77
1.15.1 Linear Stability Analysis	78
1.15.2 Hamiltonian Diagonalization	79
1.16 (2 nd Pass) General Coordinates on Phase Space	81
1.17 Summary and Additional Reading	84

2 Nonrelativistic Classical Mechanics	86

2.1 Galilean Boost Symmetry	87
2.2 Time Translational Symmetry	92
2.3 Translational Symmetry	95
2.4 Rotational Symmetry	98
2.5 Interpreting the Galilean Lagrangian	107
2.6 Equations of Motion	110
2.7 Effective Theories, Top Down and Bottom Up	115
2.8 Incorporating Constraints	132

2.8.1	Holonomic Constraints	133
2.8.2	Velocity Constraints	136
2.8.3	(2 nd Pass) Phase Space Constraints	138
2.8.4	Inequality Constraints	149
2.9	Rigid Bodies	156
2.9.1	The Axis-Angle Lagrangian for a Rigid Body	156
2.9.2	Angular Velocity and the Principal Axes	159
2.9.3	Rigid Body Action in Frame-Angular Velocity Coordinates	161
2.9.4	Spin Angular Momentum and the Hamiltonian	162
2.9.5	Angular Momentum Poisson Brackets	163
2.10	Summary and Additional Reading	176
3	Nonrelativistic Interactions	178
3.1	The Potentials as Variables	178
3.1.1	The Continuity Equation	179
3.1.2	Charge Conservation Causes Gauge Symmetry	180
3.2	Classical Field Theory	184
3.2.1	The Action in Classical Field Theory	184
3.2.2	The Hamiltonian in Classical Field Theory	185
3.2.3	Locality	186
3.3	Accounting for Symmetries	193
3.3.1	Transformation Properties of the Potentials	193
3.3.2	Gauge Symmetry	194
3.3.3	Rotational Symmetry	196
3.3.4	Galilean Boost Symmetry	198
3.3.5	Parity Symmetry	199
3.4	Gauss' Law	201
3.4.1	Solving the Poisson Equation	202
3.4.2	Effective Equations of Motion	205
3.4.3	Effective Lagrangian	207
3.5	Ampere's Law	210
3.6	Newtonian Gravity	215
3.7	Electrostatics	230
3.8	Magnetostatics	250
3.9	Electromagnetic Coexistence and Causality	264
3.9.1	A Big Bold Leap	264
3.9.2	Electromagnetic Waves	265
3.9.3	Much Ado About Boosting	267
3.10	Problems with Point Matter	274
3.11	Summary and Additional Reading	277
4	Relativistic Classical Mechanics	280
4.1	Lorentz Boost Symmetry	280
4.2	The Free Lagrangian of a Relativistic Particle	289
4.3	The Interacting Hamiltonian of a Relativistic Particle	293
4.4	Lorentz Transformation of the Fields	301
4.5	Maxwell's Equations	304
4.6	Electromagnetic Hamiltonian	312
4.7	Fixing Electromagnetism broke Gravity	345
4.8	The Failure of Point Particles	349
4.8.1	The Liénard-Wiechert Potentials	349
4.8.2	Smoothed Equations of Motion	351
4.8.3	A Wave Theory of Matter?	355
4.9	Covariant Notation, Spacetime, and Tensors	359
4.9.1	Tensors, a New Friend You Already Knew	361
4.9.2	Covariant Equations of Motion	364

4.10	The Structure of the Lorentz Group	372
4.10.1	Components of the Improper Lorentz Group	372
4.10.2	Generators of the Lorentz Group	375
4.11	Noether's Theorem (Version 2)	379
4.11.1	Field Canonical Transformations	379
4.11.2	Noether's Current	381
4.11.3	Existence of a Poincare Invariant Action	384
4.11.4	Energy-Momentum Tensor	384
4.12	Summary and Additional Reading	390
5	Classical Statistical Mechanics	393
5.1	The Role and Meaning of Probability	393
5.1.1	Defining Probability	393
5.1.2	Discrete Random Variables	398
5.1.3	Continuous Random Variables	403
5.1.4	(2 nd Pass) Overly Philosophical Rambling	410
5.2	The Liouville Equation	422
5.3	The First Law of Thermodynamics	430
5.4	Microcanonical Ensemble	432
5.5	Canonical Ensemble	435
5.6	Information Theory and Entropy	448
5.7	The Second Law of Thermodynamics	459
5.8	Thermal Quasidynamics	467
5.9	Quasistatics and Thermodynamic Potentials	473
5.9.1	Identical Particles and Boltzmann Statistics	475
5.9.2	Example: Nonrelativistic Ideal Gases	477
5.10	Thermodynamic Processes and Stability	484
5.10.1	Phase Transitions	487
5.10.2	Example: Van der Waals Fluid	489
5.10.3	Chemical Reactions and the Grand Canonical Ensemble	495
5.11	Linear Response Theory	502
5.12	The Ultraviolet Catastrophe	509
5.12.1	An aside on Fourier Series	510
5.12.2	Electromagnetism in a Conducting Box	512
5.12.3	Black Body Radiation	518
5.12.4	Planck's Law	519
5.13	Summary and Additional Reading	523
6	Continuum Mechanics	525
6.1	Degrees of Freedom in Continuum Mechanics	525
6.2	Nonrelativistic Transport Equations	529
6.3	Nonrelativistic Kinetic Theory	534
6.3.1	Particle Transfer	534
6.3.2	Momentum Transfer	536
6.3.3	Energy Transfer	538
6.4	Nonrelativistic Constitutive Relations	543
6.4.1	Gases	543
6.4.2	Fluids	546
6.4.3	Solids	549
6.4.4	Plasma	552
6.5	Nonrelativistic Continuum Mechanical Actions	563
6.5.1	Active Formulation	563
6.5.2	Passive Formulation	568
6.6	Relativistic Transport Equations	572
6.7	Relativistic Ideal Continuum Mechanics	581
6.8	Relativistic Dissipative Continuum Mechanics	585

6.9	Summary and Additional Reading	588
7	General Relativity	589
7.1	Diffeomorphism Symmetry	589
7.1.1	What Does Gravity Interact With?	589
7.1.2	What is a Diffeomorphism?	591
7.1.3	General Coordinate Transformations	592
7.1.4	Lie Derivatives	596
7.2	Differentiation on Manifolds	601
7.2.1	Connection and Covariant Differentiation	601
7.2.2	Geodesic Equation	608
7.2.3	Local Inertial Frames	610
7.3	General Relativistic Particle	613
7.4	Integration on Manifolds	618
7.4.1	Spacetime Integration	618
7.4.2	Surface Integration	620
7.4.3	Stokes' Theorem	624
7.5	Spacetime Curvature	626
7.5.1	Riemann Curvature Tensor	626
7.5.2	Wilson Loops	630
7.6	Classical Field Theory in Curved Spacetime	636
7.6.1	Covariant Equations of Motion	636
7.6.2	Field Canonical Transformations	638
7.6.3	Noether's Theorem (Version 3)	639
7.6.4	Spacetime Symmetries	642
7.6.5	Energy-Momentum Tensor	644
7.7	Einstein-Hilbert Action	649
7.7.1	Gibbons-Hawking-York Boundary Term	650
7.7.2	Cosmological Constant	654
7.7.3	Newtonian Limit	657
7.7.4	Vierbein Description and the Spin Connection	658
7.8	Arnowitt-Deser-Misner Formalism	664
7.9	Summary and Additional Reading	688
7.10	Conclusion to Part I	690
II	Quantum Physics	692
8	Single Particle Quantum Mechanics	694
8.1	The Linear Algebra of Fields	697
8.2	The Schrödinger Equation	701
8.2.1	Hermitian vs. Self-Adjoint	704
8.2.2	The Spectral Theorem	705
8.2.3	Adiabatic Invariants in Quantum Mechanics	710
8.3	Wigner's Theorem	714
8.4	Continuous Transformations in Quantum Mechanics	720
8.5	Summary and Spread Coordinates	727
8.5.1	Operator Spreads	733
8.5.2	The Classical Limit	737
8.5.3	The meaning of $\hbar$	740
8.5.4	Rigged Hilbert Space	742
8.5.5	The Phenomenological Born Rule	743
8.6	Scalar Theory - The Galilean Schrödinger Equation	755
8.6.1	Interaction with Electromagnetism	758
8.6.2	Gauge Transformation Geometry	760
8.6.3	Charge Conservation	765

8.7	Angular Momentum	778
8.7.1	Representations of $SU(2)$	780
8.7.2	Spherical Harmonics	786
8.8	Spinor Theory - The Pauli Equation	799
8.9	Scattering Theory	812
8.9.1	The Interaction Picture	813
8.9.2	The Dyson Series	814
8.9.3	The Lippmann-Schwinger Equation	816
8.9.4	The Transition Matrix	820
8.9.5	Transition Rates and Fermi's Master Equation	822
8.9.6	Analytic Properties of the S Matrix	824
8.9.7	Nonrelativistic Single Particle Scattering	827
8.9.8	Scattering in 1 Spatial Dimension	829
8.9.9	Scattering in 3 Spatial Dimensions	831
8.10	Another Big Bold Leap	839
8.10.1	Trouble with Multi-particle Statistics	839
8.10.2	Quantum Field Theory to the Rescue	840
8.11	Summary and Additional Reading	854
9	Quantum Mechanics in General	857
9.1	Why Quantum Mechanics?	857
9.1.1	Quantum Ex Nihilo	857
9.1.2	Why Density Matrices?	864
9.1.3	Entanglement	867
9.1.4	Canonical Structure of Density Matrices	870
9.2	The Classical Limit	875
9.2.1	The Weyl Transform	875
9.2.2	Classicality Conditions	879
9.2.3	Groenewold's theorem	883
9.2.4	Quantum Mechanics in Classical Phase Space	885
9.3	The Measurement Problem	892
9.4	Misinterpretations of Quantum Mechanics	901
9.4.1	Copenhagen Interpretation	902
9.4.2	Post-Schrödinger Dynamics	905
9.4.3	Many Worlds Interpretation	905
9.4.4	The Damned Cat	907
9.4.5	Bell-type Theorems and Their Consequences	909
9.5	The Path Integral	912
9.5.1	The Path Integral for Time Evolution	912
9.5.2	Important Subtleties	914
9.5.3	The Path Integral for Vacuum Expectation Values	916
9.5.4	The Path Integral for the Quantum Harmonic Oscillator	920
9.6	Quantum Statistical Mechanics	925
9.6.1	The First Law of Thermodynamics	925
9.6.2	Thermodynamic Equilibrium	926
9.6.3	Von Neumann Entropy	928
9.6.4	Planck's Law	932
9.6.5	Bose-Einstein and Fermi-Dirac Statistics	932
9.6.6	The Lindblad Equation	936
9.7	Summary and Additional Reading	947
10	Quantum Field Theory	948
10.1	Summary and Additional Reading	949
11	Gauge Theory	950

12 The Standard Model	951
12.1 Summary and Additional Reading	952
13 Quantum Gravity	953
A Mathematical Identities	954
A.1 Coordinate Systems	954
A.2 Fourier Transform Conventions	956
A.3 Asymptotic notation	957
B Systems of Units	959
B.1 Discussion of Different Systems	959
B.2 Conversion Chart	963
C How to write your Lagrangian	965
D References	966

What is the point?

Note for the graduate student likely reading this. The chapters in this book most closely line up with typical graduate courses as follows:

Graduate Classical Mechanics	→	Chapters 1, 2, 3, 4, 6
Graduate Electromagnetism	→	Chapters 3, 4, 6
Graduate Statistical Mechanics	→	Chapters 5, 9
Graduate Quantum Mechanics	→	Chapters 8, 9
Graduate General Relativity	→	Chapter 7
Graduate Quantum Field Theory	→	Chapters 10, 11, 12, 13.

Warning: This book is a work in progress. It contains typos, pieces of incomplete reasoning, and likely flawed arguments. Every section is in need of proofreading and editing. Part I is basically “complete”. Part II is currently under development and may fluctuate between being reasonable, incoherent, or empty. Don’t take Part II seriously yet. If you find errors you think I’m unaware of, please let me know. Throughout this book I include more steps of algebra than is typical for physics. I will trim these down with time while trying to keep the important steps. I will box equations which are important “results” to be clearly distinct from equations which are stepping stones. Please judge this work by the standard of a project not yet completed.

There comes a time in every physicist’s life when they realize they learned everything in the wrong order. We tend to learn the most specific and least general models first (Newton’s laws, Coulomb’s law, etc.) and then later use them to “derive” more general versions (Lagrangian or Hamiltonian mechanics, Gauss’ law) which we are led at least initially to believe are equivalent. We teach this way because this was the order things happened historically. However, the old versions and new versions are **NOT** equivalent. In physics education we tend to cling to these false equivalences by introducing misleading concepts (such as “relativistic mass”) or ignoring true discoveries (such as incorrectly deeming the vector potential unphysical) to try to hold the old worldview together as long as possible. This becomes progressively more untenable as one gets deeper into their physics education. One day one is forced to abandon their original worldview and is left uncertain what the right starting principles actually are or how the old ones were selected. Some students give up trying to have a coherent picture of physics altogether and learn to be cynical; they learn to “shut up and calculate”. I believe we can do better.

Most undergraduates learn physics just by being told what are the right things to do. Maxwell’s equations, thermodynamics, et cetera simply fall onto them from the sky with no clear picture how they could have come up with those theories themselves. This results in most students understanding physics as a loose collection of facts with a poor conception of what is more fundamental than what. Organizing physics this way is inefficient and obfuscates many deeper principles. The common argument for organizing the material this way is that the real stuff – the Lagrangian/Hamiltonian/action formalism – is too abstract for young students. At the graduate level this is entirely inappropriate but still common. The lucky students eventually learn how symmetries restrict the form of the Lagrangian and just how powerful and general the variational approach is. The even luckier come to learn that the variational approach (the Lagrangian/Hamiltonian formalism) is fundamental to every single branch of physics and is the most conceptually clear way to understand all of them. But, by then even these luckiest students have had to spend so much time redoing the hierarchy of information of physics in their minds. What if we just started with the fundamental principles first so that nothing has to be undone? That is the goal of this work.

This is a graduate level book that exists to explain and apply the “metatheory” of how to “come up with a theory” of physics. We will see how following some very believable assumptions about the universe using some math and experimental guidance, you will naturally be led to Newtonian mechanics, then to replace it

with relativistic classical mechanics, single particle quantum mechanics, and so on eventually arriving at our status quo understanding of theoretical physics that everything is an effective theory of which our best present model is Lorentz invariant quantum field theory with a need to incorporate gravity in a way not yet well understood. Consequently, this is ultimately a book about “effective theory” and what goes right and wrong with common effective theories of interest. While we will discuss many different theories, our understanding of all of them will be consistently born out of the fundamental ideas of analytical mechanics. Analytical mechanics provides a single core algorithm that forms the foundation of how to do useful theoretical physics. The basic outline of the algorithm is:

1. Based on your system of interest, decide which variables are needed to describe your system with an action.
2. Decide what symmetries you believe your system to have.
3. Based on your desired experimental resolution, decide what order in Taylor expansion you need to be accurate to in your action.
4. Compute the most general possible action consistent with your desired symmetries to the desired order of approximation.
5. From that action compute the equations of motion of your theory and from those equations of motion compute the observables of the theory, again to the desired order of approximation.

While we will cover many different theories with correspondingly different domains of validity, this algorithm will always apply. We will see that all of the theories which seem to just materialize out of nowhere when learning physics for the first time can be justified as outputs of this more modern perspective with just some basic experimental guidance to help with pulling off the first three steps. While a typical physics book would present theories as the final dishes of a master chef, hopefully this one can teach you what ingredients to use and how to use them to cook that dish for yourself.

Each section has accompanying homework questions. Some are just practice but others introduce or expand on concepts to be used later. The especially important homework questions are marked with a ★ symbol and a list of them is given at the end of each chapter in the summary section. **It is essential for understanding this work that you at the very least solve the homework questions marked with ★.** In undergrad, Kyoungchul Kong told me to really claim to have read a physics book you have to solve at least half of its homework questions; at the time I thought that was too strict, now I see it is quite wise.

We will spend the overwhelming majority of our time on general theoretical results. Most specific experimental predictions will be homework questions. References to experimental results will be made as necessary to judge the viability of the theory. We will cover many topics and most of them go much deeper than we discuss. I will try to give good references to additional reading on topics as we cross them. We will discuss how to come up with a theory and check some basic properties of it. It is then another task for another book to calculate the detailed consequences of theories of interest and yet another task to test those consequences experimentally. To say we are doing science, a theory must eventually in some way connect to experiment.

This book is physics graduate level in general. The required math background will mostly be just standard vector calculus, linear algebra, and differential equations. There will be times where deeper knowledge is needed, especially in the later chapters. When more mathematics is necessary, references for learning will be given. For students needing to refresh their knowledge of vector calculus, I suggest [111], [17], [18]; for linear algebra, I suggest [30], [84]; and for differential equations, I suggest [10], [115].

Importantly, this is a physics book. Mathematical deductions and derivations which culminate in “theorems” will not be proven or stated as rigorously as they would be by a mathematician. Some derivations and conclusions may need to be rigorized to be satisfying to a mathematician. For example, we will typically work as if all unspecified functions we are working with are analytic or at least smooth. We will work with the Dirac delta distribution without a discussion of measure theory or a treatment of test functions. We will commute limits without proving if it is safe to do so (although we will comment on some places where it is not safe to do so). When we do quantum mechanics we will only mention briefly the difference between Hermitian and self-adjoint and then neglect the distinction. We may refer to the “position basis” and “momentum basis” even though neither the position nor momentum “eigenstates” are in the Hilbert space of square integrable functions (or even functions at all in the case of position eigenstates). These are just some examples of the mathematical imperfections we will endure. I personally place a high value on rigorous mathematics and so all “theorems” here are intended to be understood as “proven at the standards of a physicist” by proofs which are “correct in spirit”. That is, when the proofs given lack full rigor, there typically exist proofs which have a similar line of thinking starting from appropriately formalized hypotheses but with full rigor which

prove the appropriately rigorized conclusion of the theorem and that the rigorous conclusion will have the same meaning for all intents and purposes of this work as the less rigorously stated version. In essence, I have attempted to the best of my ability to give results essentially provable by rigorous mathematics formulated in a way which is more palatable to a typical physicist but which has not lost the heart of the underlying mathematics.

All of the effort of this text serves to explain Figure 1. Our journey through physics will lead us through three different theories of the geometry of the universe of increasing generality, power, and challenge. First we will have flat space with invariant time (Euclidean with Galilean Symmetry). Then, flat space with invariant speed of light (Minkowskian with Poincare Symmetry). And finally, we will arrive at curved spacetime with invariant speed of light (Lorentzian with Diffeomorphism Symmetry). We will also go through two different theories of matter. The first will be classical physics in which matter is described (most naively) by interacting point particles moving in space or (more generally) by interacting wave-packets moving in space. The second will be quantum physics in which matter and all forces are different interacting modes of one big wave on the space of classical configurations. These two independent selections lead to a grid of six different regimes of physics. Each regime but the bottom right corner has known issues with theoretical consistency and/or matching experiment which led to the discover of a new regime. For each regime I have selected a pair of concepts in red which are experimentally necessary but theoretically at odds within that regime; reconciling these pairs requires the discovery of the new regime it points to. Then, the new regime reduces approximately to the old regime when the circumstance shown in green is valid. The bottom right corner, which by the logic of the diagram would be our ultimate theory, is at the time not well understood theoretically and even once understood may very well have new problems. It is also presently inaccessible experimentally. The exact meanings of all these words, precise analyses of how to come up with each regime and see its failures, and some discussion of why the obvious ways of attempting this final theory don't work is the meat of this work. Importantly, note that the overwhelming majority of ongoing physics research is done in the 5 "non-final" regimes, which each still contain exciting questions and applications, not in the final one, which presently is too far out experimentally to warrant saying much about with any confidence.

In order to get this started, Chapter 1 describes Analytical Mechanics, which is the mathematical framework that everything we do will be based on. Its goal is to derive all of the common tools of physics (the Hamiltonian, the Lagrangian, the Action, Noether's Theorem, et cetera) rather than to assert them without justification. In order to do so, a little bit of discussion about Lie algebras and Lie groups is necessary, which is likely to be new content to the reader. We will not need to go into much detail on the topic, but to supplement our discussion for the interested reader I highly recommend [41], [81], [80], [83], [2], [48]. As well, additional topics and practice on analytical mechanics can be found in [117], [37] although they only discuss analytical mechanics in the particular context of classical mechanics. To get a treatment of classical mechanics which appropriately supplements our discussion of analytical mechanics, I recommend [2], [48], [120].

Chapter 2 covers non-relativistic (more correctly, Galilean relativistic) classical mechanics and so sits within the topics discussed in [117], [37], [2]. The goal of chapter 2 is to derive the equations of motion for Galilean classical mechanical matter (which may also be called Newtonian mechanics, depending on one's precise categorization scheme) from symmetry but other reading will significantly supplement how to usefully apply those equations of motion. If a more introductory background on Galilean classical mechanics is felt necessary to the reader, [56] provides a strong but very traditional introduction.

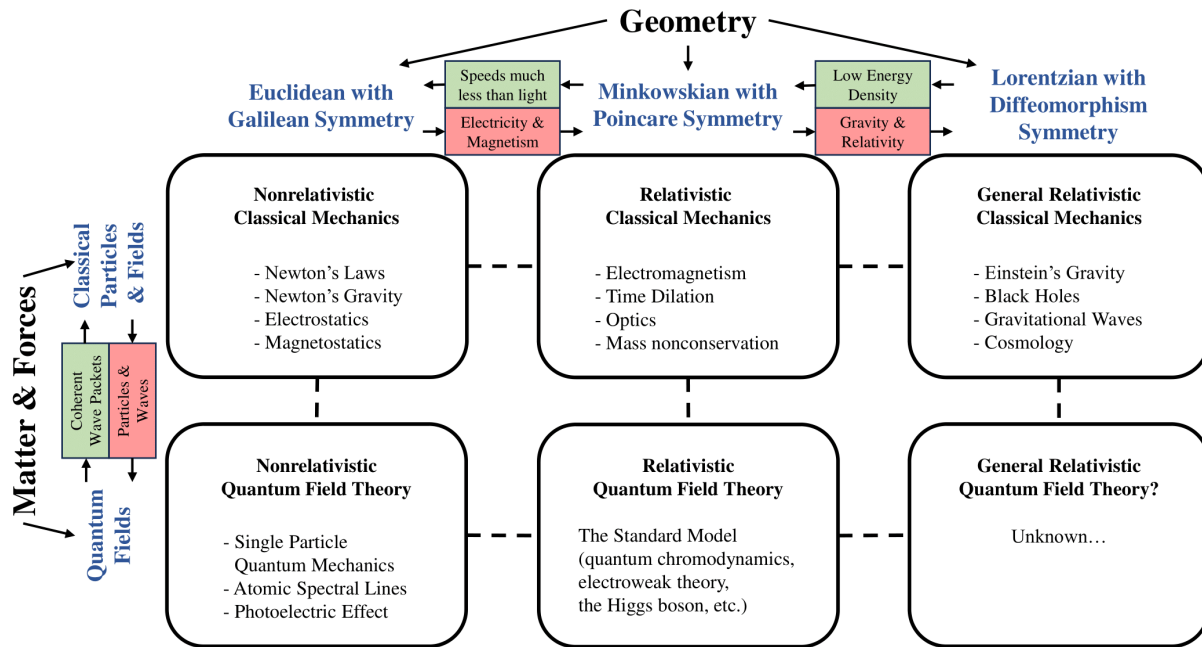


Figure 1: The map of the regimes of physical theories together with just some of the successes of each theory.

Chapter 3 covers Galilean mechanical interactions, meaning electrostatics, magnetostatics, and Newtonian gravity. These are covered in the mentioned classical mechanics texts as well as in the early chapters of common electromagnetism texts. The goal of chapter 3 is again to derive those theories from symmetry rather than to just assert them. In totality, the first three chapters culminate in our first candidate theory of physics, Galilean Classical Mechanics, and an analysis of some of its successes and failures.

Chapter 4 introduces (special) relativity, the classical mechanics of relativistic particles, and electromagnetism as a classical field theory while deriving the latter two from the assumptions of the first. These topics are expanded on in several of the mentioned classical mechanics texts. [121] provides the best foundation for electromagnetism (but is short) and [89] provides a strong introduction at a lower level for the unfamiliar student. Using [121] to guide your thinking, there are many more examples and problems to get your hands on in [52] and [128], and so they are useful for practice. Because chapter 4 (and chapter 3 as well) brings us firmly into the domain of classical field theory, [109] is a good companion. These first 4 chapters will culminate in another flawed theory of physics, Relativistic Classical Mechanics, which far outperforms the original Galilean theory. At the end of this chapter we will explore the breakdown of relativistic classical mechanics due to the fundamental problem with point particles. Special relativity is incompatible with Newton's gravity and so in this chapter we will find that an improved theory of gravity is necessary, but not yet try to look for it.

Before resolving that breakdown, we will make a slight detour in Chapter 5 to study statistical mechanics and the physics of large systems comprised of many similar (or identical) constituents. Statistical mechanics is necessary to understand the physics of the everyday world as most systems in daily life consist of just so very many things. Somewhat surprisingly, statistical mechanics will prove itself to make fundamental statements about what theories can and cannot possibly describe our universe. Statistical mechanics requires a proper knowledge of probability, which is a math topic which you should learn from a mathematician. I recommend [123]. For applying the theory of probability in the form of statistics to physics, [20], [53], [19] are very useful. For additional reading on statistical mechanics, [57], [116], and [106] are very good. The laws of statistical mechanics culminate in the nicely self-contained theory of thermodynamics, for which [13] provides the strongest foundation. We will find in this chapter that there is a fundamental tension between the theories of statistical mechanics and classical field theory. We will see this tension repeatedly until we resolve it in Part II.

In Chapter 6 we will use our statistical mechanical results to study collective phenomena and continuum mechanics such as the dynamics of gases, fluids, solids, and plasmas. This chapter will present the basics of some of the most important ways in which the content of the first 5 chapters can be applied and show that

an interacting theory of matter with electromagnetism is possible if instead of point particles we consider continuous wave matter. We will also study some generic properties of classical wave theories (called classical field theories) in this chapter.

In Chapter 7 we will find the theory of gravity consistent with relativity, known as general relativity. This will allow us to study General Relativistic Classical Mechanics. At this point [109] is necessary. General relativity is a remarkable and successful theory of gravity but does nothing to resolve the tension between classical fields and statistical mechanics. This chapter will conclude Part I with us having two unresolved puzzles: what is the appropriate microscopic model for matter and how to resolve the inconsistency between classical field theory and statistical mechanics? These question will end classical physics.

In Part II we find that both puzzles are solved with one theoretical advancement, known as quantum mechanics. In quantum mechanics, a single matter particle is described by a wave-packet, not a moving point. This just sounds like classical field theory. While that is true for single particle quantum mechanics, in multiparticle quantum mechanics the system is described by a single wave on the space of all possible configurations of all the particles, not by an independent wave in space for each particle. This causes the statistical properties of quantum mechanics to be significantly different from classical field theory and resolves the tension with statistical mechanics. Quantum mechanics also allows changes in the numbers of particles, as they can be created or annihilated in interactions. The full theory of changing particle number is known as quantum field theory, in which the entire universe is a single large quantum system.

We will start Part II with Chapter 8 which derives all of the fundamental results of single particle quantum mechanics from basic definitions and symmetries. For further exposition see [3], [76], [98]. Ultimately, chapter 8 allows us to describe a single quantum particle interacting with electromagnetism. It will also lead us to discover the necessity of quantum field theory for describing more than one particle.

Chapter 9 will derive the general structure of quantum mechanics and its common tools (density matrices, the von Neumann equation, the path integral, the difference between classical and quantum symmetries, the classical limit, the theory of measurement).

Chapter 10 will use the general properties of quantum mechanics to understand the basics of quantum field theory. This will include free field theory and the famous spin-statistics theorem, which characterizes the statistical behavior of particle systems in a way determined by their spin. The spin-statistics theorem is necessary for explaining the macroscopic properties of matter and the periodic table of elements.

Chapter 11 will develop gauge theory, which is a general formulation of all three forces that are relevant in particle physics, electromagnetism, the nuclear weak force, and the nuclear strong force. Studying these will also let us develop the essential calculation tools of quantum field theory, such as renormalization and how to extract scattering observables from the path integral. From this point, [86] and [112] are helpful supplements.

Chapter 12 will combine quantum electrodynamics, quantum chromodynamics, and further fields (due to the nuclear weak interaction, neutrinos, and the Higgs boson) to form the standard model of particle physics, which is the most successful theory of physics to date. As a quantum field theory, the standard model is able to explain almost every phenomenon we have observed in nature.

Unfortunately, one of the most glaring failures of the standard model is its lack of a theory of gravity. Chapter 13 will discuss why it is so difficult to adapt the standard model to include a theory of gravity and discuss what are considered future prospects for physics beyond the standard model.

The underlying philosophy and content of this work are strongly inspired by conversations with John P. Ralston.

Part I

Classical Physics

Physics can be understood, and it can be understood by you.

Chapter 1

Analytical Mechanics

From definition by reason all follows.

This chapter is the foundation of everything else going forward. While it is essential to read this chapter before continuing, it is not expected that the reader should feel *completely* comfortable with the material of this chapter before moving on. At first, much of this chapter is likely to feel abstract but it will become easier to understand as it is applied in later chapters. Several later sections in this chapter can be skipped on a first read and returned to once they become relevant later on. Those sections are labeled as “2nd pass”. It may seem odd to write the first chapter in this way, but I saw no other way to organize the material without jeopardizing the fidelity of it.

On a first read through, the reader should focus on completely understanding sections 1.1 and 1.2, following at a conceptual level what is broadly going on in sections 1.3-1.11, and understanding what the theorems tell you are true in sections 1.4-1.11. Sections 1.12-1.15 are all 2nd pass sections. Understanding every calculation detail and logical step in sections 1.3-1.11 can be saved for later and will be easier after the reader has gotten some familiarity with applying the tools in those sections in examples. That familiarity will be developed by reading further. But, I insist that the reader should return back to this chapter and read it again once they are ready. Physics is often best read multiple times and in a different order each time ¹.

1.1 Physics is Dynamics

When we say we are doing physics we mean that we are trying to answer some variant of the question: given what a **system** of interest is doing now, what will it be doing later? (Variations include: what was it doing earlier? or what will it do in the long-run?) Fundamentally, this question is about **time evolution**. Something called time happens and systems evolve with it. The entire enterprise of physics is devoted to understanding *how* different systems evolve with it. Because we are attempting to describe the time evolution of the real world, we must use the only known technique for studying the real world consistently: the scientific method. Altogether this means that:

Physics is the science of time evolution.

The business of time evolution can be handled very efficiently and effectively by a kind of mathematics called **Analytical Mechanics**. Analytical mechanics describes how the state of a system changes with time using some special mathematical tools that we will develop over the rest of this chapter. Time appears to pass continuously in an ordered way (we can order the events we see from earlier to later). So, if we were to consider all of the events which occur during some duration of time, we could identify a real number t_0 with the first event in that duration and another real number t_f with the last event in that duration. To any other events between these two, we assign a real number t which is greater than all of the values of t for events before that event and less than all of the values of t for events after that event. In this way, we can identify any particular time with a real number t that gives “what time it is right now”. A time t_1 which is

¹Of course, the reordering should be purposeful as opposed to haphazard.

less than some other time t_2 would always be “before” t_2 and t_2 would always be “after” t_1 . For any given duration, the times t_0 and t_f could be chosen to be anything. Often, we choose t_0 for a duration of interest to be defined to be $t_0 = 0$. Alternatively t_f is usually measured by using a device which can measure durations of time (more on that later). By the **state** of a system we mean “the way the system is right now” where a system is just any set of things in the world. A system could mean a block, a gas, a person, a stock market, a planet, a galaxy, or the whole universe. The way a system is (the state) generally changes with time. The set of all possible states the system can take is called the **phase space** $\mathbb{P}$ of the system. At each particular time t then, the state at that time will be some element of that set. Thus, we can think of the whole lifetime of our system as a function which takes the time t as input and gives as output the state at that time t . We call the state Φ and so the function $\Phi(t)$ describes the entire lifetime (or history, or trajectory) of our system. Mathematically, it is a map from the real numbers (time) into the phase space: $\Phi(t) : \mathbb{R} \rightarrow \mathbb{P}$. In practice we describe our state by some list of numbers $\Phi^1, \dots, \Phi^N$ where N is however many numbers it takes to successfully describe our system (these superscripts are not meant as exponents, just as an index to tell you which number in the list you are looking at). Then, each of these Φ^a (a is used as an index running from 1 to N) will be real-valued² functions of time and so we write $\Phi(t) = (\Phi^1(t), \dots, \Phi^N(t))$. If our system was the stock market this list could be the price of each stock or if our system was a box of gas it could be the position of every molecule of the gas within the box. The ultimate achievement of physics as a whole would be to take the system to be everything which exists (everything which exists is also called **the Universe**).

Calling some initial time $t_0 = 0$ and the state at that time $\Phi(0)$, time evolution then takes our system to a new state $\Phi(t)$ at a later time t . If in our definition of the phase space we have included all of the variables which define and affect our system then anything about our system can be expressed in terms of those variables by definition³. In order for physics to be possible, meaning time evolution is predictable, then all exact knowledge of all of the properties of our system now must determine all of the exact properties of our system later. So, there must exist some function $U(t, \Phi)$ which relates the later state to the initial state:

$$\Phi(t) = U(t, \Phi(0)). \quad (1.1.1)$$

Note that it is only true that the U in equation (1.1.1) exists because we assumed that the Φ are all of the variables affecting our system. A system which includes all of the variables affecting that system is called an **isolated system**. If there are variables outside of our Φ which affect the Φ (meaning our system is not isolated), just knowing the Φ 's alone won't tell us everything and thus we can't guarantee that the Φ 's at a later time can be determined from the Φ 's now. In reality, no system is exactly and entirely isolated except the whole universe. However, if we include all of the variables which have a big enough effect on our system for that effect to be noticeable in a given experiment, then the system will be as if it were isolated for the purposes of that experiment. This is why physics is reasonably straightforward to apply to a swinging pendulum (where the list of relevant variables is manageable) but not so easy to apply to the stock market (where the list of relevant variables is completely unmanageable). In principle, the logic works for either but the number of meaningful variables which affect tomorrow's stock prices beyond just today's stock prices makes the endeavor of including all of them nearly pointless. For our purposes, we will assume that when we are talking about a phase space we have accounted for all of the variables and thus equation (1.1.1) exists. Accomplishing this practically is another issue. Physics is not hopeless for systems for which not all of the factors can be accounted for but we will delay discussing such systems until Chapter 5. Assuming we have defined our phase space to include a complete list of variables, we have that the U in (1.1.1) exists. We shall assume $U(t, \Phi)$ is a smooth function of time (systems evolve smoothly in time; we can take as many time derivatives as we desire) and invertible as a function of the state Φ (exact knowledge of the present would allow one to calculate the past) with a smooth inverse which we call $U^{-1}(t, \Phi)$. Then, taking the derivative of equation (1.1.1), we have:

$$\frac{d\Phi}{dt}(t) = \frac{\partial U}{\partial t}(t, \Phi(0)). \quad (1.1.2)$$

As well, the inverse function by definition would take our state $\Phi(t)$ now and give us back our $\Phi(0)$ from

²We choose real-numbers because many physical properties are apparently continuous, such as length. Complex numbers are implicitly included as well as a complex number is just an ordered pair of real numbers with an additional multiplication rule. If you study enough math, you will come to appreciate that real numbers are horrendously complicated and that real valued functions of real numbers don't have any of the nice properties you might want. It happens instead that complex numbers are much simpler and work much more like how you would hope. Not so surprisingly then, complex numbers appear all over the place in physics. I like to say that the only *real* numbers are the complex numbers.

³If a property of our system could not be computed from our set of variables, our set of variables would not be complete.

earlier:

$$U^{-1}(t, U(t, \Phi(0))) = \Phi(0) \implies U^{-1}(t, \Phi(t)) = \Phi(0). \quad (1.1.3)$$

By substituting equation (1.1.3) into equation (1.1.2), we can actually write $\frac{d\Phi}{dt}$ in a way which does not depend on the initial conditions $\Phi(0)$:

$$\frac{d\Phi}{dt} = \frac{\partial U}{\partial t}(t, U^{-1}(t, \Phi(t))). \quad (1.1.4)$$

Define then the velocity field $V(t, \Phi) : \mathbb{R} \times \mathbb{P} \rightarrow \mathbb{P}$ such that:

$$V(t, \Phi) \stackrel{\text{def}}{=} \frac{\partial U}{\partial t}(t, U^{-1}(t, \Phi)). \quad (1.1.5)$$

This gives us:

Theorem 1.1: Existence of the equation of motion

If the system state Φ as a function of time t evolves smoothly and invertibly as a function of Φ with a smooth inverse, then there exists a function $V(t, \Phi)$ so that:

$$\frac{d\Phi}{dt} = V(t, \Phi(t)). \quad (1.1.6)$$

Equation (1.1.6) in words says that if you give me the state now and plug it into the function V , I can tell you how that state will change with time (the time derivative on the left hand side) and thus can tell you the future of that state. It is a differential equation, which the reader is assumed to be familiar with solving. (For students who need a refresher, see [10] for a solid introduction and [115] for a continuation up to the level necessary for this book.) The literature of differential equations gives conditions to guarantee the existence and uniqueness of solutions to equation (1.1.6) which are very broadly satisfied in physics⁴. If a solution to (1.1.6) exists and is unique then it must be our original map U as it is a solution by definition. Hence the requirements that time evolution be a deterministic, differentiable, invertible map imply that time evolution can be written in the form of equation (1.1.6) and suitable theorems of mathematics guarantee (1.1.6) can recover our original map in equation (1.1.1). Equation (1.1.6) is called a **dynamical system** or **equation of motion** and the key observation for us is that equation (1.1.6) tells us everything about what a system does in time. Therefore, because physics is all about time, to do physics we simply need to work with equation (1.1.6).

In all physics to date, the hypotheses necessary to prove Theorem 1.1 have given results consistent with experiment⁵. Therefore, we will assume them to be true for the rest of this book. That is, we assume:

Assumption :: PHSXI - Smoothness of time

Time is continuous and time evolution is deterministic, smooth, and smoothly invertible.

Note that this assumption is labeled “PHSX”. All assumptions labeled “PHSX” are always to be assumed true and are apparently actually true by experiment⁶.

Exercises

Problem 1.1: Manually finding V from U . Let Φ , the system state, be real number valued with time evolution map $U(t, \Phi_0)$ given by $U(t, \Phi_0) = e^{rt}\Phi_0$ for some constant r .

- (a) Following the steps of this section differentiate and invert $U(t, \Phi_0)$ to find $V(t, \Phi)$.

⁴There are particular instances in which existence or uniqueness fail which we will encounter but the default situation for us is that existence and uniqueness of solutions will be reliable.

⁵Later it will be useful for us to use descriptions of various systems which include redundant degrees of freedom known as gauge degrees of freedom. These variables are literally arbitrary but can be convenient to include for mathematical simplicity. Because they are arbitrary they do not have deterministic time evolution until you supply a choice for how they should evolve. However, all of the nonarbitrary variables in the system will still have deterministic evolution unaffected by the choice of the behavior of the gauge variables.

⁶Maybe one day any or all of them will be shown to be wrong. But given their overwhelming success so far, that would require quite an extraordinary observation and more than a bit of explanation.

(b) From the function $V(t, \Phi)$, solve the equation of motion and recover $U(t, \Phi_0)$.

Problem 1.2: Manually finding U from V . Let Φ , the system state, be real number valued with velocity field $V(t, \Phi)$ given by $V(t, \Phi) = r\Phi^2$ for some constant r .

(a) From the function $V(t, \Phi)$, solve the equation of motion and find $U(t, \Phi_0)$.

(b) Following the steps of this section, differentiate and invert $U(t, \Phi_0)$ to recover $V(t, \Phi)$.

Problem 1.3: From second order to first order. Suppose you have found that your system is described by a second order differential equation in one variable ϕ : $\ddot{\phi} = f(t, \phi, \dot{\phi})$. (Throughout this book dots above a symbol indicate the number of time derivatives.) Show that with the correct definition of the phase space, this can be rewritten as a pair of first order differential equations in the form of (1.1.6) and identify $V(t, \Phi)$ in that case.

Problem 1.4: From N^{th} order to first order. Suppose you have found that your system is described by an order N differential equation in one variable: $\overset{\cdot N}{\phi} = f(t, \phi, \dot{\phi}, \ddot{\phi}, \dots, \overset{\cdot N-1}{\phi})$. Show that with the correct definition of the phase space, this can be rewritten as N first order differential equations in the form of (1.1.6) and identify $V(t, \Phi)$ in that case.

Problem 1.5: From anything to first order. Suppose you have found that your system is described by k variables each satisfying a differential equation of order N_n : $\overset{\cdot N_n}{\phi}_n = f_n(t, \phi, \dot{\phi}, \dots)$ for $1 \leq n \leq k$ and each f_n only depending on ϕ_m (for $1 \leq m \leq k$) up to differentiation of order $N_m - 1$ or less. Show that with the correct definition of the phase space, this can be rewritten as a list of first order differential equations in the form of (1.1.6) and identify $V(t, \Phi)$ in that case.

1.2 Physics as a Science

There are three important theoretical issues with (1.1.6). First, in order to even write it down we need to know what the Φ 's are. We need to understand how to write all the properties which define the state of our system mathematically as variables. We call this **the problem of interpretation** because the issue is in identifying how to interpret a real physical system into a space of variables. Once the space of variables is known we then need to write the other side of equation (1.1.6). This requires knowledge of the $V(t, \Phi)$ functions that define the dynamics of the system. We call this **the problem of dynamics**. Finally, once both sides of the equation can be written we need to solve the differential equation. We call this **the problem of calculation**. Once all of these problems are solved, the predictions of the theory are known and it is now an experimental question if your theory is consistent with actual reality. Essentially, these are the only three problems in theoretical physics. Once solved, the theorist hands the problem off to the experimenter, the experimenter compares the predictions against reality, and then the experimenter returns with news for the theorist about whether they need to try again. This back and forth is the core of the scientific method.

The problem of interpretation can roughly be divided into three parts. First, one must determine what properties of a system affect how it behaves; second, one must translate those properties into mathematical variables; and third, one must identify which of these variables are in principle experimentally accessible. This first step (called defining your system) is essentially handled by trial and error. You must make a very detailed description of the system, listing all properties you can identify. Then, you take that description and go to the second step (called encoding your system). If everything after that goes successfully, your definition of your system was correct enough for your present purposes. If it does not, it was incorrect and you must try again with more detail. How specific you have to be and which variables to pick to define your system is often informed by experience with similar problems, but is at its core just educated trial and error (at some level science always is).

Once you have specified your description of your system, you need to encode that description into mathematical variables in order to use (1.1.6). In order to do this, you need a way to assign numbers to physical properties. This is done by a **unit system**. A unit system is a set of reference properties which the properties of actual physical systems can be measured relative to. For example, if you had a stick you could encode the length of any other object by giving the real number that you would have to multiply the length of the stick by to get the length of that object. Essentially, “how many copies” of your stick would you have to lay end-to-end to equal the object of interest in length. This stick then provides a “unit of length”. For example, if the stick were a meter stick (the world’s most popular stick), then it would take 1 full stick and 82% of a second stick to equal my height, so my height is 1.82 m where m is an abbreviation for meters. This comparison to reference values allows properties of physical objects, like height or length, to be converted into real numbers. The reference value (in this case the meter) is then called a unit of that quantity (the meter is a unit of length). Because the numerical value of that property depends on the reference value, one must **always** specify what reference value (that is, what unit) is being used. Saying my height is 1.82 m is okay but saying my height is 1.82 is not. Does 1.82 mean 1.82 meters? 1.82 feet? 1.82 times the height of my best friend’s dog? There is no way to tell! Different types of quantities may require different units. For example, having a unit of length on its own doesn’t give you a way to measure amounts of time. You need either a new unit for the passage of time or a way to convert lengths to times. You could define 1 second (1 s) by making reference to some arbitrary periodic process in nature such as $1/86400^{\text{th}}$ of a day. This gives a new unit of time. Or, you could define 1 s as the time it would take light to travel 299792458 meters. This latter way defines the unit of time by a conversion factor from an existing unit of length (the meter).

Once you have either through reference units (like the stick) or conversion factors (like $1 \text{ s} = \text{the time in which light travels } 299792458 \text{ meters}$) defined enough units to encode all of the described properties of your system into mathematical variables, all you have left to do in the problem of interpretation is specify how those properties in your theory are supposed to present themselves in experiment. Generally for one reason or another many of the variables of a system will not be directly experimentally observable, especially without significantly interfering with the system. So, in order to make a meaningful theory we must identify which variables of our system ought to be accessible in an experiment and specify how they may be accessed. It is obvious enough how to measure lengths of everyday objects with a ruler but not so obvious how to measure the pressure of a tank of gas. It would be even less obvious how to measure the velocity of an individual gas molecule. A well defined theory needs to be able to specify which of these variables are measurable and how. The correspondence between the resulting mathematical description of your system by a list of Φ 's in

appropriate units and your actual real life system is called the interpretation. That is, the interpretation of a system in physics is the dictionary which converts theory stuff (the variables and equations) into experiment stuff (what will I see happen, what does my measurement device read) and back.

Supposing you have solved the problem of interpretation and identified the correct space of variables, the next problem is the problem of dynamics. How do we know what $V(t, \Phi)$ to write down? We have two great tools at our disposal for answering this question: approximation and symmetry. Every number coming from an experiment has some quantifiable amount of uncertainty because every measuring tool has limited precision. Because of the finite precision of every measurement, every experimentally measured value must be reported with an error bar. For example, I am 1.82(1) m tall, meaning mean that I have a height of 1.82 meters with an error bar of 0.01 meters (parenthetical numbers at the end of measured value give the uncertainty in the last decimal places of that value). Similarly, the (low-energy) measured value of the fine-structure constant, which determines the strength of the electromagnetic interaction, is 0.0072973525693(11) (so it has best estimate value 0.0072973525693 with an error bar of 0.0000000000011). Because all experiments are done at some finite precision, we don't actually need to make exact predictions to know if our theory matches experiment. **We only need to predict with precision equal to or better than experiment** to know if we are right (more carefully, right enough for the purpose at hand). Conveniently, this allows us to neglect effects smaller than our experimental error and truncate approximations at finite order, greatly reducing the possible dynamics we need to consider. Consider for example an experiment in which a variable $x(t)$ is near 0, so close to 0 that the fourth power x^4 is always too small for the experiment to detect it. Then, rather than considering arbitrary smooth functions of x for V , we only need to Taylor expand V up to the order which our experiment can detect: $V(t, x) \approx a_0(t) + a_1(t)x + a_2(t)x^2 + a_3(t)x^3$. Anything higher than that we would never notice. That is, the finite precision of all experiments creates an equivalence class of theories giving experimentally indistinguishable predictions at that precision. This allows us to only have to work with the mathematically most convenient representative in that equivalence class rather than deal with each element. Instead of considering every possible theory, we only have to consider theories which are experimentally distinguishable.

No theory of physics has ever included every variable in the universe. Even if a theory claimed to do so, it would only really be able to experimentally claim to describe every variable known so far and eventually as experiments get more precise it could be discovered that there were effects unaccounted for. It is not really in the domain of science to ever claim a permanent exact description of the universe. Approximation is intrinsic to physics because the exact ultimate truth of the universe is not known and we would likely not know how to prove we were at the end even if we were. A theory which is valid (meaning makes experimentally correct predictions within an allowed tolerance) under certain circumstances is called an **effective theory** and the certain circumstances required are called the **domain of validity** of the theory. Because all theories are only applied within the limits of what is currently possible, **all theories are effective theories** and are subject to being replaced and explained by a more general theory as time goes on. The alternative of a naive “fundamental theory” which is permanently unaltered by future experiments is not something we have any reason to believe we will find in finite time. Presumably some exact description of the universe exists but scientifically we have no way of finding it; we only have the ability to get closer and closer asymptotically with time. We can still say that one theory is more fundamental than another if the second theory is a special case of the first. In this way, we are always trying to find more and more fundamental theories.

In addition to only needing to include terms in our theories which are relevant at the experimentally necessary precision, we also use **symmetry** to restrict which terms we need. A symmetry is any transformation of our system which leaves the dynamics of our system unchanged. For example, we observe the same laws of physics every day at all times and so under the transformation of translating everything forward in time, the dynamics (the equations of physics) remain the same. Therefore, we say the universe has time-translational symmetry. Consequently, whenever we make models of the universe we only include terms in the model which also have time-translation symmetry (which is actually very restrictive). This reduces the possibilities for the right hand side of (1.1.6). Because symmetries are so good at restricting what a system can do, in physics we try to find as many of them as possible and have developed a mathematical formalism called Analytical Mechanics which processes symmetries highly efficiently. More mathematically, a **transformation** T is any invertible map from the space of system states into itself: $T(\Phi) : \mathbb{P} \rightarrow \mathbb{P}$. A **symmetry** is any transformation which is preserved dynamically. That is, if $\Phi(0)$ is my untransformed state at time 0 and $\Phi'(0) = T(\Phi(0))$ is my transformed state at time 0, then the transformation T is a symmetry if and only if $T(\Phi(t)) = \Phi'(t)$ for all t where $\Phi'(t)$ is what the time evolution of $\Phi'(0)$ would be (we will often use Φ' to mean that the variable Φ has been transformed in some way, not to mean differentiation of any kind). Equivalently stated in terms

of the time evolution function in (1.1.1):

$$U(t, T(\Phi)) = T(U(t, \Phi)) \text{ for all } t \text{ and } \Phi \iff T \text{ is a Symmetry.} \quad (1.2.1)$$

So, the function composition of U and T must be the same as of T and U . This is said as “ T and U commute”. Another way of understanding this is through a commutative diagram. A transformation is a symmetry whenever applying the transformation either before or after applying the time evolution gives the same result. That is, both routes on this diagram lead to the same place:

$$\begin{array}{ccc} \text{Initial State } \Phi(0) & \xrightarrow{\text{Time Evolution}} & \text{Final State } \Phi(t) \\ \downarrow \text{Transformation} & & \downarrow \text{Transformation} \\ \text{Transformed Initial State } \Phi'(0) & \xrightarrow{\text{Time Evolution}} & \text{Transformed Final State } \Phi'(t). \end{array} \quad (1.2.2)$$

The symmetry condition (1.2.1) can also be stated very nicely and usefully in terms of the equations of motion. From $\Phi' = T(\Phi)$ and $\Phi = T^{-1}(\Phi')$ we can develop an equation of motion for Φ' regardless of whether T is a symmetry:

$$\frac{d\Phi'}{dt} = \frac{d}{dt}T(\Phi) = \frac{\partial T}{\partial \Phi}(\Phi) \frac{d\Phi}{dt} \quad (1.2.3)$$

$$= \frac{\partial T}{\partial \Phi}(T^{-1}(\Phi'))V(t, T^{-1}(\Phi')). \quad (1.2.4)$$

We identify then from (1.1.6) that the velocity field $V'(t, \Phi')$ for the Φ' coordinates is:

$$V'(t, \Phi') = \frac{\partial T}{\partial \Phi}(T^{-1}(\Phi'))V(t, T^{-1}(\Phi')). \quad (1.2.5)$$

Again, this holds true whether the transformation T is a symmetry or not. If we differentiate (1.2.1) we can see though what the symmetry condition tells us:

$$U(t, T(\Phi)) = T(U(t, \Phi)) \quad (1.2.6)$$

$$\implies \frac{\partial U}{\partial t}(t, T(\Phi)) = \frac{\partial T}{\partial \Phi}(U(t, \Phi)) \frac{\partial U}{\partial t}(t, \Phi) \quad (1.2.7)$$

$$\implies V(t, \Phi') = \frac{\partial T}{\partial \Phi}(\Phi)V(t, \Phi) \quad (1.2.8)$$

$$\implies V(t, \Phi') = V'(t, \Phi'). \quad (1.2.9)$$

Hence, we see the symmetry condition actually implies that the velocity field V' of the transformed coordinates is the exact same function as the velocity field V of the untransformed coordinates. In reverse, if V' and V are the exact same function, then trivially using either results in the same time evolution. So, in terms of the equations of motion, **a transformation is a symmetry if and only if it leaves the equations of motion unchanged as functions.**

To gain some intuition, consider two objects connected by a spring and sitting on a table. If I have two exactly identical copies of this two object system but one is just slid a few feet down the table from the other and I start them in exactly the same way, they will both do the exact same oscillations and will maintain the few feet of separation in time. Therefore sliding the two blocks down the table and then letting them move due to the spring is the same as letting them move due to the spring and then sliding them down the table. This means the two blocks on a spring system has translational symmetry (presuming they don't reach the end of the table and fall off) because its dynamics (moving due to the spring) are unchanged by translating the whole system on the table. If instead I considered a single block attached by a spring to a fixed wall and I took just the single moving block as my system, it would not have translational symmetry because starting the block different distances from the wall (which are all just a translation away from each other) gives oscillations of different amplitude and so the motions are not related by a simple overall translation. This shows also that symmetry depends on the definition of your system because if we included the wall in our system together with the block, then that system would have translational symmetry. We try to come up with what symmetries a system has by observation just as with the space of variables. So again, it is somewhat guesswork. However, once we have defined our symmetries and specified the order of approximation to which we will go, we can actually derive the equation of motion (1.1.6) highly systematically. We will see how to do this soon. In this way although identifying which symmetries you should assume is guesswork, what to do once you have those symmetries is systematic.

Once we have defined our space of variables, all the symmetries of our system, and the precision with

which we would like to calculate, we can find our equations of motion. These properties together act as the **defining assumptions** which specify a **theory of physics**, the set of all logical consequences of those assumptions. We have already seen one such assumption (PHSXI). A theory of physics is a mathematical model with the additional underlying requirement that the predictions of the theory of physics are intended to reproduce the properties observed in a system which truly exists in the world. That is, in physics there ultimately has to be a system to interpret in the problem of interpretation. Mathematics has no such restriction. In mathematics, one picks the assumptions and looks at their interesting consequences (theorems). In physics, one observes the consequences (experiments) and tries to infer the underlying assumptions and then cyclically tries to predict new consequences to look for⁷. Actually trying to compute the consequences of a theory brings us to the third problem: solving the equations of motion. No one knows how to solve differential equations exactly in general. It is too hard. However, solving differential equations by hand or on a computer, exactly or approximately, is one of the most explored topics in mathematics and thousands of texts exist for how to handle this problem systematically. So, while exact solutions are not usually known, approximate solutions can be made at will and often to whatever precision you desire with enough computational power. For solid help solving differential equations, consult [10], [115], [82]. Teaching solution methods for differential equations will not be the focus of this book; we will only do so occasionally for specific cases as needed.

To begin solving these theoretical problems, you must choose the system you would like to describe. Each choice (and its corresponding solution to the problem of interpretation) essentially defines a branch of physics. When your phase space is the space of positions and momenta of particles, you are doing classical mechanics. When your phase space is the set of probability distributions for the state of a classical system, you are doing classical statistical mechanics. When your phase space is the set of states of a wave propagating through space, you are doing classical field theory. When your phase space is the set of states of a wave propagating through the configuration space of an underlying theory, you are doing quantum mechanics. When you are doing quantum mechanics and the underlying configuration space is a space of fields, you are doing quantum field theory. We will get to all of these in time; at this point it should simply be mentioned that to treat physics in more in more detail we will first have to consider bigger and bigger phase spaces (there are more variables at work the more honest you make your theory). The problem of dynamics will be the principal focus of this series as it is the most under-served in typical presentations. However, in order to solve the problem of dynamics we need to first introduce some mathematical tools (which will be accomplished in the rest of this chapter).

Once the three theoretical problems are solved, the theory is defined and all of its predictions are knowable with sufficient calculation. It then goes to the experimental side of physics to design the scenario necessary to see if the predictions match what actually happens. If the experimental results and theoretical predictions match, the theory is said to be consistent with observation and gets to live on. If the experimental results and theoretical predictions do not match, the theory is inconsistent with observation and is therefore wrong. **Because physics is a science and therefore seeks to describe reality, experimental results always supersede the theory.** If a theory is found to be wrong, the underlying assumptions have to be modified to have another chance or discarded completely if no adequate modification is possible. Throughout this book we will discuss the experimental successes and failures of some historical theories of physics, showing for what are they valuable and why some had to be left behind. It is possible for different theories to give many of the same theoretical predictions. For this reason, while a theory failing an experimental test means it must be wrong (and thus failure is called “evidence against” the theory), a theory passing an experimental test does not mean it is correct (and thus it is only said to be “consistent with” the evidence). It is not correct to say that an experimental test which a theory passes acts as “evidence for” that theory. Theories are to be stricken down by their failures and only that which is left with no failures may survive. A theory can never be proven definitively right, but it can be proven definitively wrong. The best a theory can be is “consistent, so far”. Only predictions that can be tested and thus which could in principle be found to be wrong tell you anything about whether a theory is correct. So, a strictly necessary criterion for a meaningful scientific theory is that it has **falsifiability** – the potential for its claims to be proven wrong⁸. If a theory

⁷Often physicists will spend a great deal of time studying mathematical models which they know do not likely correspond to any real existing system. This is because studying artificially simple models can be a great way to isolate and study interesting features of more realistic but difficult systems. So, while physicists *eventually* have to make it back to the real world, it is entirely sane and healthy to sometimes indulge in easier artificial systems.

⁸It may be the case that a valid scientific claim will be out of reach of experiment in the present or even for many years. This is not a violation of falsifiability, it just means we need to be patient in working toward being able to test that particular claim. But, that claim is only scientifically meaningful if it is possible in principle that an experiment could eventually be performed which could prove it wrong.

has assumptions which are not even in principle falsifiable, those assumptions are not legitimate scientific hypotheses because by definition they cannot meaningfully be tested by the scientific method.

Experimenters face a different set of fundamental problems than theorists. In order for an experiment to meaningfully test a theory, it has to be able to in principle observe results which could contradict the particular theory in question. Thus, experiments have to be designed to be able to distinguish what a theory predicts from possible alternatives. To do so the experimenter must identify which predictions of a theory are susceptible to tests by existing technology (or technology that experimenter and their team are capable of inventing) within some scenario that the experimenter can imagine. As well, in order for any experimental result to be trustworthy, it has to be **reproducible** and done in a way to be maximally **unbiased** toward any particular outcome. The **problem of design** for such an experiment meeting these criteria of reproducibility, unbiasedness, and power to falsify requires marvelous ingenuity and tackling it has directly or indirectly invented many of the fundamental technologies of the modern world. Once the experimenter has devised a testing scenario for a theory and the equipment necessary to perform the test, they must collect data which faithfully represents the variables involved in the experiment. Even measuring the position of an ordinary object in time is difficult. One needs precise alignment of a position/distance measuring device to act as a “meter stick”, a high quality timer, and the ability to associate positions and times of the object (such as through taking a video and watching the video frame by frame). All measuring tools measure with some degree of uncertainty and how to manage, reduce, calibrate, and optimize these uncertainties make up the **problem of calibration**. In order to test precise theories, one needs precise experiments. Once all of the equipment is optimized and all data is collected, the experimenter must process that data and determine what it actually means. This process of turning data into meaning is the **problem of statistics**.

We will not discuss the experimental problems; they are not the focus of this book. We will at times reference important experiments or experimental results but how to actually work through the problem of design and problem of calibration is best learned in an actual lab in person in practice from a real experimenter. The problem of statistics, being more theoretical, can be studied more formally (I recommend [7], [4], [20], [53]) but again it is necessarily supplemented by actual practice. While we will not be covering experimental methods, make no mistake that experiment is in every way as important as theory; it is what makes physics a science. There is of course much more depth to the philosophy of the scientific method and how it is applied to physics than covered here. For a good introduction, see [113].

Exercises

Problem 1.6: State of a spec. What might be an appropriate choice of state for a spec of dust moving in the air (which is well approximated in your experiment by a point)? Why do you believe this choice of state is reasonable? How would your answer change if instead of dust you were considering a small rock (which now has some definite non-point-like shape)?

Problem 1.7: Equation of motion with symmetry. Suppose you are developing a theory in which the position $\vec{x}(t)$ of an object as a function of time satisfies some differential equation: $\ddot{\vec{x}} = \vec{f}(t, \vec{x}, \dot{\vec{x}})$. Argue that if this system has time-translational symmetry then $\vec{f}$ should not depend explicitly on t .

Problem 1.8: Investigating approximations. Suppose you have found that your system is described by a single variable θ satisfying an equation of the form $\ddot{\theta} = f(\sin \theta)$ for some unknown smooth function f .

- Suppose further that you know that $\theta = 0$ is an equilibrium of the system (if $\theta = 0$ and $\dot{\theta} = 0$ at a particular time then $\theta = 0$ for all time). Find $f(0)$.
- Suppose the hypotheses of (a) with the additional assumption that the equilibrium is a stable equilibrium (if θ is sufficiently close to 0 then θ is accelerated toward 0). Find the sign of $f'(0)$ (assume $f'(0) \neq 0$).
- Now assume in addition to (a) and (b) that for your experimental purposes you are only concerned with the lowest order contributions from f to the equations of motion. Taylor expand f and show that to lowest order θ satisfies the equation of motion: $\ddot{\theta} = -\omega^2 \sin \theta$ for some constant ω .
- Taking the equation of motion in (c), suppose that θ is sufficiently small that it is reasonable to Taylor expand $\sin \theta$ to first order in θ . Write the corresponding equation of motion and solve this approximate equation of motion exactly using the techniques of differential equations.
- Exactly solve the equation of motion in (c) using a computer or an elliptic integral. Plot the solutions to (c) and (d) alongside each other. Do this for several choices of initial conditions and comment on the quality of the approximation in (d).

1.3 Writing Transformations

1.3.1 The Generator of a Transformation

We will now build up the mathematics which lets us use the symmetries of our system to figure out its dynamics. Because symmetries are transformations under which our dynamics are unchanged, we first need to develop a theory of transformations. In physics we are typically interested in a certain class of transformations called **continuous transformations**. A continuous transformation is a transformation which depends smoothly on a real-valued parameter so that at each stage in the transformation we are applying it in the same way. A symmetry under a continuous transformation is called a **continuous symmetry**. For example, translating an object in space is a continuous transformation; the amount of the transformation can take any real value, what the transformation actually does to the position of the object depends smoothly on the parameter (the amount of translation), and the rule for applying the transformation does not depend on how much any previous transformation has been applied. A translation can be inverted by translation again by the negative of the original amount. The common transformations of time translation, space translation, and rotation are all continuous transformations. A symmetry under time translation, space translation, or rotation would then be a continuous symmetry. Let $T(\alpha, \Phi) : \mathbb{R} \times \mathbb{P} \rightarrow \mathbb{P}$ be a continuous transformation with parameter α . Then our transformed state Φ is related to our untransformed Φ_0 by definition as:

$$\Phi = T(\alpha, \Phi_0). \quad (1.3.1)$$

Note the striking similarity between (1.3.1) and (1.1.1). In fact, almost all of the conditions on T are the same as those on U without the interpretation of the parameter α as time. The only additional requirement is that the transformation must be applied the same way at each stage, which we have yet to include formally in our equations, whereas we did not have such a condition on time evolution. Because T satisfies all of the conditions that U did, we can immediately recycle Theorem 1.1 and say that for our transformation T we can find a function $F(\alpha, \Phi) : \mathbb{R} \times \mathbb{P} \rightarrow \mathbb{P}$ so that:

$$\frac{d\Phi}{d\alpha} = F(\alpha, \Phi). \quad (1.3.2)$$

Now let us specify what is meant by “the same at each stage” for our continuous transformation. The form of equation (1.3.2) is appropriate if the map between Φ_0 and Φ is just some generic path in the space of possible states of our system. However, by a continuous transformation we don’t intend just a generic continuous path, we mean that we are continuously applying the same transformation. This is the distinction between holding an object (so that Φ includes its position) and flailing it around chaotically (which could be represented by some $F(\alpha, \Phi)$ so that at each α the rate of change of the object’s position is adjusted accordingly) and simply swinging that object in a circle (which can be represented by some $F(\Phi)$ that simply gives how at each point to apply a rotation about the same unchanging axis). When applying a time translation, space translation, rotation or other continuous transformation of interest, at each step in the transformation how much the system state changes ($F(\alpha, \Phi)$) depends only on the system’s present state Φ , not on how much it has previously been transformed α . Therefore, for a continuous transformation, we really have $F(\Phi)$, not $F(\alpha, \Phi)$.

We will find shortly that the phase space $\mathbb{P}$ used in physics has a very particular structure. To head toward that structure, it is useful to start with a different space of variables. Suppose in studying our system, we find that it possesses an independent list of variables $Q = (Q^1, \dots, Q^D)$ (where D is some natural number) which naively seem to describe its state. We call this list the configuration of the system and the space of possible configurations (the set of all variables these variables can take) the configuration space $\mathbb{Q}$. It may sound like we should use this configuration as the state and the configuration space as the phase space, however, it turns out there is a natural way to associate each Q^a (with a an index running from 1 to D) with a partner “conjugate” variable P_a . We define the state Φ by the list of all Q ’s and all P ’s. Thus, the phase space will have dimension $2D$. This doubled space of variables (the phase space) will have much more convenient mathematical properties and give us a much simpler description than the basic configuration space. Over the rest of this and the next section we will see how this is done and gradually see why it is helpful.

In our initial description, we have treat the configuration coordinates $Q^1, \dots, Q^D$ as the list of variables defining our system. Then, if we consider a continuous transformation of the configuration of our system (called a point transformation), (1.3.2) with the condition of being a continuous transformation is written as:

$$\frac{dQ^a}{d\alpha} = f^a(Q) \quad (1.3.3)$$

where the functions $f^a(Q) : \mathbb{Q} \rightarrow \mathbb{R}$ are called the components of F . An extremely helpful notation which we will use for the rest of this book is the **Einstein summation notation**. This notation defines that in products in which an index label occurs twice and is once a superscript and once a subscript, it is intended that the expression is summed over all values that index could take⁹. That is, if A^a and B_a are indexed lists with a taking values from $1, 2, \dots, N$:

$$A^a B_a \stackrel{\text{def}}{=} \sum_{a=1}^N A^a B_a. \quad (1.3.4)$$

Summation would not be implied over the product $A^a B_b$ (because neither index a nor b is repeated in the product) and in the rare event implicit summation is not desired when an index is repeated, the indices which should not be implicitly summed over will be underlined as above. Similarly, summation would not be implied over the product $A_a B_a$ because there the index occurs twice as a subscript (for now this is the only difference in meaning between whether we write an index as a superscript or subscript). Of course, this notation only makes sense when the repeated index has the same domain in both cases (if the index of A^a ran from 1 to 3 but for B_a it ran from 0 to 5, the meaning of $A^a B_a$ would be completely unclear). Whether an index is written as a superscript or subscript for now is purely conventional and carries no meaning. Later (Chapter 4) we will expand on our definition of indices to make a more meaningful distinction between superscripts and subscripts but until then it does not matter. This notation does not change anything (no notation ever does), but it makes some equations shorter without losing anything. For the wary reader, it is a good idea to work out all expressions both in and out of this notation for a while until you become comfortable with it. Now that we have how the state changes under our transformations with (1.3.3), we can compute how any smooth function $u(Q) : \mathbb{Q} \rightarrow \mathbb{R}$ on the configuration space changes as well by using the chain rule:

$$\frac{du}{d\alpha} = \frac{\partial u}{\partial Q^a} \frac{dQ^a}{d\alpha} = f^a(Q) \frac{\partial u}{\partial Q^a}. \quad (1.3.5)$$

This is useful because as the Q 's completely specify the configuration of our system, any property of the configuration can be expressed as some function $u(Q)$. Therefore, (1.3.5) lets us calculate how any property ($u(Q)$) of our system's configuration changes under a transformation. As is not surprising (because the derivative is a linear operator), the right hand side of (1.3.5) depends linearly on u . This allows us to define the linear operator $\hat{F}$ which acts on smooth functions of the state and returns smooth functions of the state as:

$$\hat{F} = f^a(Q) \frac{\partial}{\partial Q^a} \implies \frac{du}{d\alpha} = \hat{F}u. \quad (1.3.6)$$

A linear operator $\hat{F}$ so that the rate of change ($\frac{d}{d\alpha}$) of a property (u) of our system under a transformation (T) is given by that operator acting on the property ($\hat{F}u$) is called the **generator** of the transformation T . That is, the generator of a transformation is whatever operator appears on the far right side of (1.3.6). Because the operator $\hat{F}$ acting on a function gives the rate of change of that function under the transformation, integrating that derivative gives the full change of the function under T and so T can be recovered from $\hat{F}$. This is the motivation for the language “ $\hat{F}$ generates T ”. The situation here gets more interesting when we consider multiple smooth functions of the state (u and v), multiple transformations (T and S with parameters α and β), and consequently multiple generators ($\hat{F}$ for T and $\hat{G}$ for S). Then, it makes sense to consider how one transformation changes due to another:

$$\frac{du}{d\alpha} = \hat{F}u, \quad \frac{du}{d\beta} = \hat{G}u, \quad \forall u \quad (1.3.7)$$

$$\implies \hat{G}\hat{F}u = \frac{d}{d\beta}(\hat{F}u). \quad (1.3.8)$$

The second line comes from using that $\hat{G}v$ is the β derivative of v by definition for any v and then setting $v = \hat{F}u$. In order to go further we need to develop a sort of product rule for linear operators. Let $\hat{F}(\beta)$ be $\hat{F}$ when it has been transformed by the transformation generated by $\hat{G}$ by an amount β and let $u(\beta)$

⁹Some books do not require a mix of subscript and superscript to intend summation in a product and would sum over $A_a B_a$ for example. We will NEVER intend notation in this way, as this alternate convention encourages a bad habit of writing down equations with incorrect transformation properties for reasons that will become clear in chapter 4.

be when u has been similarly transformed. Then, by the definition of the derivative:

$$\frac{d}{d\beta}(\hat{F}u) = \lim_{h \rightarrow 0} \frac{\hat{F}(\beta+h)u(\beta+h) - \hat{F}(\beta)u(\beta)}{h} \quad (1.3.9)$$

$$= \lim_{h \rightarrow 0} \frac{\hat{F}(\beta+h)u(\beta+h) - \hat{F}(\beta)u(\beta+h) + \hat{F}(\beta)u(\beta+h) - \hat{F}(\beta)u(\beta)}{h} \quad (1.3.10)$$

$$= \lim_{h \rightarrow 0} \left(\frac{\hat{F}(\beta+h) - \hat{F}(\beta)}{h} u(\beta+h) + \hat{F}(\beta) \frac{u(\beta+h) - u(\beta)}{h} \right) \quad (1.3.11)$$

where in the last line we have applied the linearity of $\hat{F}$ to reorganize the expression and we have defined the operator $\frac{1}{h}(\hat{F}(\beta+h) - \hat{F}(\beta))$ as the linear operator so that:

$$\frac{\hat{F}(\beta+h) - \hat{F}(\beta)}{h} v = \frac{1}{h} \hat{F}(\beta+h)v - \frac{1}{h} \hat{F}(\beta)v \quad \forall v(Q). \quad (1.3.12)$$

Then, if $\hat{F}$ is continuous in the sense that it commutes with sufficiently quickly converging limits:

$$\lim_{h \rightarrow 0} \hat{F}(\beta) \frac{u(\beta+h) - u(\beta)}{h} = \hat{F}(\beta) \lim_{h \rightarrow 0} \frac{u(\beta+h) - u(\beta)}{h} \quad (1.3.13)$$

we are able to write:

$$\frac{d}{d\beta}(\hat{F}u) = \lim_{h \rightarrow 0} \frac{\hat{F}(\beta+h) - \hat{F}(\beta)}{h} \lim_{h \rightarrow 0} u(\beta+h) + \hat{F}(\beta) \lim_{h \rightarrow 0} \frac{u(\beta+h) - u(\beta)}{h} \quad (1.3.14)$$

$$= \frac{d\hat{F}}{d\beta} u + \hat{F} \frac{du}{d\beta} \quad (1.3.15)$$

thus giving us an operator product rule. Continuing from (1.3.8) then:

$$\hat{G}\hat{F}u = \frac{d}{d\beta}(\hat{F}u) = \frac{d\hat{F}}{d\beta} u + \hat{F} \frac{du}{d\beta} = \frac{d\hat{F}}{d\beta} u + \hat{F}\hat{G}u \quad (1.3.16)$$

$$\implies \frac{d\hat{F}}{d\beta} u = \hat{G}\hat{F}u - \hat{F}\hat{G}u. \quad (1.3.17)$$

Equation (1.3.17) holds for all u and therefore we can state it more simply as:

$$\frac{d\hat{F}}{d\beta} = [\hat{G}, \hat{F}]. \quad (1.3.18)$$

This bracket notation is called the commutator of two operators:

$$[\hat{F}, \hat{G}] \stackrel{\text{def}}{=} \hat{F}\hat{G} - \hat{G}\hat{F}. \quad (1.3.19)$$

So, while (1.3.6) gives how functions evolve under a continuous transformation, (1.3.18) gives how generators evolve under a continuous transformation. To understand intuitively what it means for one generator to change under another, consider rotations in three dimensions about the x axis and about the y axis as an example. A small rotation of the x axis about the y axis produces a new x' axis which is slightly misaligned with the x axis because it now has a nonzero z component. Rotations about this new axis will have a slightly different generator than rotations about the x axis. If β is the angle by which we rotated about the y axis and $\hat{F}(\beta)$ is the generator of rotations about the x' axis after rotating by that angle, then $\frac{d\hat{F}}{d\beta}$ at $\beta = 0$ by this argument will be (up to a multiplier) the generator of rotations about the z axis. At this point, it looks like we have these two separate classes of objects, the functions and the generators. However, these two can actually be unified into one description by defining the operator $\hat{u}$ as the operator which simply multiplies by the function u :

$$\hat{u}v(Q) = u(Q)v(Q). \quad (1.3.20)$$

Then, with this definition, it immediately follows from our previous reasoning that:

$$\frac{d\hat{u}}{d\beta} = [\hat{G}, \hat{u}]. \quad (1.3.21)$$

Because $u = Q^a$ is a smooth function, (1.3.20) implicitly defines the coordinate operators $\hat{Q}^a$ as the linear operators which simply multiply by Q^a . Hence, we can unify our definitions to use equation (1.3.18) to describe the evolution of anything related to the configuration space in operator form under continuous

transformation. This is quite surprising! We have found essentially that from our configuration space we can construct this space of linear operators and that the algebra of the operator commutators tells us everything there is to know about continuous transformations (even ones which act nonlinearly on our coordinates) of the configurations including how even other transformations are transformed. The incredible result here is that we started with nonlinear differential equations (1.3.3) and reformulated everything in terms of linear operators. You should know from your math education that if things are linear, you have a chance at actually being able to accomplish something!

1.3.2 The Lie Bracket

The (negative) commutator of generators is also called the **Lie bracket**:

$$\hat{F} \angle \hat{G} = -[\hat{F}, \hat{G}]. \quad (1.3.22)$$

The Lie bracket as we can see acts on two operators and returns back an operator. It satisfies a number of important algebraic properties. For constants a, b and operators $\hat{F}, \hat{G}, \hat{H}$:

$$(a\hat{F} + b\hat{G}) \angle \hat{H} = -[a\hat{F} + b\hat{G}, \hat{H}] = -a[\hat{F}, \hat{H}] - b[\hat{G}, \hat{H}] = a\hat{F} \angle \hat{H} + b\hat{G} \angle \hat{H} \quad (1.3.23)$$

$$\hat{F} \angle (a\hat{G} + b\hat{H}) = -[\hat{F}, a\hat{G} + b\hat{H}] = -a[\hat{F}, \hat{G}] - b[\hat{F}, \hat{H}] = a\hat{F} \angle \hat{G} + b\hat{F} \angle \hat{H}. \quad (1.3.24)$$

These two properties together are known as bilinearity. Further:

$$\hat{F} \angle \hat{G} = -[\hat{F}, \hat{G}] = -\hat{F}\hat{G} + \hat{G}\hat{F} = [\hat{G}, \hat{F}] = -\hat{G} \angle \hat{F}. \quad (1.3.25)$$

This property is known as antisymmetry¹⁰. Finally:

$$\hat{F} \angle (\hat{G} \angle \hat{H}) + \hat{G} \angle (\hat{H} \angle \hat{F}) + \hat{H} \angle (\hat{F} \angle \hat{G}) = [\hat{F}, [\hat{G}, \hat{H}]] + [\hat{G}, [\hat{H}, \hat{F}]] + [\hat{H}, [\hat{F}, \hat{G}]] \quad (1.3.26)$$

$$\begin{aligned} &= \hat{F}\hat{G}\hat{H} - \hat{F}\hat{H}\hat{G} - \hat{G}\hat{H}\hat{F} + \hat{H}\hat{G}\hat{F} + \hat{G}\hat{H}\hat{F} - \hat{G}\hat{F}\hat{H} - \hat{H}\hat{F}\hat{G} + \hat{F}\hat{H}\hat{G} \\ &+ \hat{H}\hat{F}\hat{G} - \hat{H}\hat{G}\hat{F} - \hat{F}\hat{G}\hat{H} + \hat{G}\hat{F}\hat{H} = 0. \end{aligned} \quad (1.3.27)$$

This last property is called the Jacobi identity. Further, notice from (1.3.6) that any $\hat{F}$ which is the generator of a point transformation can be written as a linear combination of the partial derivatives with respect to the coordinates. This motivates defining a basis (in the sense of linear algebra) of generators called the **conjugate momenta** $\hat{P}_a$. Each $\hat{P}_a$ is defined as the generator of translations of the coordinate Q^a on the configuration space:

$$\hat{P}_a u \stackrel{\text{def}}{=} \frac{\partial u}{\partial Q^a} \implies \hat{F} = f^a(Q) \frac{\partial}{\partial Q^a} = f^a(Q) \hat{P}_a. \quad (1.3.28)$$

From (1.3.28) one can see what we mean by “ $\hat{P}_a$ is the generator of translations of Q^a ”. The generator of a transformation acting on a function gives the rate of change of that function under the transformation. Under the act of translating the variable Q^a , Q^a is simply shifted. Therefore, the rate of change of a function of Q^a under the transformation is the rate of change of that function under shifting Q^a , which is precisely the definition of a partial derivative with respect to Q^a . The momenta $\hat{P}_a$ form a basis of generators of point transformations because as seen in (1.3.6) any generator of a point transformation can be written as a linear combination of them. The Lie brackets between the Q ’s and P ’s are called the canonical Lie brackets:

$$(\hat{Q}^a \angle \hat{Q}^b)u = (\hat{Q}^b \hat{Q}^a - \hat{Q}^a \hat{Q}^b)u = (Q^b Q^a - Q^a Q^b)u = 0 \quad (1.3.29)$$

$$(\hat{Q}^a \angle \hat{P}_b)u = (\hat{P}_b \hat{Q}^a - \hat{Q}^a \hat{P}_b)u = \frac{\partial}{\partial Q^b} (Q^a u) - Q^a \frac{\partial u}{\partial Q^b} = \frac{\partial Q^a}{\partial Q^b} u + Q^a \frac{\partial u}{\partial Q^b} - Q^a \frac{\partial u}{\partial Q^b} = \delta_b^a u \quad (1.3.30)$$

$$(\hat{P}_a \angle \hat{P}_b)u = (\hat{P}_b \hat{P}_a - \hat{P}_a \hat{P}_b)u = \frac{\partial}{\partial Q^b} \frac{\partial u}{\partial Q^a} - \frac{\partial}{\partial Q^a} \frac{\partial u}{\partial Q^b} = \frac{\partial^2 u}{\partial Q^a \partial Q^b} - \frac{\partial^2 u}{\partial Q^b \partial Q^a} = 0. \quad (1.3.31)$$

The symbol δ_b^a is called the Kronecker delta. It is the function of a and b defined by the property that it equals 1 when $a = b$ and 0 when $a \neq b$. Because (1.3.29)-(1.3.31) hold for all u , we have:

$$\hat{Q}^a \angle \hat{Q}^b = 0 \quad (1.3.32)$$

$$\hat{Q}^a \angle \hat{P}_b = \delta_b^a \quad (1.3.33)$$

$$\hat{P}_a \angle \hat{P}_b = 0. \quad (1.3.34)$$

¹⁰Mathematicians often define the Lie bracket to have the slightly weaker property that $\hat{F} \angle \hat{F} = 0$. As long as the field of constants one is working over is such that division by 2 is defined and one has bilinearity, these two requirements are equivalent. Because we always work over spaces for which there is such thing as division by 2, this distinction will not be important for us.

By using the algebraic properties, (1.3.23), (1.3.24), (1.3.25), (1.3.27); the canonical brackets, (1.3.32), (1.3.33), (1.3.34); and one further property, we can calculate the brackets of any analytic functions of $\hat{Q}$ and $\hat{P}$. This further property is called the Leibniz property¹¹:

$$\hat{F}\angle(\hat{G}\hat{H}) = -[\hat{F}, \hat{G}\hat{H}] = -\hat{F}\hat{G}\hat{H} + \hat{G}\hat{H}\hat{F} = -(\hat{F}\hat{G} - \hat{G}\hat{F})\hat{H} + \hat{G}(\hat{H}\hat{F} - \hat{F}\hat{H}) \quad (1.3.35)$$

$$= (\hat{F}\angle\hat{G})\hat{H} + \hat{G}(\hat{F}\angle\hat{H}). \quad (1.3.36)$$

Summary 1.1: Lie Bracket Summary

The Lie Bracket $\angle$ between two generators satisfies the following properties (for constants a, b and operators $\hat{F}, \hat{G}, \hat{H}$):

$$\text{Bilinearity: } (a\hat{F} + b\hat{G})\angle\hat{H} = a\hat{F}\angle\hat{H} + b\hat{G}\angle\hat{H} \quad (1.3.37)$$

$$\hat{F}\angle(a\hat{G} + b\hat{H}) = a\hat{F}\angle\hat{G} + b\hat{F}\angle\hat{H} \quad (1.3.38)$$

$$\text{Antisymmetry: } \hat{F}\angle\hat{G} = -\hat{G}\angle\hat{F} \quad (1.3.39)$$

$$\text{Jacobi Identity: } \hat{F}\angle(\hat{G}\angle\hat{H}) + \hat{G}\angle(\hat{H}\angle\hat{F}) + \hat{H}\angle(\hat{F}\angle\hat{G}) = 0 \quad (1.3.40)$$

$$\text{Leibniz Property: } \hat{F}\angle(\hat{G}\hat{H}) = (\hat{F}\angle\hat{G})\hat{H} + \hat{G}(\hat{F}\angle\hat{H}). \quad (1.3.41)$$

The evolution of a linear operator $\hat{F}$ under a continuous transformation parameterized by β and generated by $\hat{G}$ is given by:

$$\frac{d\hat{F}}{d\beta} = \hat{F}\angle\hat{G}. \quad (1.3.42)$$

The configuration coordinate operators $\hat{Q}^a$ and their conjugate momenta $\hat{P}_a$ operators defined as the generators of translations of the coordinates satisfy the canonical brackets:

$$\hat{Q}^a\angle\hat{Q}^b = 0 \quad (1.3.43)$$

$$\hat{Q}^a\angle\hat{P}_b = \delta_b^a \quad (1.3.44)$$

$$\hat{P}_a\angle\hat{P}_b = 0. \quad (1.3.45)$$

1.3.3 The Phase Space

Using the information in the Lie bracket summary box, we can compute the brackets of any analytic function of $\hat{Q}$ and $\hat{P}$. Notice that by (1.3.28), any linear operator $\hat{F}$ which generates continuous transformations of the configuration space into itself can be represented for some functions $f^a(Q)$ as a linear combination in $\hat{P}_a$. So, linear functions of $\hat{P}_a$ are distinguished from nonlinear functions of them even though we can compute brackets of nonlinear functions if we desire. Because any continuous transformation from the configuration space into itself has a generator which is linear in the $\hat{P}_a$, any generator not a linear function of $\hat{P}_a$ then does not simply generate transformations on the configuration. Let us see what happens for the simplest case of a generator which is not linear in $\hat{P}$. Consider a 1 dimensional configuration space and the generator $\hat{F} = \frac{\hat{P}^2}{2}$:

$$\frac{d\hat{Q}}{d\alpha} = \hat{Q}\angle\left(\frac{\hat{P}^2}{2}\right) = \frac{1}{2}\left((\hat{Q}\angle\hat{P})\hat{P} + \hat{P}(\hat{Q}\angle\hat{P})\right) = \frac{1}{2}(\hat{P} + \hat{P}) = \hat{P}. \quad (1.3.46)$$

So, the transformation generated by a function which is not linear in P gives evolution for the configuration Q which depends on both Q and P . While this is not what we initially expected to work with when we wrote the math down, it is something we are capable of doing using the generator and bracket formalism. If we choose to allow generators which are generic smooth functions of Q and P , then we will have transformations which mix the coordinates and the momenta into each other. Once the coordinates and their momenta start to mix under a transformation, we are dealing with a transformation on a much bigger space. Whereas the point transformations mapped the configuration space $\mathbb{Q}$ of Q states into itself, these transformations map the **phase space** $\mathbb{P}$ of (Q, P) into itself. Because for each Q there is a P , the phase space has double the dimension of the configuration space. The space of transformations on phase space is much larger than the

¹¹Mathematicians do not require the Leibniz property because they may sometimes work on spaces on which $\hat{F}\angle\hat{G}$ and $\hat{F}\angle\hat{H}$ exist but $\hat{F}\angle(\hat{G}\hat{H})$ does not. Again, this generalization will not be a concern for us and so we will always have the Leibniz property.

space of point transformations. The full set of transformations from old t , coordinate Q , and momenta P to a new time t' , coordinate Q' , and momenta P' is called the set of **canonical transformations**. This manual doubling of the dimension allows us to use all of these structures we have defined for general functions of Q and P . It is not obvious at the moment that the doubling of dimension does anything useful for us but as we will see next section it turns out to be a extremely helpful. So, we will not assume that our generators are required to only be linear functions of the conjugate momenta. If they happen to be non-linear, we will be fine with that. It will also sometimes be useful to discuss the **extended configuration space** (t, Q) of both the time parameter t and coordinates Q and transformations on this space, called **extended point transformations**. We call the set (t, Q, P) the **the extended phase space**. More on all of this later in section 1.9.

Because all of the properties of the Lie bracket in the summary box are sufficient to compute the brackets of any analytic functions of Q and P and the brackets of functions of Q and P give how variables in our system evolve under transformation, the information in the summary box is sufficient to compute all of our transformations (including time evolution). A particular formula for the bracket is not actually necessary. This is convenient because it allows us to consider a **representation** of the abstract generators and bracket we have been discussing. A representation is a map (which is linear over constants) R from these linear operators and the bracket into other math objects such as variables and functions which preserves the structure of the abstract objects. That is for $\hat{F}$, $\hat{G}$ any of the generators we have defined so far, a representation R will define a new object $R(\hat{F})$ (called the representation of $\hat{F}$) and new object $R(\hat{G})$ so that the representation of the bracket $(\cdot\angle_R\cdot)$ acting on the representatives $R(\hat{F})$ and $R(\hat{G})$ gives the representation of $R(\hat{F}\angle\hat{G})$:

$$R(\hat{F}\angle\hat{G}) = (R(\hat{F}))\angle_R(R(\hat{G})) \quad (1.3.47)$$

and all of the properties in the Lie bracket summary box are required to hold for the representative bracket $\angle_R$. This means the bracket of the representatives must be the representation of the bracket. Or, R must “commute” with the bracket $\cdot\angle\cdot$. This just means that everything about our abstract brackets and generators can be translated into a corresponding statement in terms of the representation. This is highly convenient because we know how to measure numbers (through units/reference values as described last section) but not so much how to measure differential operators. So, by making a representation which takes all of these abstract generators and the Lie bracket and turns them into real numbers and real valued functions, we will keep all of this mathematical structure but arrive as something much more directly useful for doing physics and comparing to experiment. Making such a representation, called the **Poisson representation**, is the goal of the next section.

(This next paragraph contains a large amount of jargon which you won’t be able to parse until later. It is perfectly alright and expected to not know at all what the following few sentences mean.) The original representation we started with is called the defining representation of the **Moyal algebra**. This bracket structure we have developed is used to define a particular kind of math object called a **Lie algebra**. In physics, we use two representations of the Moyal algebra, the **Poisson representation** which we will discuss next (and which gives classical physics) and the **Schrödinger representation** which we will discuss in Chapter 9 (and which gives quantum physics).

Exercises

Problem 1.9: Closure of point transformations. For two generators of point transformations $\hat{F} = f^a(Q)\frac{\partial}{\partial Q^a}$ and $\hat{G} = g^a(Q)\frac{\partial}{\partial Q^a}$ compute $\hat{F}\angle\hat{G}$. Notice that $\hat{F}\angle\hat{G}$ is itself a generator of a point transformation $\hat{H} = h^a\frac{\partial}{\partial Q^a}$ for some functions h^a and identify those functions.

Problem 1.10: Computing brackets. Using the algebraic properties of the Lie bracket, compute the following (assume a 1 dimensional configuration space and that all functions appearing are analytic):

- (a) $\hat{Q}\angle\hat{Q}^2$ (b) $\hat{Q}\angle\hat{F}(\hat{Q})$ (c) $\hat{Q}^2\angle\hat{P}^2$ (d) $\hat{Q}\angle\hat{G}(\hat{P})$.

1.4 Hamilton's Equations

All of the math in the previous section is well and good but a bit too abstract to be immediately helpful for physics. We can measure numbers, so let us try to come up with a representation of the generators and brackets by real numbers. By this we mean we will try to represent $\hat{Q}$ and $\hat{P}$ by real valued functions of time so that our phase space is the space of values of these coordinates and their corresponding momenta. It is not obvious that such a representation “exists” mathematically in the sense that you don't really know before you try it if it will work. But, it is certainly the first thing to try. We will go through all of the requirements this representation, called the Poisson representation, must satisfy in order to exist and show that indeed one does by constructing it. The Lie bracket in the Poisson representation is called the Poisson bracket and is written with curly braces $\{, \}$. Previously, we had that generators $\hat{F}$ were analytic functions of $\hat{Q}$ and $\hat{P}$. Now that $\hat{Q}$ and $\hat{P}$ are to be represented by real valued variables Q and P , we have that the generators are represented by analytic functions $f(Q, P)$. Stating then the conditions on the Poisson bracket, from (1.3.18) we have that for a generator $\hat{F}$ with representation f and transformation parameter α , any function $u(Q, P)$ on the phase space should change under that transformation by:

$$\frac{du}{d\alpha} = \{u, f\}. \quad (1.4.1)$$

We also have the algebraic properties and Leibniz rule for constants a, b and functions f, g, h :

$$\{af + bg, h\} = a\{f, h\} + b\{g, h\} \quad (1.4.2)$$

$$\{f, ag + bh\} = a\{f, g\} + b\{f, h\} \quad (1.4.3)$$

$$\{f, g\} = -\{g, f\} \quad (1.4.4)$$

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 \quad (1.4.5)$$

$$\{f, gh\} = \{f, g\}h + g\{f, h\}. \quad (1.4.6)$$

Finally, we have the canonical brackets:

$$\{Q^a, Q^b\} = 0, \quad \{Q^a, P_b\} = \delta_b^a, \quad \{P_a, P_b\} = 0. \quad (1.4.7)$$

If we can find a formula for the Poisson bracket which satisfies all of these properties, we will successfully have a representation. Consider a generator g corresponding to a continuous transformation with parameter β and use the chain rule:

$$\frac{df}{d\beta} = \frac{\partial f}{\partial Q^a} \frac{dQ^a}{d\beta} + \frac{\partial f}{\partial P_a} \frac{dP_a}{d\beta} \quad (1.4.8)$$

$$\Rightarrow \{f, g\} = \frac{\partial f}{\partial Q^a} \{Q^a, g\} + \frac{\partial f}{\partial P_a} \{P_a, g\}. \quad (1.4.9)$$

Now consider $g = Q^a$ and use the canonical brackets and anti-symmetry property. Then,

$$\{f, Q^a\} = \frac{\partial f}{\partial Q^b} \{Q^b, Q^a\} + \frac{\partial f}{\partial P_b} \{P_b, Q^a\} \quad (1.4.10)$$

$$\{f, Q^a\} = \frac{\partial f}{\partial Q^b} 0 - \frac{\partial f}{\partial P_b} \delta_b^a \Rightarrow \{f, Q^a\} = -\frac{\partial f}{\partial P_a}. \quad (1.4.11)$$

Doing the same thing with $g = P_a$:

$$\{f, P_a\} = \frac{\partial f}{\partial Q^b} \{Q^b, P_a\} + \frac{\partial f}{\partial P_b} \{P_b, P_a\} \quad (1.4.12)$$

$$\{f, P_a\} = \frac{\partial f}{\partial Q^b} \delta_b^a + \frac{\partial f}{\partial P_b} 0 \Rightarrow \{f, P_a\} = \frac{\partial f}{\partial Q^a}. \quad (1.4.13)$$

Using the anti-symmetry property and inserting these into (1.4.9), we find for a generic g :

$$\{f, g\} = \frac{\partial f}{\partial Q^a} \{Q^a, g\} + \frac{\partial f}{\partial P_a} \{P_a, g\} = -\frac{\partial f}{\partial Q^a} \{g, Q^a\} - \frac{\partial f}{\partial P_a} \{g, P_a\} \quad (1.4.14)$$

$$= \frac{\partial f}{\partial Q^a} \frac{\partial g}{\partial P_a} - \frac{\partial f}{\partial P_a} \frac{\partial g}{\partial Q^a}. \quad (1.4.15)$$

And so (1.4.15) allows us to compute the Poisson bracket of any two functions on the phase space. As well, it is the unique possible formula for the bracket satisfying our properties required so far. To have properly established the Poisson representation, we simply need to verify that (1.4.15) satisfies all of the required properties in Summary 1.1. All of these properties can be checked by a direct calculation using the formula

(1.4.15). Hence, the Poisson representation genuinely does exist.

Now that we have a representation, we can really accomplish something. As time passes, Q and P evolve and change values continuously into new coordinates and momenta. So, at each time t , there will be some generator which acts as the generator of time evolution at that time. Call that function $\mathcal{H}(t, Q, P)$. If our system behaves in some way physically differently at different times, then the generator of time evolution at one time will not necessarily be the generator of time evolution at a different time, which is why $\mathcal{H}$ may in principle explicitly change with t . The generator of time evolution $\mathcal{H}(t, Q, P)$ is called the **Hamiltonian**. By (1.4.1), we have that for $f(Q, P)$:

$$\frac{df}{dt} = \{f, \mathcal{H}\}. \quad (1.4.16)$$

For the special cases of taking $f = Q^a$ or $f = P_a$, we have:

$$\frac{dQ^a}{dt} = \{Q^a, \mathcal{H}\} = \frac{\partial Q^a}{\partial Q^b} \frac{\partial \mathcal{H}}{\partial P_b} - \frac{\partial Q^a}{\partial P_b} \frac{\partial \mathcal{H}}{\partial Q^b} = \frac{\partial \mathcal{H}}{\partial P_a} \quad (1.4.17)$$

$$\frac{dP_a}{dt} = \{P_a, \mathcal{H}\} = \frac{\partial P_a}{\partial Q^b} \frac{\partial \mathcal{H}}{\partial P_b} - \frac{\partial P_a}{\partial P_b} \frac{\partial \mathcal{H}}{\partial Q^b} = -\frac{\partial \mathcal{H}}{\partial Q^a}. \quad (1.4.18)$$

Equations (1.4.17) and (1.4.18) are called **Hamilton's equations**. So, given the Hamiltonian function we know how all the variables, the Q 's and the P 's, change in time. Thus **all of time-evolution comes down to specifying the Hamiltonian**. This turns the problem of dynamics into the singular problem of finding the right Hamiltonian. Because all of time-evolution is in the Hamiltonian and physics is the science of time-evolution, **all of the physics of a system is in its Hamiltonian**. Writing down the Q 's solves the problem of interpretation; finding the Hamiltonian solves the problem of dynamics. It is hard to overstate the accomplishment here. **The Hamiltonian is the universe in 1 function**. Hamilton's equations are the key. They are it. Let us write them loudly:

Summary 1.2: Hamilton's Equations

$$\frac{dQ^a}{dt}(t) = \frac{\partial \mathcal{H}}{\partial P_a}(t, Q, P), \quad \frac{dP_a}{dt}(t) = -\frac{\partial \mathcal{H}}{\partial Q^a}(t, Q, P).$$

With these, we can really see the advancement we made by going from the configuration space to the phase space. Using the configuration space only, one needs to specify an equation of motion function for each coordinate Q^a . Using the Hamiltonian, one needs only to specify a single function (and that function generally transforms very nicely under the relevant symmetries of interest). Figuring out what the right Hamiltonian to use and computing what it does is essentially the job description of a theoretical physicist. Collecting the results of an experiment based on the predictions of a Hamiltonian is essentially the job description of an experimental physicist. $\mathcal{H}$ and some related quantities called the Lagrangian and the action will be the core objects of this book and are without exaggeration the core objects of all physics. Any system which we use a Hamiltonian to describe is called a Hamiltonian system.

Occasionally, we will consider functions of the extended phase space $f(t, Q, P)$, meaning they are allowed to be explicitly dependent on time in addition to their implicit dependence on time through the coordinates and momenta. Then, using the chain rule we can see that (1.4.16) is simply modified to:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial f}{\partial P_a} \frac{dP_a}{dt} \quad (1.4.19)$$

$$= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \frac{\partial \mathcal{H}}{\partial P_a} - \frac{\partial f}{\partial P_a} \frac{\partial \mathcal{H}}{\partial Q^a} \quad (1.4.20)$$

$$= \frac{\partial f}{\partial t} + \{f, \mathcal{H}\} \quad (1.4.21)$$

Theorem 1.2: Hamilton-Poisson Theorem

For any system of N variables $Q = (Q^1, \dots, Q^N)$ with differentiable invertible dynamics, we can embed that system into a $2N$ variable (Q, P) phase space with conjugate momenta $P = (P_1, \dots, P_N)$, the generators of translations of the corresponding Q . For any two functions f and g on the phase space, their Lie bracket (called the Poisson bracket in this notation) is given by:

$$\{f, g\} = \frac{\partial f}{\partial Q^a} \frac{\partial g}{\partial P_a} - \frac{\partial f}{\partial P_a} \frac{\partial g}{\partial Q^a}. \quad (1.4.22)$$

The dynamics of the system are determined by Hamilton's equations of motion:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a} \quad (1.4.23)$$

where the Hamiltonian $\mathcal{H}(t, Q, P)$ is the generator of time evolution. The time evolution of any function $f(t, Q, P)$ on the extended phase space is given by:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, \mathcal{H}\}. \quad (1.4.24)$$

We have proven that the Poisson representation of our bracket structure in section 1.3 exists (assuming you do the homework). There is another important question: is it faithful? A faithful representation is a representation R which is “invertible” in the sense that for each of our abstract operators $\hat{F}$, if we associate to it a function on phase space $f = R(\hat{F})$, then it should be possible to recover $\hat{F}$ by some map $R^{-1}(f)$ which should preserve the bracket structure so that in addition to (1.3.47) the inverse holds:

$$R^{-1}(f) \angle R^{-1}(g) \stackrel{!}{=} R^{-1}(\{f, g\}). \quad (1.4.25)$$

Faithfulness is an important property because it means that the representation is “lossless”. Everything about our abstract operator formulation can be recovered from it identically from a faithful representation by applying the inverse R^{-1} , whatever it happens to be. However, we will prove in Chapter 9 that the Poisson representation is **NOT** faithful. Something is lost there. The essential origin of what is lost is that simply in the operator formalism the operators $\hat{Q}\hat{P}$ and $\hat{P}\hat{Q}$ are not equal because the operators $\hat{Q}$ and $\hat{P}$ do not commute while in the Poisson representation QP and PQ are equal because the numbers Q and P do commute. This difference has statistical effects that lead to the difference between classical mechanics and quantum mechanics. This all likely seems like a technical point. We have proven that through the Poisson representation we can represent all of our abstract transformation properties by real valued functions evolving in time on phase space. From there it is reasonable to make concrete measurable predictions. If those predictions agree with experiment, who cares if in some abstract sense the Poisson representation is not identical to the more abstract and less obviously meaningful operator formulation? That thinking is reasonable. But, we will see much later on that naive use of standard Poisson representation runs into real experimental trouble. Returning to a faithful representation and understanding why it matters will be a job for Part II.

Exercises

Problem 1.11: ★ Poisson bracket properties. Verify by direct calculation that the formula for the Poisson bracket in (1.4.22) satisfies all the necessary properties, (1.4.2)-(1.4.7).

Problem 1.12: Our favorite Hamiltonian. Consider the Hamiltonian $\mathcal{H} = \frac{P^2 + \omega^2 Q^2}{2}$ for some real parameter ω .

- Using Hamilton's equations, compute the equations of motion implied by this Hamiltonian.
- From the equations of motion in (a), by algebra and differentiation eliminate P and find a second order differential equation for Q only. Notice that there is no way from Hamilton's equations to reduce to a first order equation of motion for Q . This is due to us manually doubling the dimension of the variable space when we introduced P . We will see that you can, if you desire, undouble it in section 1.13.

Problem 1.13: Coordinate Clean-Up. Consider the Hamiltonian $\mathcal{H} = \frac{P^2 - Q^2}{2}$.

- Using Hamilton's equations, compute the equations of motion implied by this Hamiltonian.

- (b) From the equations of motion in (a), by algebra and differentiation eliminate P and find a second order differential equation for Q only.
- (c) Consider the new coordinates Q', P' defined by:

$$Q' = \frac{Q + P}{\sqrt{2}}, \quad P' = \frac{P - Q}{\sqrt{2}}.$$

Assuming Hamilton's equations apply equally well to these coordinates (we will be able to justify this later), rewrite the Hamiltonian in terms of these coordinates and find the associated equations of motion. Notice that in these coordinates we do get an equation of motion for Q' and thus have effectively undone the dimension doubling by using the right coordinates. This is possible in general but not typically useful.

Problem 1.14: Clarifying Theorem 1.2.

- (a) Consider the equations of motion $\dot{x} = x$, $\dot{y} = y$. Show, by direct calculation, that there does not exist a Hamiltonian $\mathcal{H}$ so that $x = Q$, $y = P$, and the equations of motion given are produced by Hamilton's equations. While Hamilton's equations can be applied to any dynamical system, they are only so general when we take the right list of variables. An initial list of N variables is not guaranteed to have a Hamiltonian description in terms of only those variables. However, any list of N variables is guaranteed to have a Hamiltonian description in $2N$ variables, and possibly fewer.
- (b) Consider a dynamical system with equations of motion:

$$\frac{dQ^a}{dt} = V^a(t, Q).$$

Show that the Hamiltonian $\mathcal{H}(t, Q, P) = P_a V^a(t, Q)$ reproduces this system's dynamics and thus confirm by construction the claim that any N dimensional dynamical system has a Hamiltonian on $2N$ dimensional phase space.

1.5 Functional Differentiation

We will continue our study of dynamics in a moment but first it will help to study a new kind of mathematical object called a functional. A **functional** is a map from a space of functions into a space of numbers (in physics, into $\mathbb{R}$ or $\mathbb{C}$). A common example is the length of a path, called the arclength. The arclength of a curve depends on the whole specification of the function between the two endpoints considered and based on that function returns a non-negative real number. Consider a path in $\mathbb{R}^N$ parameterized by $t \in \mathbb{R}$: $\vec{x}(t) : \mathbb{R} \rightarrow \mathbb{R}^N$ (we will call t time for linguistic convenience). Then, for fixed endpoints $\vec{x}(t_0) = \vec{x}_0$ and $\vec{x}(t_f) = \vec{x}_f$, the arclength S between those two endpoints is:

$$S[\vec{x}](t_0, t_f, \vec{x}_0, \vec{x}_f) = \int_{t=t_0}^{t=t_f} |d\vec{x}| = \int_{t=t_0}^{t=t_f} \left| \frac{d\vec{x}}{dt} \right| dt = \int_{t=t_0}^{t=t_f} |\dot{\vec{x}}| dt. \quad (1.5.1)$$

Throughout this book, a dot overhead of a variable is used to indicate a time derivative of that variable with multiple dots meaning multiple derivatives. Functionals will often also be functions. By that I mean that a functional might be a functional of some variables (as S here is a functional of the path $\vec{x}(t)$) while also being an ordinary function of other variables (as S here is a function of the boundary conditions $t_0, t_f, \vec{x}_0, \vec{x}_f$). As a notational issue, square brackets $[\]$ are used around the functional dependence and parentheses $(\)$ are used around the variable dependence. For compactness of notation, the variable dependence of our functionals may sometimes be suppressed (meaning not written explicitly). Although functionals are now a more sophisticated mathematical object than an ordinary function, we can define many of the same concepts including differentiation and integration but naturally they are more technically challenging.

1.5.1 Motivating the Definition

For an ordinary function $f(x_1, \dots, x_N) : \mathbb{R}^N \rightarrow \mathbb{R}$, the derivative of f with respect to the variable x_n is defined as:

$$\frac{\partial f}{\partial x_n} \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{f(x_1, \dots, x_n + \varepsilon, \dots, x_N) - f(x_1, \dots, x_n, \dots, x_N)}{\varepsilon}. \quad (1.5.2)$$

That is, the partial derivative is the limit of the difference quotient in which only one variable is changed and the amount of the change goes to 0. This expression can be put into two nicer forms by defining $\vec{x} = (x_1, \dots, x_N)$ and the basis vectors $\vec{e}_1 = (1, 0, 0, \dots, 0)$, $\vec{e}_2 = (0, 1, 0, \dots, 0)$, ..., $\vec{e}_N = (0, 0, \dots, 0, 1)$. Then:

$$\vec{x} = \sum_{n=1}^N x_n \vec{e}_n \quad (1.5.3)$$

$$\frac{\partial f}{\partial x_n} = \lim_{\varepsilon \rightarrow 0} \frac{f(\vec{x} + \varepsilon \vec{e}_n) - f(\vec{x})}{\varepsilon}. \quad (1.5.4)$$

As well, looking at the components directly and using the Kronecker delta we see:

$$\vec{x} + \varepsilon \vec{e}_n = \sum_{k=1}^N x_k \vec{e}_k + \varepsilon \vec{e}_n = \sum_{k=1}^N (x_k + \varepsilon \delta_{nk}) \vec{e}_k \quad (1.5.5)$$

$$\frac{\partial f}{\partial x_n} = \lim_{\varepsilon \rightarrow 0} \frac{f(x_k + \varepsilon \delta_{nk}) - f(x_k)}{\varepsilon}. \quad (1.5.6)$$

(Here we have used a common abuse of notation by writing $f(x_k)$ with k a “dummy index” to mean $f(\vec{x})$ where $\vec{x}$ has components x_k .) For a constant vector $\vec{u}$ by the chain rule of multivariable calculus:

$$\lim_{\varepsilon \rightarrow 0} \frac{f(\vec{x} + \varepsilon \vec{u}) - f(\vec{x})}{\varepsilon} = \frac{\partial f}{\partial \vec{x}} \cdot \vec{u} = \sum_{n=1}^N \frac{\partial f}{\partial x_n} u_n. \quad (1.5.7)$$

A list of variables x_n is defined by the value of the list at each value of the discrete index n . Partial differentiation of a function $f(\vec{x})$ is defined as the rate of change of that function under adjusting the value of x_n at a particular n . Similarly, a function $x(t)$ is defined by the value it takes for each continuous t and functional differentiation of a functional $f[x]$ is defined as the rate of change of that functional under adjusting the value of $x(t)$ at a particular t . We can develop this analogy by acknowledging that continuous functions form a vector space under pointwise addition and scalar multiplication by real numbers. Thus, whereas before we thought of x_n as component n of the vector $\vec{x}$, for a function $x(t)$ we can think of the value $x(t)$ at a particular t as the t component of the function/vector $\vec{x}$. Thus, the difference between a list of variables

x_n and a function $x(t)$ is whether there is a discrete set of components or continuous set of components. Correspondingly, whereas in (1.5.3) we wrote $\vec{x}$ as the sum over its components and basis vectors, we now do the same but we have to range over all t continuously, thus giving an integral. As well, we now need a basis vector for each t just as we did before for each n :

$$\vec{x} = \int_a^b x(t) \vec{t}_t dt. \quad (1.5.8)$$

Here constants a and b just indicate the minimum and maximum values of t , just as before 1 and N indicated the minimum and maximum values of n . Then, we would like to have functional differentiation simply defined to generalize (1.5.4) when f is a functional:

$$\frac{\delta f}{\delta x(t)} \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{f[\vec{x} + \varepsilon \vec{t}_t] - f[\vec{x}]}{\varepsilon}. \quad (1.5.9)$$

Functional differentiation is written with these δ 's by convention and it is good practice to write in the arguments of the function in the denominator so that it is clear what variables the right hand side depends on (just like you write the subscript n in the left hand side of the partial derivative in (1.5.4)). Looking at the expression $\vec{x} + \varepsilon \vec{t}_t$ in terms of the components:

$$\vec{x} + \varepsilon \vec{t}_t = \int_a^b x(t') \vec{t}_{t'} dt' + \varepsilon \vec{t}_t \quad (1.5.10)$$

$$= \int_a^b (x(t') + \varepsilon \delta(t - t')) \vec{t}_{t'} dt'. \quad (1.5.11)$$

Here $\delta(t)$ is the Dirac delta distribution¹² defined by the property that for all $x(t)$ which are continuous at $t = 0$:

$$\int_{-\infty}^{\infty} \delta(t) x(t) dt = x(0). \quad (1.5.12)$$

This object $\delta(t - t')$ is the continuous replacement for the Kronecker delta δ_{nk} which appeared in the discrete case. Just as the Kronecker delta is 0 everywhere $n \neq k$ with a bump up to 1 at $n = k$, the Dirac delta can be thought of in a sense as being 0 everywhere $t \neq t'$ with a bump which has area 1 at $t = t'$. The precise relationship between the two is explored in problem 1.15 and so please do that problem carefully if the Dirac delta is new to you. Importantly, the Dirac delta is only defined through how it behaves in a product under an integral. In (1.5.11) we see that the map $\vec{x} \rightarrow \vec{x} + \varepsilon \vec{t}_t$ on the vectors is the same as the map $x(t') \rightarrow x(t') + \varepsilon \delta(t - t')$ on the components just as the map $\vec{x} \rightarrow \vec{x} + \varepsilon \vec{t}_n$ on the vectors is the same as the map $x_k \rightarrow x_k + \varepsilon \delta_{nk}$ on the components in the discrete case (1.5.5). Therefore, functional differentiation can be written in the same form as (1.5.6) by:

$$\frac{\delta f}{\delta x(t)} \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{f[x(t') + \varepsilon \delta(t - t')] - f[x(t')]}{\varepsilon} \quad (1.5.13)$$

where here t' is acting as the “dummy index”.

1.5.2 Relationship with Partial Differentiation

We can make the above heuristic idea of functional differentiation more well-defined by relating it to ordinary partial differentiation. Consider a smooth real-valued function $x(t)$ defined on an interval $[a, b]$. Then, we can divide up that interval into N sub-intervals $[t_n, t_{n+1}]$ with $t_n \stackrel{\text{def}}{=} a + \frac{b-a}{N}n$. Define as well $\Delta t = t_{n+1} - t_n = \frac{b-a}{N}$. Then the values $x_n \stackrel{\text{def}}{=} x(t_n)$ of our function at each of the interval endpoints gives a discrete list of real-valued variables. In the limit $N \rightarrow \infty$ this list becomes infinite and simply specifies the original function $x(t)$. For finite N , the list of x_n is not enough to determine the original $x(t)$. However, suppose we have some way of “smoothly interpolating” our discrete data $x(t_n) = x_n$. That is, let us have a map I which takes as input the t_n and the x_n but which gives as output a smooth function $y_N(t)$ which passes through all the required points: $y_N(t_n) = x_n$ and is monotone inbetween each pair of consecutive data

¹²One may be tempted to write “Dirac delta function” as is often done in physics. However, properly the Dirac delta distribution is not a real function as it is not a map from real numbers to real numbers. Instead, it is an object which has a particularly defined behavior when it is integrated in a product with a function. This behavior can be achieved through the limit of functions but in a rigorous way the Dirac delta is not a proper ordinary function, it is a distribution.

points:

$$y_N(t) = I(N, t, t_0, x_0, \dots, t_N, x_N). \quad (1.5.14)$$

At finite N this can always be done with a polynomial of degree N . While for finite N generally $y_N(t)$ and $x(t)$ will not be the same, in the limit $N \rightarrow \infty$ they exactly match (due to continuity of $x(t)$):

$$\lim_{N \rightarrow \infty} y_N(t) = x(t). \quad (1.5.15)$$

For a given functional $f[x]$, we can approximate its value by $f[y_N]$ and if that functional is continuous¹³ then in the limit $N \rightarrow \infty$ that approximation will become exact:

$$f[x(t)] = f\left[\lim_{N \rightarrow \infty} y_N(t)\right] = \lim_{N \rightarrow \infty} f[y_N(t)]. \quad (1.5.16)$$

At finite N , $f[y_N]$ is just a function of the x_n because they determine y_N . Therefore, we can define the function $F_N(x_n)$ given by that explicit variable dependence:

$$F_N(x_n) \stackrel{\text{def}}{=} f[y_N] = f[I(N, t, t_0, x_0, \dots, t_N, x_N)] \quad (1.5.17)$$

$$\implies f[x(t)] = \lim_{N \rightarrow \infty} F_N(x_n). \quad (1.5.18)$$

Such an F_N we have constructed is called a discretization of the functional f . Because F_N is now just a real-valued function of $N + 1$ real-valued variables, we can just use multivariable calculus on it! Then, at the end, all we have to do is take the limit $N \rightarrow \infty$ to recover f . Using (1.5.6):

$$\frac{\partial F}{\partial x_n} = \lim_{h \rightarrow 0} \frac{F_N(x_{n'} + h\delta_{n,n'}) - F_N(x_{n'})}{h} \quad (1.5.19)$$

$$= \lim_{h \rightarrow 0} \frac{F_N(x_{n'} + h\Delta t \frac{\delta_{n,n'}}{\Delta t}) - F_N(x_{n'})}{h} \quad (1.5.20)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{F_N(x_{n'} + \varepsilon \frac{\delta_{t_n, t_{n'}}}{\Delta t}) - F_N(x_{n'})}{\varepsilon} \Delta t \quad (1.5.21)$$

$$\implies \frac{1}{\Delta t} \frac{\partial F_N}{\partial x_n} = \lim_{\varepsilon \rightarrow 0} \frac{F_N(x_{n'} + \varepsilon \frac{\delta_{t_n, t_{n'}}}{\Delta t}) - F_N(x_{n'})}{\varepsilon} \quad (1.5.22)$$

$$\implies \lim_{N \rightarrow \infty} \frac{1}{\Delta t} \frac{\partial F_N}{\partial x_n} = \lim_{N \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} \frac{F_N(x_{n'} + \varepsilon \frac{\delta_{t_n, t_{n'}}}{\Delta t}) - F_N(x_{n'})}{\varepsilon}. \quad (1.5.23)$$

As $N \rightarrow \infty$, $\Delta t = \frac{b-a}{N} \rightarrow 0$. As well, as $\Delta t \rightarrow 0$, $\frac{\delta_{t_n, t_{n'}}}{\Delta t}$ becomes $\delta(t - t')$, the Dirac delta (shown in Problem 1.15). Assuming our function F is smooth enough for these limits to commute, the $N \rightarrow \infty$ limit gives (using (1.5.18)):

$$\lim_{N \rightarrow \infty} \frac{1}{\Delta t} \frac{\partial F_N}{\partial x_n} = \lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} \frac{F_N(x_{n'} + \varepsilon \frac{\delta_{t_n, t_{n'}}}{\Delta t}) - F_N(x_{n'})}{\varepsilon} \quad (1.5.24)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{f[x(t') + \varepsilon \delta(t_n - t')] - f[x(t')]}{\varepsilon} = \frac{\delta f}{\delta x(t_n)}. \quad (1.5.25)$$

Thus we literally can consider functional differentiation as just the limit of ordinary partial differentiation in which we discretize our function $x(t)$ to a finite set of points, differentiate with respect to each point as an ordinary real-valued variable, and then take the point-separation to 0 (and thus number of points to infinity) at the end.

This discretization formulation gives another nice result. The change in a smooth function $\Delta f \stackrel{\text{def}}{=} f(x + \delta x) - f(x)$ under a change in its argument is related to its derivative by:

$$\Delta f = \sum_{n=1}^N \frac{\partial f}{\partial x_n} \delta x_n + \mathcal{O}(\delta x^2) \quad (1.5.26)$$

(which follows immediately from (1.5.7) by setting $\delta x_n = \varepsilon u_n$). Then, using a discretization F_N of a functional f we have:

$$\Delta F_N = F_N(x_n + \delta x_n) - F_N(x_n) = \sum_{n=0}^N \frac{\partial F}{\partial x_n} \delta x_n + \mathcal{O}(\delta x^2) \quad (1.5.27)$$

¹³By this I mean evaluation of the functional commutes with limits which converge sufficiently well.

$$\implies \lim_{N \rightarrow \infty} \Delta F_N = \lim_{N \rightarrow \infty} F_N(x_n + \delta x_n) - \lim_{N \rightarrow \infty} F_N(x_n) = \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{\partial F}{\partial x_n} \delta x_n + \mathcal{O}(\delta x^2) \quad (1.5.28)$$

$$\implies \Delta f = f[x + \delta x] - f[x] = \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{1}{\Delta t} \frac{\partial F}{\partial x_n} \delta x_n \Delta t + \mathcal{O}(\delta x^2). \quad (1.5.29)$$

Now using (1.5.25) and recognizing that the right hand side is just a Riemann sum, we have:

$$\Delta f = f[x + \delta x] - f[x] = \int_a^b \frac{\delta f}{\delta x(t)} \delta x(t) dt + \mathcal{O}(\delta x^2). \quad (1.5.30)$$

The lowest order change in a function or functional is called its variation, δf , therefore we identify:

$$\delta f = \int_a^b \frac{\delta f}{\delta x(t)} \delta x(t) dt. \quad (1.5.31)$$

So, if one can compute δf , one can indirectly find the functional derivative of f by just reading off the coefficient multiplying δx under the integral.

1.5.3 The Euler-Lagrange Formula

Now that we have defined functional derivatives, let us find an easy formula for computing them. In our applications, functionals will usually be in the form of an integral of some function of x and its derivatives over an interval, along the lines of:

$$f[x] = \int_a^b \mathcal{L}(t, x(t), \dot{x}(t), \ddot{x}(t), \dots) dt. \quad (1.5.32)$$

For example, the arclength we started with was of this form with $\mathcal{L} = |\dot{x}|$. Here the ellipsis is to indicate that the function $\mathcal{L}$ may depend on arbitrarily high orders of differentiation of x . Let us say that the function $\mathcal{L}$ depends on derivatives of x up to order N and write the n^{th} derivative of x with respect to t as $\dot{x}^n$. Under a variation of $x(t)$ to a new function $x'(t) = x(t) + \delta x(t)$ it immediately follows that the new time derivative is $\dot{x}'(t) = \dot{x}(t) + \frac{d}{dt} \delta x$ and so we write $\delta \dot{x} = \frac{d}{dt} \delta x$ as a short hand. This notation continues at each higher order of differentiation. By direct calculation:

$$f[x + \delta x] = \int_a^b \mathcal{L}(t, x(t) + \delta x(t), \dot{x}(t) + \delta \dot{x}(t), \dots, \dot{x}^N(t) + \delta \dot{x}^N(t)) dt \quad (1.5.33)$$

$$= \int_a^b \left(\mathcal{L}(t, x, \dots, \dot{x}^n) + \frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \dot{x} + \dots + \frac{\partial \mathcal{L}}{\partial \dot{x}^N} \delta \dot{x}^N + \mathcal{O}(\delta x^2) \right) dt. \quad (1.5.34)$$

Equation (1.5.34) follows from (1.5.33) by the chain rule of ordinary multivariable calculus. Continuing by distributing the integral:

$$f[x + \delta x] = f[x] + \int_a^b \frac{\partial \mathcal{L}}{\partial x} \delta x dt + \int_a^b \frac{\partial \mathcal{L}}{\partial \dot{x}} \frac{d}{dt} (\delta x) dt + \dots + \int_a^b \frac{\partial \mathcal{L}}{\partial \dot{x}^N} \frac{d^N}{dt^N} (\delta x) dt + \mathcal{O}(\delta x^2). \quad (1.5.35)$$

We can integrate the second integral by parts once and then each successive integral in the sum one more time than the previous one to move all derivatives off of δx and onto the terms depending on $\mathcal{L}$. Doing so will give many boundary terms (meaning evaluated at a and b). If we choose our variations δx to vanish at the boundaries a and b to all orders of differentiation less than the highest order of differentiation in $\mathcal{L}$, then all the boundary terms we get from integrating by parts are automatically 0. It may seem like a lot to ask of our variations δx for this to be the case, but if one considers the Dirac deltas which we used to define functional differentiation in (1.5.13), for any t which is in the interval (a, b) , such a Dirac delta and all of its derivatives vanish at a and b as the “spike” of the delta is located at neither end point. Thus, such an assumption on the variations is precisely consistent with our previous definition.¹⁴ Taking this and applying sufficient integration by parts gives:

$$f[x + \delta x] = f[x] + \int_a^b \left(\frac{\partial \mathcal{L}}{\partial x} - \left(\frac{d}{dt} \right) \frac{\partial \mathcal{L}}{\partial \dot{x}} + \dots + (-1)^N \left(\frac{d}{dt} \right)^N \frac{\partial \mathcal{L}}{\partial \dot{x}^N} \right) \delta x dt + \mathcal{O}(\delta x^2). \quad (1.5.36)$$

¹⁴There are some subtleties here because of course the Dirac deltas are not smooth functions or even functions at all. Later when we take the functional derivative we will often have to think carefully about boundary terms.

The $(-1)^N$ is because each integration by parts picks up a minus sign on the new integral and so having performed it N times gives N minus signs. By (1.5.31), we can now immediately read off the functional derivative:

$$\frac{\delta f}{\delta x(t)} = \frac{\partial \mathcal{L}}{\partial x} - \left(\frac{d}{dt} \right) \frac{\partial \mathcal{L}}{\partial \dot{x}} + \dots + (-1)^N \left(\frac{d}{dt} \right)^N \frac{\partial \mathcal{L}}{\partial \dot{x}^N}. \quad (1.5.37)$$

Equation (1.5.37) is called the Euler-Lagrange equation and is usually the most useful way of actually computing functional derivatives. There are times when it isn't and in those cases (1.5.31) is nearly always the most efficient alternative. Directly applying (1.5.13) is rarely efficient. All of this gives us:

Theorem 1.3: Functional Derivative Formula

For a functional f and F_N a discretization of f :

$$f = \lim_{N \rightarrow \infty} F_N \quad (1.5.38)$$

$$\frac{\delta f}{\delta x(t)} = \lim_{N \rightarrow \infty} \frac{1}{\Delta t} \frac{\partial F_N}{\partial x_n}. \quad (1.5.39)$$

The change in f , $\Delta f = f[x + \delta x] - f[x]$, due to changing its argument is given by:

$$\Delta f = \delta f + \mathcal{O}(\delta x^2) = \int_a^b \frac{\delta f}{\delta x(t)} \delta x(t) dt + \mathcal{O}(\delta x^2). \quad (1.5.40)$$

If the functional f can be written in the form $f[x] = \int_a^b \mathcal{L}(t, x, \dot{x}, \dots, \dot{x}^N) dt$,

$$\frac{\delta f}{\delta x} = \frac{\partial \mathcal{L}}{\partial x} - \left(\frac{d}{dt} \right) \frac{\partial \mathcal{L}}{\partial \dot{x}} + \dots + (-1)^N \left(\frac{d}{dt} \right)^N \frac{\partial \mathcal{L}}{\partial \dot{x}^N}. \quad (1.5.41)$$

For a quick example of how to apply functional differentiation, let us return to the arclength of a curve. The arclength of a curve parameterized by t connecting two endpoints $\vec{x}_0$ and $\vec{x}_f$ is given by (1.5.1):

$$S[\vec{x}(t)] = \int_0^{t_f} |\dot{\vec{x}}| dt. \quad (1.5.42)$$

With this, we can show that the shortest path between two points is a line. We know that at a local minimum (or maximum) of a function, all its partial derivatives must vanish. Because the partial derivatives become a functional derivative in the continuum limit, at a minimum or maximum of a functional, its functional derivative must vanish. So, let us take the functional derivative of the arclength. We can identify that the functional is in the form necessary for (1.5.41) with $\mathcal{L} = |\dot{\vec{x}}| = \sqrt{|\dot{\vec{x}}|^2}$. Therefore:

$$\frac{\delta S}{\delta \vec{x}(t)} = \frac{\partial \mathcal{L}}{\partial \vec{x}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = 0 - \frac{d}{dt} \left(\frac{\dot{\vec{x}}}{|\dot{\vec{x}}|} \right). \quad (1.5.43)$$

In order to find the shortest path, we need to find the critical points of the arclength and thus must set its functional derivative to 0. For convenience, let $\lambda(t)$ be defined so that $\lambda(0) = 0$ and $\dot{\lambda} = |\dot{\vec{x}}|$. Then:

$$\frac{\delta S}{\delta \vec{x}(t)} = -\frac{d}{dt} \left(\frac{\dot{\vec{x}}}{|\dot{\vec{x}}|} \right) = -\frac{d}{dt} \left(\frac{\left(\frac{d\vec{x}}{dt} \right)}{\left(\frac{d\lambda}{dt} \right)} \right) = -\frac{d\lambda}{dt} \frac{d^2 \vec{x}}{d\lambda^2} \stackrel{!}{=} 0 \implies \vec{x}(t) = \dot{\vec{x}}(0) \lambda(t) + \vec{x}(0). \quad (1.5.44)$$

This indeed is the equation of a line. To show that this is a minimum is a little harder. It can be done by a functional version of the second derivative test. If we take another functional derivative, we can define the second variation $\delta^2 S$ as the second order change S (meaning that is proportional to two powers of $\delta \vec{x}(t)$). Doing so will yield:

$$\delta^2 S = \frac{1}{2} \int_0^{t_f} \int_0^{t_f} \delta \vec{x}(t) \cdot \frac{\delta^2 S}{\delta \vec{x}(t) \delta \vec{x}(t')} \cdot \delta \vec{x}(t') dt' dt. \quad (1.5.45)$$

Just as with the usual second derivative test, the stationary variation is a local minimum (/maximum) whenever this second variation is positive (/negative) for all allowed variations. Of course, it could be neither as well (and often for us it will be neither). These minimum/maximum conditions generalize the notion of concave up versus concave down from ordinary calculus. The minimum (/maximum) condition can also be stated as saying that the second functional derivative is a positive (/negative) operator. This is the equivalent

of how a minimum is guaranteed when the second derivative matrix of a function is a positive matrix.¹⁵ For the case of a line above you can check directly that in fact $\delta^2 S > 0$ for nonzero variations around the line solution. The essential use of the functional derivative for physics will be that we will find a way to rewrite Hamilton's equations as coming from setting the functional derivative of a particular functional equal to 0. That functional is called the **Action**. While we will require that action to have vanishing variation, it will not generally be a minimum or maximum.

Exercises

Problem 1.15: ★ Introduction to the Dirac delta. The Dirac delta distribution $\delta(t)$ is a curious kind of mathematical object called a generalized function or distribution. Properly, the Dirac delta is not an ordinary function in the sense that it is not a map from the reals into the reals. The Dirac delta is the limit of a “thin-spike” centered at 0 as the width of the spike goes to 0, the height of the spike goes to infinity, and the area under the spike stays constant at 1. The goal of this question is to make this seem reasonable mathematically.

- (a) Let the function $b_\varepsilon(t)$ (for $\varepsilon > 0$) be the piecewise function: $b_\varepsilon(t) = 0, \quad \forall t : |t| > \varepsilon/2$ and $b_\varepsilon(t) = 1/\varepsilon, \quad \forall t : |t| \leq \varepsilon/2$ (called the box function). Show that for all $\varepsilon > 0$:

$$\int_{-\infty}^{\infty} b_\varepsilon(t) dt = 1$$

- (b) Let $x(t)$ be a function of t which is continuous at $t = 0$. Show that:

$$\lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} b_\varepsilon(t) x(t) dt = x(0).$$

- (c) Graph the function $b_\varepsilon(t)$ for several values of ε .
 (d) Formally, the Dirac delta distribution is only defined through its action under an integral on another function (this is generically true for generalized functions, also called distributions). It is defined so that:

$$\int_{-\infty}^{\infty} \delta(t) x(t) dt = x(0)$$

for all $x(t)$ which are continuous at $t = 0$. Matching with the integral property satisfied by $b_\varepsilon(t)$, it is common to write:

$$\delta(t) = \lim_{\varepsilon \rightarrow 0^+} b_\varepsilon(t).$$

Considering this relationship between $\delta(t)$ and $b_\varepsilon(t)$ and your graphs of $b_\varepsilon(t)$ from (c), explain how $\delta(t)$ is a “thin-spike” as described before.

- (e) Using the defining property of the Dirac delta, show that for a function $f(t)$:

$$f(t) = \int_{-\infty}^{\infty} f(t') \delta(t - t') dt'$$

and explain how conceptually this can be read as “a function $f(t)$ can be written as a linear combination of Dirac deltas with different centers acting like basis vectors and with components of combination $f(t')$ ”.

Problem 1.16: ★ The Harmonic Oscillator. Consider the following action S a functional of x for a constant ω :

$$S[x] = \int_0^{t_f} \left(\frac{1}{2} \dot{x}^2 - \frac{1}{2} \omega^2 x^2 \right) dt.$$

- (a) Find the function $x_c(t)$ (with specified boundary conditions) which makes this functional stationary (meaning makes its functional derivative 0).
 (b) Is the function $x_c(t)$ in (a) a maximum, minimum, or neither for this action? If you know Fourier series, you can answer this question directly using them. If you don't, assume that we let the system evolve long enough that $t_f > \frac{\pi}{\omega}$; consider a variation of $x(t)$ so that $x(t) = x_c(t) + A \sin\left(\frac{\pi t}{t_f}\right)$. Show this variation is allowed by the boundary conditions and compare the value of the action along this path to the value of the action along x_c . Let N be an integer so that $N > \frac{\omega t_f}{\pi}$. Consider the variation

¹⁵A positive operator $\hat{M}$ is an operator for which $\vec{v} \cdot (\hat{M}\vec{v}) > 0$ for all vectors $\vec{v} \neq 0$.

$x(t) = x_c(t) + A \sin\left(\frac{N\pi t}{t_f}\right)$. Show this variation is allowed by the boundary conditions and compare the value of the action along this path to the value of the action along x_c .

1.6 The Existence of an Invariant Action

Now consider the functional, called the Action, defined by:

$$S[Q, P](t_f, t_0, Q_f, Q_0) \stackrel{\text{def}}{=} \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}(t, Q, P)) dt. \quad (1.6.1)$$

Then, its functional derivatives along the path taken by the equations of motion are:

$$\frac{\delta S}{\delta P_a} = \frac{\partial}{\partial P_a} (P_b \dot{Q}^b - \mathcal{H}) - \frac{d}{dt} \frac{\partial}{\partial \dot{P}_a} (\dot{Q}^b P_b - \mathcal{H}) = \dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} = 0 \quad (\text{By Hamilton's first equation}) \quad (1.6.2)$$

$$\frac{\delta S}{\delta Q^a} = \frac{\partial}{\partial Q^a} (P_b \dot{Q}^b - \mathcal{H}) - \frac{d}{dt} \frac{\partial}{\partial \dot{Q}^a} (\dot{Q}^b P_b - \mathcal{H}) = -\frac{\partial \mathcal{H}}{\partial Q^a} - \dot{P}_a = 0 \quad (\text{By Hamilton's second equation}). \quad (1.6.3)$$

Hence Hamilton's equations are exactly equivalent to the condition that the actual path taken by the system in phase space is a stationary point of this action. **We have Hamilton's equations if and only if $\delta S = 0$.** This allows us to reformulate our Hamiltonian dynamics in terms of the action's variation vanishing.

An especially nice property of using the action is that the stationarity of the derivative does not depend on which variables we use and so we can transparently work in whatever coordinates we want. Define $\Phi = (Q, P)$ to be our list of $2N$ phase space variables and Φ' to be $2N$ other variables for which there exists an invertible function relating Φ to Φ' . Then, referring to equation (1.5.40) and using the chain rule:

$$\delta S = \int_{t_0}^{t_f} \frac{\delta S}{\delta \Phi^a} \delta \Phi^a dt \quad (1.6.4)$$

Because we assume the relationship between Φ and Φ' is invertible, we can write:

$$\Phi^a = \Phi^a(\Phi'). \quad (1.6.5)$$

Then, taking the derivative of this:

$$\delta \Phi^a = \frac{\partial \Phi^a}{\partial \Phi'^b} \delta \Phi'^b \quad (1.6.6)$$

by the chain rule. Returning this to the variation of S :

$$\delta S = \int_{t_0}^{t_f} \frac{\delta S}{\delta \Phi^a} \frac{\partial \Phi^a}{\partial \Phi'^b} \delta \Phi'^b dt \quad (1.6.7)$$

By (1.5.40) we can immediately read off the functional derivative of S with respect Φ' :

$$\frac{\delta S}{\delta \Phi'^b(t)} = \frac{\delta S}{\delta \Phi^a(t)} \frac{\partial \Phi^a(t)}{\partial \Phi'^b(t)}. \quad (1.6.8)$$

Equation (1.6.8) is called the functional chain rule. If we have stationarity in the coordinates Φ , the functional derivative of S with respect to Φ vanishes. Then, by (1.6.8) the functional derivative of S with respect to the arbitrary other coordinates Φ' also vanishes. Hence regardless of which coordinates are used, the same action and the same stationarity condition gives the equations of motion. So, we see the stationarity of the action is **invariant** with respect to which coordinates we use. This is convenient because the universe goes on the same way regardless of which coordinates we choose to use to describe it and so a description which also works the same way regardless of which coordinates are chosen adds the least arbitrariness. It is important to note that this invariance property is only true in a restricted way for Hamilton's equations; the Q 's and P 's cannot be changed independently at will. Because each P is related to its corresponding Q through the Poisson bracket, only certain coordinate transformations preserve Hamilton's equations. Those transformations are called canonical transformations and we will study them soon. Equivalently, only certain coordinate transformations leave the integrand of the action in the same form as (1.6.1) (the canonical transformations) and we will only ever consider this subclass (if you would prefer to use completely general coordinate transformations that preserve no nice properties, how to do so is explained in section 1.16).

In (1.6.1), I have notated that S is a functional of $Q(t)$ and $P(t)$ but put that it is an ordinary function of the initial and final times, t_0 and t_f , and initial and final coordinates, Q_0^a and Q_f^a . It may be surprising that S is not written to be a function of the initial and final momenta. We will see that this is automatic in a moment. It will be very useful to see how S depends on each of these explicitly and consider all of the derivatives of S as we go on. So, consider S evaluated at varied versions of all of these for general variations:

$$S[Q + \delta Q, P + \delta P](t_f + \delta t_f, t_0 + \delta t_0, Q_f + \delta Q_f, Q_0 + \delta Q_0)$$

$$= \int_{t_0+\delta t_0}^{t_f+\delta t_f} \left((P_a + \delta P_a)(\dot{Q}^a + \delta \dot{Q}^a) - \mathcal{H}(t, Q + \delta Q, P + \delta P) \right) dt \quad (1.6.9)$$

$$= \int_{t_0+\delta t_0}^{t_f+\delta t_f} \left(P_a \dot{Q}^a + \dot{Q}^a \delta P_a + P_a \delta \dot{Q}^a - \mathcal{H}(t, Q, P) - \frac{\partial \mathcal{H}}{\partial Q^a} \delta Q^a - \frac{\partial \mathcal{H}}{\partial P_a} \delta P_a \right) dt + \text{Higher Order Terms} \quad (1.6.10)$$

$$= \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}) dt + \int_{t_f}^{t_f+\delta t_f} (P_a \dot{Q}^a - \mathcal{H}) dt + \int_{t_0+\delta t_0}^{t_0} (P_a \dot{Q}^a - \mathcal{H}) dt \\ + \int_{t_0}^{t_f} \left(\frac{d}{dt} (P_a \delta Q^a) - \dot{P}_a \delta Q^a + \dot{Q}^a \delta P_a - \frac{\partial \mathcal{H}}{\partial Q^a} \delta Q^a - \frac{\partial \mathcal{H}}{\partial P_a} \delta P_a \right) dt + \text{H.O.T.} \quad (1.6.11)$$

$$= S[Q, P](t_f, t_0, Q_f, Q_0) + (P_a(t_f) \dot{Q}^a(t_f) - \mathcal{H}_f) \delta t_f - (P_a(t_0) \dot{Q}^a(t_0) - \mathcal{H}_0) \delta t_0 \\ + P_a(t_f) \delta Q^a(t_f) - P_a(t_0) \delta Q^a(t_0) + \int_{t_0}^{t_f} \left(\left(\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} \right) \delta P_a - \left(\dot{P}_a + \frac{\partial \mathcal{H}}{\partial Q^a} \right) \delta Q^a \right) dt + \text{H.O.T.} \quad (1.6.12)$$

$$\implies \delta S = (P_{fa} \dot{Q}_f^a - \mathcal{H}_f) \delta t_f - (P_{0a} \dot{Q}_0^a - \mathcal{H}_0) \delta t_0 + P_{fa} \delta Q^a(t_f) - P_{0a} \delta Q^a(t_0) \\ + \int_{t_0}^{t_f} \left(\left(\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} \right) \delta P_a - \left(\dot{P}_a + \frac{\partial \mathcal{H}}{\partial Q^a} \right) \delta Q^a \right) dt. \quad (1.6.13)$$

We will use the short hand that we use the subscripts f and 0 for any functions of time evaluated at the final and initial times. Note that $\delta Q(t_f)$ and δQ_f are not the same thing. $\delta Q(t_f)$ is the variation $\delta Q(t)$ evaluated at the time t_f whereas δQ_f is the amount by which the final coordinate is varied. Because the final time has varied, $Q(t_f)$ is no longer the same as Q_f . Instead, the final time is now $t_f + \delta t_f$. As well, because the final coordinate is varied by δQ_f the final coordinate is now $Q_f + \delta Q_f$. So the new boundary condition is:

$$Q^a(t_f + \delta t_f) = Q_f^a + \delta Q_f^a. \quad (1.6.14)$$

$\delta Q(t_f)$ which can be computed from this boundary condition as:

$$Q^a(t_f) + \delta t_f \dot{Q}^a(t_f) + \text{H.O.T.} = Q_f^a + \delta Q_f^a \quad (1.6.15)$$

$$\implies Q^a(t_f) - Q_f^a = \delta Q_f^a - \dot{Q}^a(t_f) \delta t_f + \text{H.O.T.} \quad (1.6.16)$$

$$\implies \delta Q^a(t_f) = \delta Q_f^a - \dot{Q}^a(t_f) \delta t_f. \quad (1.6.17)$$

The identical argument holds for the initial time, giving:

$$\delta Q^a(t_0) = \delta Q_0^a - \dot{Q}^a(t_0) \delta t_0. \quad (1.6.18)$$

If we now return these to δS , we have:

$$\delta S = P_{fa} \delta Q_f - \mathcal{H}_f \delta t_f - P_{0a} \delta Q_0^a + \mathcal{H}_0 \delta t_0 + \int_{t_0}^{t_f} \left(\left(\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} \right) \delta P_a - \left(\dot{P}_a + \frac{\partial \mathcal{H}}{\partial Q^a} \right) \delta Q^a \right) dt. \quad (1.6.19)$$

We can see automatically that this variation depends on the variations of the paths δQ and δP between the initial and final times but it only depends on the boundary data (meaning at the initial and final times) for t and Q^a but not for P_a . Thus, S genuinely is not a function of the initial and final momenta. Together we have:

Theorem 1.4: Stationary Action Theorem - Hamiltonian Form

For any Hamiltonian system, Hamilton's equations of motion are equivalent to the condition that the variation of the action:

$$S[Q, P](t_f, t_0, Q_f, Q_0) = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H}(t, Q, P) \right) dt \quad (1.6.20)$$

with respect to $Q^a(t)$ and $P_a(t)$ between the initial and final times vanishes for all variations which keep the boundary values $Q(t_0) = Q_0$ and $Q(t_f) = Q_f$ fixed. The vanishing variation of the action

holds in all coordinates. Under general variations of all its parameters, the action's variation is:

$$\delta S = P_{f_a} \delta Q_f - \mathcal{H}_f \delta t_f - P_{0a} \delta Q_0^a + \mathcal{H}_0 \delta t_0 + \int_{t_0}^{t_f} \left(\left(\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} \right) \delta P_a - \left(\dot{P}_a + \frac{\partial \mathcal{H}}{\partial Q^a} \right) \delta Q^a \right) dt. \quad (1.6.21)$$

If the reader has not done Problem 1.16, they should go back and do it now. They may be surprised to find that the solution of the harmonic oscillator (the most standard of all systems in physics) is **NOT** a minimum of that action. For a reader with some physics background used to hearing the name “Principle of Least Action” instead of “Stationary Action Theorem”, this may be unsettling. Confucius said “*the beginning of wisdom is to call things by their proper names*”. It is left to the reader what this implies about physicists.

Exercises

Problem 1.17: The Chain rule by hand. Consider the action S which is a functional of x :

$$S = \int_0^{t_f} \frac{1}{2} \dot{x}^2 dt.$$

- (a) Compute $\frac{\delta S}{\delta x}$.
- (b) Let $y(t) = (x(t))^{1/3}$. Rewrite S as a functional of y and compute $\frac{\delta S}{\delta y}$.
- (c) Using the results of (a) and (b), show by direct calculation that:

$$\frac{\delta S}{\delta y}[y] = \frac{\delta S}{\delta x}[x(y)] \frac{\partial x(y)}{\partial y}.$$

Problem 1.18: Variational practice. Find the equations of motion implied by the following action S :

$$S[Q, P] = \int_0^{t_f} (P\dot{Q} - QP^2) dt.$$

1.7 The Lagrangian

In our action we have to vary two sets of variables, the coordinates Q and the momenta P . The coordinates Q are the variables we originally wrote down and so presumably they are the variables we “understand” (meaning have developed an interpretation for). The momenta on the other hand we don’t know anything about in advance other than that they generate translations of the coordinates. We introduced them from a rather abstract place mathematically and only find how they relate to our Q ’s through Hamilton’s equations. Because we have a more tangible grasp of the Q ’s, it is a worthwhile idea to see if we can solve for the momenta and eliminate them to leave us with something in terms of the Q only. Let us see how this works out. The variation of P in the action (1.6.2) gave us Hamilton’s first equation:

$$\dot{Q}^a = \frac{\partial \mathcal{H}}{\partial P_a}(t, Q, P). \quad (1.7.1)$$

To invert this and solve for the momenta we first need the relationship it defines between $\dot{Q}^a$ and P_a to even be invertible. Conveniently, it typically is¹⁶. For now assuming that (1.7.1) is invertible we can invert it to define:

$$P_a = P_a(t, Q, \dot{Q}) \text{ so that } \frac{\partial \mathcal{H}}{\partial P_a}(t, Q, P(t, Q, \dot{Q})) = \dot{Q}^a. \quad (1.7.2)$$

Inserting this inverted relationship back into the action, we get now a functional of Q only:

$$S[Q, P(t, Q, \dot{Q})] = \int_{t_0}^{t_f} \left(\dot{Q}^a P_a(t, Q, \dot{Q}) - \mathcal{H}(t, Q, P(t, Q, \dot{Q})) \right) dt. \quad (1.7.3)$$

The integrand here is quite clunky to write so let us give it a name. It is called the Lagrangian:

$$\boxed{\mathcal{L}(t, Q, \dot{Q}) \stackrel{\text{def}}{=} P_a(t, Q, \dot{Q}) \dot{Q}^a - \mathcal{H}(t, Q, P(t, Q, \dot{Q}))}. \quad (1.7.4)$$

$$\implies S[Q, P(t, Q, \dot{Q})] = \int_{t_0}^{t_f} \mathcal{L}(t, Q, \dot{Q}) dt. \quad (1.7.5)$$

Let us take the variation of this reduced action using the chain rule:

$$\delta S[Q, P(t, Q, \dot{Q})] = \int_{t_0}^{t_f} \left(\left. \frac{\delta S}{\delta Q^a} \right|_{P=P(t, Q, \dot{Q})} \delta Q^a + \left. \frac{\delta S}{\delta P_a} \right|_{P=P(t, Q, \dot{Q})} \delta P_a(t, Q, \dot{Q}) \right) dt. \quad (1.7.6)$$

The vertical bar next to the derivatives indicates that the action is first differentiated in the usual way for general arguments Q and P and then after the derivative is taken P is evaluated at $P(t, Q, \dot{Q})$.

Because $P_a(t, Q, \dot{Q})$ satisfies (1.7.1) by definition and (1.7.1) is equivalent to $\frac{\delta S}{\delta P_a} = 0$ by (1.6.2), the variation with respect to P_a term automatically vanishes:

$$\delta S[Q, P(t, Q, \dot{Q})] = \int_{t_0}^{t_f} \left. \frac{\delta S}{\delta Q^a} \right|_{P=P(t, Q, \dot{Q})} \delta Q^a dt \quad (1.7.7)$$

$$\implies \frac{\delta S[Q, P(t, Q, \dot{Q})]}{\delta Q^a} = \left. \frac{\delta S[Q, P]}{\delta Q^a} \right|_{P=P(t, Q, \dot{Q})}. \quad (1.7.8)$$

That is to say, the variation of our reduced action with respect to Q^a is the same as the variation of our unreduced action with respect to Q^a when it is then evaluated at momenta which satisfy Hamilton’s first equation. In other words, taking the variation of the action after applying Hamilton’s first equation is the same as taking the variation of the action before applying Hamilton’s first equation.¹⁷ Because Hamilton’s equations are equivalent to the stationary variation of our unreduced action by (1.6.3), the right hand side of (1.7.8) vanishes when we use the equations of motion. As such, our reduced action will have stationary variation as well! Therefore, we can get our equation of motion for Q by setting its variation to 0. In terms of the Lagrangian, this is given by Theorem 1.3:

$$\frac{\delta S[Q, P(t, Q, \dot{Q})]}{\delta Q^a} = \frac{\partial \mathcal{L}}{\partial Q^a} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^a} = 0 \quad (1.7.9)$$

¹⁶There are some very important times we will encounter when it is not. We will address what to do in such cases in section 2.8.3

¹⁷This is only true because the variation of the unreduced action with respect to the momenta is 0. In general, evaluating a function and taking derivatives of that function absolutely do not commute. But, they do at points where the derivative of that function vanishes, like in our case.

$$\implies \boxed{\frac{\partial \mathcal{L}}{\partial Q^a} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^a}} \quad (1.7.10)$$

This is called the Euler-Lagrange equation of motion. Because the Lagrangian depends only on t , Q , and $\dot{Q}$, this gives a second order differential equation for the coordinates with no direct reference to the momenta!

Because the Euler-Lagrange equation of motion is supposed to be equivalent to Hamilton's equations, we really ought to relate them. Returning to the definition of the Lagrangian, consider its derivative with respect to $\dot{Q}^a$ (remember that $\mathcal{H}$ implicitly depends on $\dot{Q}$ in (1.7.4) and so we must use the chain rule):

$$\frac{\partial \mathcal{L}}{\partial \dot{Q}^a} = \frac{\partial P_b}{\partial \dot{Q}^a} \dot{Q}^b + P_a - \frac{\partial \mathcal{H}}{\partial P_b} \frac{\partial P_b}{\partial \dot{Q}^a} = \frac{\partial P_b}{\partial \dot{Q}^a} \dot{Q}^b + P_a - \dot{Q}^b \frac{\partial P_b}{\partial \dot{Q}^a} = P_a. \quad (1.7.11)$$

Hence, from the Lagrangian we can recover the momenta by:

$$\boxed{P_a(t, Q, \dot{Q}) = \frac{\partial \mathcal{L}}{\partial \dot{Q}^a}(t, Q, \dot{Q})}. \quad (1.7.12)$$

This is the equivalent of Hamilton's first equation as it is what defined $P_a(t, Q, \dot{Q})$ in the first place. Further calculating the Q derivatives of the Lagrangian (again remembering to use the chain rule for the implicit dependence of P on Q):

$$\frac{\partial \mathcal{L}}{\partial Q^a} = \frac{\partial P_b}{\partial Q^a} \dot{Q}^b - \frac{\partial \mathcal{H}}{\partial Q^a} - \frac{\partial \mathcal{H}}{\partial P_b} \frac{\partial P_b}{\partial Q^a} = \frac{\partial P_b}{\partial Q^a} \dot{Q}^b - \frac{\partial \mathcal{H}}{\partial Q^a} - \dot{Q}^b \frac{\partial P_b}{\partial Q^a} = -\frac{\partial \mathcal{H}}{\partial Q^a}. \quad (1.7.13)$$

Now then the Euler-Lagrange equation becomes:

$$\frac{\partial \mathcal{L}}{\partial Q^a} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{Q}^a} \right) \implies -\frac{\partial \mathcal{H}}{\partial Q^a} = \frac{d}{dt} P_a \implies \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a}. \quad (1.7.14)$$

Thus, the Euler-Lagrange equation does genuinely simply give us back Hamilton's second equation. The two are equivalent!

There are a number of meaningful observations to make here. First, this business of transforming from the Hamiltonian to the Lagrangian is called the **Legendre transformation** and it can also be done in reverse. That is, starting from the Lagrangian, P_a can be defined by (1.7.12) just as starting from the Hamiltonian, $\dot{Q}^a$ could be defined by (1.7.1). Then, the steps to get the Hamiltonian from the Lagrangian follow just like we did to get the Lagrangian from the Hamiltonian. Second, the only condition for the Legendre transform to exist (meaning the Lagrangian to exist given the Hamiltonian and the Hamiltonian to exist given the Lagrangian) is that the relationship between the momentum and $\dot{Q}$ (given by (1.7.1) or equivalently (1.7.12)) be invertible. This is usually true in application, and we will learn what to do when it isn't in section 2.8.3. Third, the Legendre transformation can be derived quickly through differentials and the chain rule. Consider the total differential of the Hamiltonian and insert Hamilton's equations:

$$d\mathcal{H} = \frac{\partial \mathcal{H}}{\partial t} dt + \frac{\partial \mathcal{H}}{\partial Q^a} dQ^a + \frac{\partial \mathcal{H}}{\partial P_a} dP_a \quad (1.7.15)$$

$$= \frac{\partial \mathcal{H}}{\partial t} dt - \dot{P}_a dQ^a + \dot{Q}^a dP_a. \quad (1.7.16)$$

Now take the definition of the Lagrangian and compute the total differential:

$$\mathcal{L} = P_a \dot{Q}^a - \mathcal{H} \quad (1.7.17)$$

$$d\mathcal{L} = \dot{Q}^a dP_a + P_a d\dot{Q}^a - d\mathcal{H} \quad (1.7.18)$$

$$= \dot{Q}^a dP_a + P_a d\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial t} dt + \dot{P}_a dQ^a - \dot{Q}^a dP_a \quad (1.7.19)$$

$$= -\frac{\partial \mathcal{H}}{\partial t} dt + \dot{P}_a dQ^a + P_a d\dot{Q}^a. \quad (1.7.20)$$

We see no dP_a term and so $\frac{\partial \mathcal{L}}{\partial P_a} = 0$. Thus, the Lagrangian is in the end not a function of the momentum. Further, we see that:

$$\frac{\partial \mathcal{L}}{\partial Q^a} = \dot{P}_a = \frac{d}{dt} P_a = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^a}. \quad (1.7.21)$$

So we can recover the equation of motion. Further, we get one last equation:

$$\frac{\partial \mathcal{L}}{\partial t} = -\frac{\partial \mathcal{H}}{\partial t}. \quad (1.7.22)$$

All of these results are true and can be checked from the more explicit method using the inverse functions. The only two concerns with the differential method are that (1) it doesn't make clear that the condition for this transformation to exist is the invertibility condition discussed earlier and (2) it doesn't make clear the partials are taken in different ways. $\frac{\partial \mathcal{L}}{\partial \dot{Q}^a}$ is a partial taken at fixed t and $\dot{Q}^a$ because the Lagrangian is written as a function of $t, Q, \dot{Q}$ whereas $\frac{\partial \mathcal{H}}{\partial \dot{Q}^a}$ is a partial taken at fixed t and P_a because the Hamiltonian is written as a function of t, Q, P . Being careless about which variables are varied in a partial can be dangerous. However, this differential derivation is a useful shorthand to remember the relationships. Our fourth observation is that we now have two equally good actions, $S_{\mathcal{H}}[Q, P]$ (the Hamiltonian action) and $S_{\mathcal{L}}[Q]$ (the Lagrangian action), in which P has already been varied, solved for, and reinserted. These two actions give the same equations of motion and take the same numerical value along the solution of the equations of motion. The final observation is that because the Lagrangian doesn't reference the momenta and only mentions the coordinates Q (which we presumably have an interpretation for), it is usually easier to guess the Lagrangian of a system from the properties of that system than the Hamiltonian. Together, we have:

Theorem 1.5: Stationary Action Theorem - Lagrangian Form

If the dynamics of a system are given by the stationary variation of the action:

$$S_{\mathcal{H}}[Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H}(t, Q, P) \right) dt \quad (1.7.23)$$

and the map $\dot{Q}^a = \frac{\partial \mathcal{H}}{\partial P_a}$ can be locally inverted to give $P_a(t, Q, \dot{Q})$, then the dynamics of just the Q 's are equivalently given by the stationary variation of the action:

$$S_{\mathcal{L}}[Q] = \int_{t_0}^{t_f} \mathcal{L}(t, Q, \dot{Q}) dt \quad (1.7.24)$$

where $\mathcal{L}$, called the Lagrangian, is the Legendre transformation of $\mathcal{H}$:

$$\mathcal{L}(t, Q, \dot{Q}) = P_a(t, Q, \dot{Q}) \dot{Q}^a - \mathcal{H}(t, Q, P(t, Q, \dot{Q})). \quad (1.7.25)$$

The actions are related by:

$$S_{\mathcal{L}}[Q] = S_{\mathcal{H}}[Q, P(t, Q, \dot{Q})]. \quad (1.7.26)$$

The equation of motion given by the Lagrangian is the Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial Q^a} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{Q}^a} \right). \quad (1.7.27)$$

And, the Legendre transformation is invertible with:

$$P_a(t, Q, \dot{Q}) = \frac{\partial \mathcal{L}}{\partial \dot{Q}^a} \iff \dot{Q}^a(t, Q, P) = \frac{\partial \mathcal{H}}{\partial P_a} \quad (1.7.28)$$

$$\mathcal{H}(t, Q, P) = P_a \dot{Q}^a(t, Q, P) - \mathcal{L}(t, Q, \dot{Q}(t, Q, P)). \quad (1.7.29)$$

Thus, there are three ways of doing analytical mechanics which are joined at the hip: Hamilton's equations, the Euler-Lagrange equation, or stationary action. As well, stationary action can be done as a functional of Q and P or just Q (by eliminating P). You must know all three but which one you prefer is a matter of personal taste. Each one has its own time to shine when it is the stand-out as the easiest to use. They are all friends and should be your friend too. There is a little picture to see how they all relate in Figure 1.1.

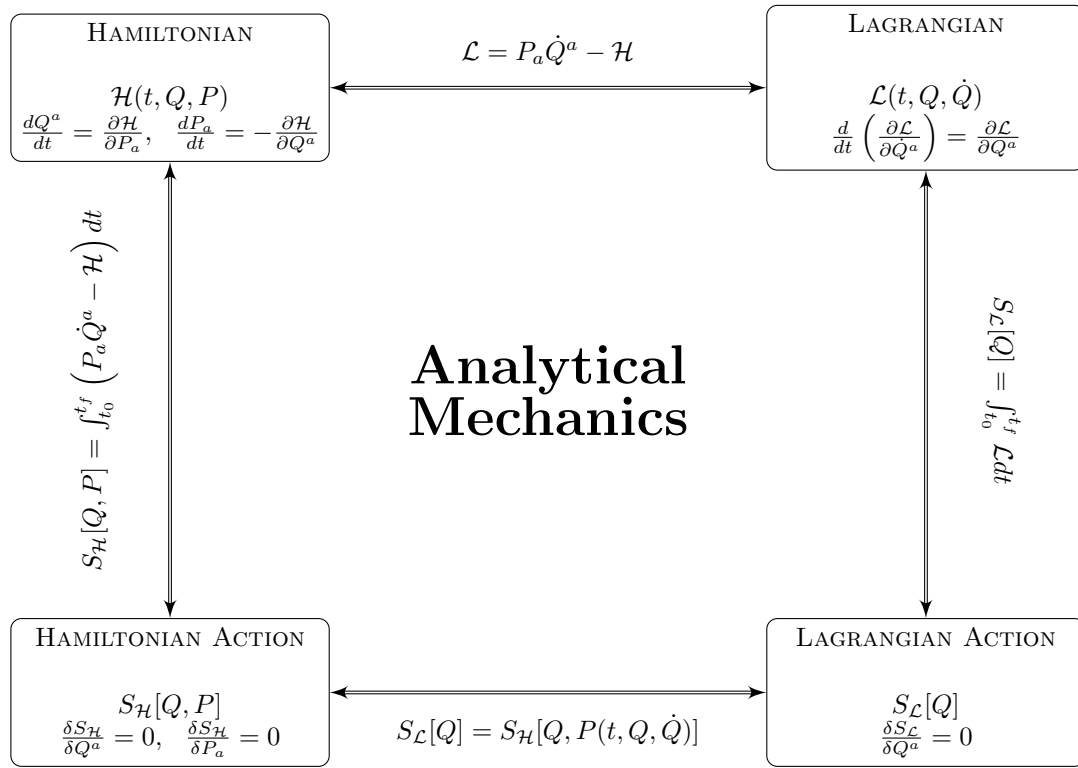


Figure 1.1: The core objects of Analytical Mechanics (and Physics by extension). If there is anything in this book you must know before you put it down, it is this chart.

Exercises

Problem 1.19: A common Hamiltonian. Consider the Hamiltonian $\mathcal{H} = \frac{P^2}{2} + U(t, Q)$ for some function $U(t, Q)$.

- Compute Hamilton's equations of motion for this Hamiltonian.
- By differentiation and algebra, produce from Hamilton's two first order equations a single second order equation for Q only.
- Write the Hamiltonian action for this Hamiltonian and vary it. Verify that its functional derivatives vanish if and only if Hamilton's equations are satisfied.
- From the first of Hamilton's equations, find $P(t, Q, \dot{Q})$ and complete the Legendre transformation to find the Lagrangian.
- From the Lagrangian, find the Euler-Lagrange equation of motion and verify that it matches what you found in (b).
- Write the Lagrangian action for this Lagrangian and vary it. Verify that its functional derivative vanishes if and only if the Euler-Lagrange equation is satisfied.

Problem 1.20: Hamiltonian for a ray of light. For a configuration $Q = \vec{x}$ for $\vec{x}$ some vector in $\mathbb{R}^N$ and conjugate momentum $P = \vec{p}$, consider the Hamiltonian $\mathcal{H} = c|\vec{p}|$.

- Compute Hamilton's equations of motion for this Hamiltonian and show that it corresponds to motion in a straight line at constant speed c .
- Show that the first of Hamilton's equations is not invertible and so the Legendre transformation cannot be completed (and thus that in this case the Lagrangian does not exist).
- Consider now the Hamiltonian $\mathcal{H}_\varepsilon = c\sqrt{|\vec{p}|^2 + \varepsilon^2}$. Show that for all $\varepsilon > 0$ the Legendre transformation can be completed and find the Lagrangian $\mathcal{L}_\varepsilon$. Verify that $\mathcal{L}_\varepsilon$ gives the same equations of motion as $\mathcal{H}_\varepsilon$.
- Show in the limit $\varepsilon \rightarrow 0$ that $\mathcal{H}_\varepsilon \rightarrow \mathcal{H}$, $|\vec{x}| \rightarrow c$, and $\mathcal{L}_\varepsilon \rightarrow 0$. This Hamiltonian is actually physically meaningful and corresponds essentially to the Hamiltonian for a single ray of light.

Problem 1.21: Lagrangian for arclength. For a configuration $Q = \vec{x}$ just like before, consider the Lagrangian $\mathcal{L} = |\dot{\vec{x}}|$.

- (a) Compute the Euler-Lagrange equations of motion for this Lagrangian and show that it corresponds to motion in a straight line where the magnitude of the momentum is fixed to be 1.
- (b) Show that the relationship between the momentum and the Lagrangian is not invertible and so the Legendre transformation cannot be completed (and thus that in this case the Hamiltonian does not exist for these coordinates).
- (c) Consider now the Lagrangian $\mathcal{L}_\varepsilon = \sqrt{|\dot{\vec{x}}|^2 + \varepsilon^2}$. Show that for all $\varepsilon > 0$ the Legendre transformation can be completed and find the Hamiltonian $\mathcal{H}_\varepsilon$. Verify that it gives the same equation of motion as the Lagrangian.
- (d) Show in the limit $\varepsilon \rightarrow 0$ that $\mathcal{L}_\varepsilon \rightarrow \mathcal{L}$, $|\vec{p}| \rightarrow 1$, and $\mathcal{H}_\varepsilon \rightarrow 0$.

1.8 The Non-uniqueness of the Action

We have found that using an action in the form in Theorem 1.4 we can generate our equations of motion by setting the variation of the action to 0. Further, we saw that when we change coordinates, we still get the new equations of motion from varying the same action. As such, the variational principle is coordinate invariant. However, it turns out that the action satisfying the properties we have so far described is not unique. It is important to understand the class of all actions of the form of either (1.7.23) or (1.7.24) which produce the same physics. Suppose we have an action $S[\Phi]$ where we take $\Phi = (Q, P)$ if we are using the Hamiltonian action or $\Phi = Q$ if we are using the Lagrangian action (we can study both choices using the same techniques here). Suppose the functional derivative of that action gives functions $F_a(t, \Phi, \dot{\Phi}, \ddot{\Phi})$:

$$\frac{\delta S}{\delta \Phi^a(t)} = F_a(t, \Phi, \dot{\Phi}, \ddot{\Phi}). \quad (1.8.1)$$

These F_a are called the equation of motion functions of the action S . Setting them to 0 gives the differential equations governing the dynamics of the system by the stationary action theorem. Because the F_a specify the dynamics of the system, two actions are only to be considered equivalent if they give the same F_a .¹⁸ So, we can study the non-uniqueness of the action by looking at the extent to which we can reconstruct S from F_a . Using an argument from [109] and [120], define $S_1[\Phi](\lambda)$, a functional of Φ and function of λ as:

$$S_1[\Phi](\lambda) \stackrel{\text{def}}{=} S[\lambda\Phi] \quad (1.8.2)$$

$$\implies S_1[\Phi](0) = S[0] \quad (1.8.3)$$

$$\implies S_1[\Phi](1) = S[\Phi]. \quad (1.8.4)$$

Then by differentiating S_1 with respect to λ and using Theorem 1.3 and the chain rule:

$$\frac{dS_1}{d\lambda} = \int_{t_0}^{t_f} \frac{\delta S}{\delta \Phi^a} [\lambda\Phi] \frac{d(\lambda\Phi^a)}{d\lambda} dt = \int_{t_0}^{t_f} F_a(t, \lambda\Phi, \lambda\dot{\Phi}, \lambda\ddot{\Phi}) \Phi^a dt. \quad (1.8.5)$$

Now using the fundamental theorem of calculus:

$$S_1[\Phi](1) = S_1[\Phi](0) + \int_0^1 \frac{dS_1}{d\lambda} d\lambda \quad (1.8.6)$$

$$\implies S[\Phi] = S[0] + \int_0^1 \int_{t_0}^{t_f} F_a(t, \lambda\Phi, \lambda\dot{\Phi}, \lambda\ddot{\Phi}) \Phi^a dt d\lambda. \quad (1.8.7)$$

Hence from the equation of motion functions F_a we can recover the action $S[\Phi]$ up to the undetermined $S[0]$, the action when the path is identically 0. Because $S[0]$ sets the path to a fixed value, it is a function only of the end points of the path (as they are not varied by definition of functional differentiation). Therefore, the equation of motion functions F_a determine the action up adding an arbitrary function $g(t_f, \Phi_f, t_0, \Phi_0)$ of the end points. Naturally because we don't vary the end points, a function of the end points is a constant with respect to the variation of the path. We can check by direct calculation that adding such an g does in fact leave the equations of motion functions unchanged. We can get another perspective by pushing g into the time integral with the fundamental theorem of calculus:

$$g(t_f, \Phi_f, t_0, \Phi_0) = g(t_0, \Phi_0, t_0, \Phi_0) + \int_{t_0}^{t_f} \frac{dg}{dt}(t, \Phi(t), t_0, \Phi_0) dt \quad (1.8.8)$$

$$\implies S'[\Phi] = S[\Phi] + g(t_f, t_0, \Phi_f, \Phi_0) \quad (1.8.9)$$

$$= \int_{t_0}^{t_f} \mathcal{L} dt + g = \int_{t_0}^{t_f} \left(\mathcal{L} + \frac{dg}{dt}(t, \Phi, t_0, \Phi_0) \right) dt + g(t_0, \Phi_0, t_0, \Phi_0). \quad (1.8.10)$$

Because the action (either Hamiltonian action or Lagrangian action) is 0 when $t_f = t_0$ (see (1.7.23) and (1.7.24)), we must have $g(t_0, \Phi_0, t_0, \Phi_0) = 0$ to keep our action of the same form. As well, the integrand of the action is not an explicit function of the initial data t_0, Φ_0 and so $\frac{dg}{dt}$ must not be either to keep our action

¹⁸It might seem that because we set the F_a to 0 to get the equations of motion, we could consider different F_a to be equivalent if one vanishes if and only if the other vanishes. This weaker condition still guarantees the same dynamics would be produced. But, the weaker condition turns out to be physically incorrect because when the system at hand interacts with another system, additional terms will be added to the equations of motion and so F_a 's which are equivalent in the weaker sense when non-interacting are typically not equivalent when interacting, even under the same interaction. This important distinction will be covered in the homework and later chapters.

of the right form. Consequently, for some function $f(t, \Phi)$:

$$\frac{d}{dt}g(t, \Phi, t_0, \Phi_0) = \frac{df}{dt} = \frac{\partial f}{\partial t}(t, \Phi) + \frac{\partial f}{\partial \Phi^a}(t, \Phi)\dot{\Phi}^a \quad (1.8.11)$$

$$\implies g(t_f, \Phi_f, t_0, \Phi_0) = g(t_0, \Phi_0, t_0, \Phi_0) + \int_{t_0}^{t_f} \frac{dg}{dt} dt = 0 + \int_{t_0}^{t_f} \frac{df}{dt} dt = f(t_f, \Phi_f) - f(t_0, \Phi_0). \quad (1.8.12)$$

Therefore, to keep our action of the correct form the function g must have this restricted form. Then, the new integrand of the action (literally the Lagrangian $\mathcal{L}(t, Q, \dot{Q})$ in the case we are using the Lagrangian action of $P_a \dot{Q}^a - \mathcal{H}$ in the case of the Hamiltonian action) is:

$$\mathcal{L}' = \mathcal{L} + \frac{df}{dt} = \mathcal{L} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \Phi^a} \dot{\Phi}^a \quad (1.8.13)$$

where in the last step we have used the chain rule. By taking the variation of our new action S' in terms of our new $\mathcal{L}'$, we can see the effect of the function f disappear more explicitly:

$$\frac{\delta S'}{\delta \Phi^a} = \frac{\partial \mathcal{L}'}{\partial \Phi^a} - \frac{d}{dt} \frac{\partial \mathcal{L}'}{\partial \dot{\Phi}^a} \quad (1.8.14)$$

$$= \frac{\partial}{\partial \Phi^a} \left(\mathcal{L} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \Phi^b} \dot{\Phi}^b \right) - \frac{d}{dt} \frac{\partial}{\partial \dot{\Phi}^a} \left(\mathcal{L} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \Phi^b} \dot{\Phi}^b \right) \quad (1.8.15)$$

$$= \frac{\partial \mathcal{L}}{\partial \Phi^a} + \frac{\partial^2 f}{\partial t \partial \Phi^a} + \frac{\partial^2 f}{\partial \Phi^a \partial \Phi^b} \dot{\Phi}^b - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\Phi}^a} + \frac{\partial f}{\partial \Phi^a} \right) \quad (1.8.16)$$

$$= \frac{\partial \mathcal{L}}{\partial \Phi^a} + \frac{d}{dt} \frac{\partial f}{\partial \Phi^a} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\Phi}^a} - \frac{d}{dt} \frac{\partial f}{\partial \Phi^a} \quad (1.8.17)$$

$$= \frac{\partial \mathcal{L}}{\partial \Phi^a} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\Phi}^a} = \frac{\delta S}{\delta \Phi^a}. \quad (1.8.18)$$

Hence as we expected the function f (called a “surface term”) cancels in the end and so is entirely arbitrary. Adding an f , a function of the end points, to the action does not affect its variation (and by our original argument is actually the most general modification keeping our action of the same form for which that is true). There is a nice intuition as to why it is always possible to add a surface term to the action without affecting the equations of motion. The derivative of a function determines that function up to boundary conditions (by integrating and using the fundamental theorem of calculus). This essentially extends to functionals; the derivative of a functional determines that functional up to boundary conditions. The boundary values of the functional S are changed by choosing different f . In this way, f is essentially the “plus C ” integration constant from trying to recover the action from its derivative.

If we are using the Lagrangian action $S_{\mathcal{L}}$ then $\Phi = Q$ and the most general addition to the action which keeps its form and does not affect the equations of motion is $f(t, Q) - f(t_0, Q_0)$. If we are using the Hamiltonian action $S_{\mathcal{H}}$ then $\Phi = (Q, P)$ and we would think we can take a general function $f(t_f, Q_f, P_f) - f(t_0, Q_0, P_0)$ as our surface term. However, we found in theorem 1.4 that the Hamiltonian action is not a function of the initial and final momenta and so the most generic surface term that can be added which preserves the form of the action and appropriate boundary conditions on the variation is also one that is not a function of the initial and final momenta. That is, we still have to take $f = f(t, Q)$ in order to preserve Hamilton’s equations¹⁹. Any such f then changes the Lagrangian according to:

$$\mathcal{L}'(t, Q, \dot{Q}) = \mathcal{L}(t, Q, \dot{Q}) + \frac{df}{dt} = \mathcal{L}(t, Q, \dot{Q}) + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \dot{Q}^a. \quad (1.8.19)$$

This new Lagrangian then changes the corresponding value of the momenta P_a to new momenta P'_a :

$$P'_a = \frac{\partial \mathcal{L}'}{\partial \dot{Q}^a} = \frac{\partial \mathcal{L}}{\partial \dot{Q}^a} + \frac{\partial f}{\partial Q^a} = P_a + \frac{\partial f}{\partial Q^a}. \quad (1.8.20)$$

Similarly, the Hamiltonian changes according to the Legendre transform:

$$\mathcal{H}'(t, Q, P') = P'_a \dot{Q}^a - \mathcal{L}' = P_a \dot{Q}^a + \frac{\partial f}{\partial Q^a} \dot{Q}^a - \mathcal{L} - \frac{\partial f}{\partial t} - \frac{\partial f}{\partial Q^a} \dot{Q}^a = \mathcal{H}(t, Q, P) - \frac{\partial f}{\partial t}. \quad (1.8.21)$$

Therefore, under adding a surface term, while the definition of the time t and the coordinates Q^a does not change, the expressions for the momentum and Hamiltonian do. This is a kind of canonical transformation known as an **action gauge transformation**. We can see that it is the most general class of modifications to

¹⁹We will see what happens if one violates this next section.

the action which does not affect its predictions (the equations of motion) for the coordinates. Because actions which are related by an action gauge transformation are equivalent in terms of the equations of motion they produce and because the composition of gauge transformations is a gauge transformation, we can define an equivalence relation between actions $\simeq$ to say that:

$$S'[Q] \simeq S[Q] \iff \exists f(t, Q) : S'[Q] = S[Q] + f(t_f, Q_f) - f(t_0, Q_0). \quad (1.8.22)$$

This then defines an equivalence class of actions which are all “gaugeomorphic” to each other (related by a gauge transformation or “gaugeomorphism”). If two actions are gaugeomorphic, we apply the same similarity symbol to their corresponding Hamiltonians and Lagrangians:

$$S' \simeq S \iff \mathcal{H}' \simeq \mathcal{H} \iff \mathcal{L}' \simeq \mathcal{L}. \quad (1.8.23)$$

Because all gaugeomorphic actions produce identical equations of motion, they make all of the same physical predictions. The gauge transformation is then a redundancy in our description of physics; all actions which differ by a surface term are equivalent for all experimental purposes.

Theorem 1.6: Action Gauge Theorem

Two actions S and S' produce the same equations of motion for the same coordinates if and only if they are related by an action gauge transformation:

$$S'[Q] = S[Q] + f(t_f, Q_f) - f(t_0, Q_0) \quad (1.8.24)$$

for some function $f(t, Q)$. Correspondingly, the canonical quantities of each are related by:

$$\mathcal{H}'(t, Q, P') = \mathcal{H}(t, Q, P) - \frac{\partial f}{\partial t}(t, Q) \quad (1.8.25)$$

$$P'_a = P_a + \frac{\partial f}{\partial Q^a}(t, Q) \quad (1.8.26)$$

$$\mathcal{L}' = \mathcal{L} + \frac{df}{dt}. \quad (1.8.27)$$

Our reconstruction of the Action from the equations of motion will also be useful to refer back to:

Theorem 1.7: Action Recovery Theorem

If there exists an action $S[\Phi]$ so that $\frac{\delta S}{\delta \Phi^a} = F_a(t, \Phi, \dot{\Phi}, \ddot{\Phi})$ for a given function $F_a(t, \Phi, \dot{\Phi}, \ddot{\Phi})$, then up to adding a function of the boundary conditions that action is given by:

$$S[\Phi] = \int_{t_0}^{t_f} \Phi^a \int_0^1 F_a(t, \lambda \Phi, \lambda \dot{\Phi}, \lambda \ddot{\Phi}) d\lambda dt. \quad (1.8.28)$$

It is important to note that the term “gauge transformation” is used for a few related but slightly different things in physics. In general, physicists call something a gauge transformation if a quantity is only defined up to modifying it by a whole *function* in a well-defined way. Most transformations of interest depend on some constant parameters, like a rotation by an angle θ , whereas any transformation that depends on a whole function worth of data to define the transformation is called a gauge transformation. Here we see the function is $f(t, Q)$ and that the action / Lagrangian / Hamiltonian are only defined up to modification by f as described in theorem 1.6. So, to be more precise this action gauge transformation is a particular kind of gauge transformation. We will see that other quantities of interest will sometimes also carry some arbitrariness due to being able to be modified by functions in a precise way, and we will also call those transformations gauge transformations. While the careful thing to do is to also call the transformation we have done here an “action gauge transformation”, the physicist in me is liable to just say gauge transformation and hope you get the context.

Exercises

Problem 1.22: A hint at boost symmetry. Consider the Lagrangian $\mathcal{L} = \frac{1}{2}\dot{Q}^2$ and the point transformation $Q' = Q + vt$ for some constant v .

- (a) Write the action S corresponding to the Lagrangian $\mathcal{L}$. Evaluate this action at the transformed coordinates (call the result S') and show that S' and S differ by a term which depends only on the

boundary conditions, not on the path. Thus these should give the same equations of motion. Explain that this means the transformation should be a symmetry of the system.

- (b) Find the Lagrangian $\mathcal{L}'$ corresponding to S' and show that it is related to $\mathcal{L}$ by the addition of a total derivative.
- (c) Show by direct calculation that Q and Q' satisfy the same equation of motion and so this transformation is in fact a symmetry.

Problem 1.23: Action of the Harmonic Oscillator. Consider the equation of motion function $F = -\ddot{Q} - \omega^2 Q$. Compute the right hand side of (1.8.28) for this function and call the result S . Show that that functional S when varied with respect to Q reproduces this equation of motion function and thus is the action with this equation of motion.

Problem 1.24: Action of the damped Harmonic Oscillator. Consider the equation of motion function $F = -\ddot{Q} - \gamma\dot{Q} - \omega^2 Q$.

- (a) Compute the right hand side of (1.8.28) for this function and call the result S . Show that that functional S when varied with respect to Q does not reproduce this equation of motion and from this conclude using Theorem 1.7 that there does not exist an action for Q only with this equation of motion function.
- (b) Consider now the equation of motion function $F' = -e^{\gamma t}(\ddot{Q} + \gamma\dot{Q} + \omega^2 Q)$. Show that $F' = 0$ if and only if $F = 0$ and so these two different equation of motion functions produce the same differential equation for Q . Compute the right hand side of (1.8.28) for this F' and call the result S' . Show that S' when varied with respect to Q does reproduce this equation of motion and thus is the action with F' as its equation of motion. It may seem bizarre that by multiplying functions onto an equation of motion with no action one can make an equation of motion with an action. This may make the equation of motion function idea seem ambiguous. However, as we will see later when we make a system interact with another system we add terms to its action which ultimately adds terms to the equation of motion function. Adding a term to F and setting the result to 0 is not the same as adding that term to F' and setting the result to 0 and so we can see that when we interact with a system it is actually enough to fix its equation of motion function uniquely. This is why actions are gaugeomorphic only when they produce the same equation of motion functions, not simply when their equation of motion functions can be transformed into each other by sufficient algebra.
- (c) It may seem weird at all that there exist equation of motion functions for which there is no action. One should be more careful and say that there exist equation of motion functions for which there is no action in only the variables appearing in that function. By our dimension doubling, we can always make an action work out. Trivially show that the variation of this action S :

$$S[Q, R] = \int_{t_0}^{t_f} R(t)F(t, Q, \dot{Q}, \ddot{Q})dt$$

with respect to the variable R gives the equation of motion function F . Generalize this argument to apply for any equation of motion function and any number of variables.

Problem 1.25: Equivalent or inequivalent? Consider the following two Lagrangians:

$$\mathcal{L}_1 = Q^2 \dot{Q}^4, \quad \mathcal{L}_2 = Q^3 \dot{Q}^6.$$

- (a) Show that the equation of motion functions F_1 and F_2 corresponding to these Lagrangians each vanish if and only if the other vanishes.
- (b) Now consider adding a term $+J(t)Q$ to each Lagrangian for J some given function of t . Show that the conclusion of (a) is now false. This term we have added physically corresponds to making the system interact with an external force J (this will be explained later) and so we see that by probing our system with this driving force, we can distinguish between the two Lagrangians $\mathcal{L}_1$ and $\mathcal{L}_2$ even though when the system is undriven or “free” they produce the same dynamics. Again, this is why we say we care about the equation of motion function precisely and don’t have the freedom to make algebraic transformations of it. Although systems with different equations of motion functions may act the same when they are not interacting with other systems, they do not act the same when they interact with other systems. You have to interact with a system to measure anything about it, so this distinction is crucial!

1.9 Canonical Transformations

Coordinate transformations which leave our analytical formalism unchanged (meaning preserve Hamilton's equations) are called canonical transformations. The set of all of them is quite large. It is the set of all transformations $t' = t'(t, Q, P)$, $Q' = Q'(t, Q, P)$, $P' = P'(t, Q, P)$ so that Hamilton's equations are satisfied using all of the primed quantities with an appropriately chosen new Hamiltonian $\mathcal{H}'(t', Q', P')$ whenever Hamilton's equations are satisfied by the unprimed variables using the old Hamiltonian $\mathcal{H}(t, Q, P)$. Suppose we have such a transformation. Then, the primed system will be described by the stationary variation of some action $S'[Q', P']$ with the boundary conditions t'_f, Q'_f, t'_0, Q'_0 fixed:

$$S'[Q', P'] = \int_{t'_0}^{t'_f} \left(P'_a \dot{Q}'^a - \mathcal{H}'(t', Q', P') \right) dt'. \quad (1.9.1)$$

Because the stationarity of the action is coordinate invariant, the stationary variation of this same action should give the equations of motion for our untransformed variables when we express it in terms of them and when we keep the boundary conditions t_f, Q_f, t_0, Q_0 fixed. That is, it must give the same variations as the unprimed action:

$$S[Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H}(t, Q, P) \right) dt. \quad (1.9.2)$$

Because these two actions give the same variations, they must differ only by a function of the boundary conditions (by using the action recovery theorem 1.7 they both must be given by that same integral for each up to a function of the boundary conditions, their difference is then a function of the boundary conditions only). The full set of boundary conditions between these two actions are provided by $t'_f, Q'_f, t'_0, Q'_0, t_f, Q_f, t_0, Q_0$. Therefore, for some function $F(t', Q', t, Q)$ we have:

$$S'[Q', P'] = S[Q, P] + F(t'_f, Q'_f, t_f, Q_f) - F(t'_0, Q'_0, t_0, Q_0). \quad (1.9.3)$$

This function $F(t', Q', t, Q)$ is called the **generating function** of the canonical transformation or simply **canonical function** of the transformation. The use of the term generating function can be confusing because this F is **NOT** the same thing as the generator of a continuous transformation discussed in section 1.3 (we will see in section 1.10 that they are related but are not equal). The generator of a continuous transformation only exists for continuous transformation while the generating function F exists for any canonical transformation, continuous or discrete. If we express both actions as integrals we have:

$$\int_{t'_0}^{t'_f} \left(P'_a \frac{dQ'^a}{dt'} - \mathcal{H}'(t', Q', P') \right) dt' = \int_{t_0}^{t_f} \left(P_a \frac{dQ^a}{dt} - \mathcal{H}(t, Q, P) + \frac{dF}{dt} \right) dt. \quad (1.9.4)$$

Let us assume the direction of time is not reversed in the canonical transformation ($\frac{dt'}{dt} > 0$) so that the transformed final and initial times are $t'_f(t_f, Q_f, P_f)$ and $t'_0(t_0, Q_0, P_0)$. Then, changing integrals to the same integration variable of t :

$$\int_{t_0}^{t_f} \left(P'_a(t') \frac{d}{dt} Q'^a(t') - \mathcal{H}'(t', Q', P') \frac{dt'}{dt} \right) dt = \int_{t_0}^{t_f} \left(P_a \frac{dQ^a}{dt} - \mathcal{H}(t, Q, P) + \frac{dF}{dt} \right) dt. \quad (1.9.5)$$

This must be true for all initial and final times and so we have that the integrands must be equal:

$$P'_a \frac{dQ'^a}{dt} - \mathcal{H}'(t', Q', P') \frac{dt'}{dt} = P_a \frac{dQ^a}{dt} - \mathcal{H}(t, Q, P) + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial F}{\partial t'} \frac{dt'}{dt} + \frac{\partial F}{\partial Q'^a} \frac{dQ'^a}{dt}. \quad (1.9.6)$$

This must hold regardless of whether the equations of motion are used (because the actions are related this way as functionals using theorem 1.7). Therefore, it holds for any time dependence of Q, t', Q' . Because the time dependence of t' can be chosen independently, the factors $\frac{dt'}{dt}$ are independent from any other time derivatives appearing here and so the terms proportional to them must cancel each other:

$$\implies -\mathcal{H}' = \frac{\partial F}{\partial t'}. \quad (1.9.7)$$

Similarly, the $\frac{dQ^a}{dt}$ terms must cancel each other:

$$\implies 0 = P_a + \frac{\partial F}{\partial Q^a}. \quad (1.9.8)$$

As well, the $\frac{dQ'^a}{dt}$ terms must cancel each other:

$$\implies P'_a = \frac{\partial F}{\partial Q'^a}. \quad (1.9.9)$$

Finally, the remaining terms with no time derivatives must cancel each other:

$$\implies 0 = -\mathcal{H} + \frac{\partial F}{\partial t}. \quad (1.9.10)$$

Collected together we have:

$$\boxed{\frac{\partial F}{\partial t'} = -\mathcal{H}', \quad \frac{\partial F}{\partial Q'^a} = P'_a, \quad \frac{\partial F}{\partial t} = \mathcal{H}, \quad \frac{\partial F}{\partial Q^a} = -P_a.} \quad (1.9.11)$$

These give the full set of four conditions for a canonical transformation which does not change the direction of time. For a given canonical function $F(t', Q', t, Q)$ we can determine $t'(t, Q, P)$, $Q'^a(t, Q, P)$, $P'_a(t, Q, P)$, $\mathcal{H}'(t', Q', P')$ by solving these four differential equations together. Once we have found the solution, that is our canonical transformation.

In practice when performing a canonical transformation one does not usually start off by knowing the generating function F . Instead, motivated by the situation of interest, one may know $Q'(t, Q, P)$ and $t'(t, Q, P)$ but not $P'(t, Q, P)$ and $\mathcal{H}'$. Or, one may know some other subset of the final transformation functions. To find the transformation functions which are not known, simply insert the ones which are known into (1.9.11) and solve those conditions for the most general F consistent with them. Then, from the derivatives of that restricted form of F compute the functions which are not known. Generally a subset of the transformation functions that relate $t, Q, P, \mathcal{H}$ to $t', Q', P', \mathcal{H}'$ will only partly determine the other functions and so for a particular canonical transformation of interest if only some of these transformation functions are known you will have some arbitrariness left in your solution for F and thus some arbitrariness left in the definitions of the unknown transformation functions.

The four conditions on F in (1.9.11) can be used to check if a proposed transformation is genuinely canonical. Taking the proposed transformation functions $t', Q', P', \mathcal{H}'$ and trying to use them to integrate those four conditions, if a solution can be found it guarantees the transformation is canonical. If it can be proven that a solution does not exist, the transformation is not canonical.

For calculations, the above F may not be the easiest way to approach a canonical transformation. By using a Legendre transform analogous to how we related the Lagrangian and Hamiltonian, it is possible to make many other “generating functions” which can help with performing a canonical transformation. Typically, $F(t', Q', t, Q)$ is called a “type-1 generating function”. A “type-2 generating function” is defined by inverting (1.9.9) to solve for Q'^a in terms of t, t', Q, P' and making the function $F_2(t', P', t, Q)$:

$$F_2(t', P', t, Q) \stackrel{\text{def}}{=} F(t', Q', t, Q) - Q'^a P'_a. \quad (1.9.12)$$

Taking partial derivatives and using the conditions on F we have:

$$\frac{\partial F_2}{\partial t'} = -\mathcal{H}', \quad \frac{\partial F_2}{\partial P'_a} = -Q'^a, \quad \frac{\partial F_2}{\partial t} = \mathcal{H}, \quad \frac{\partial F_2}{\partial Q^a} = -P_a. \quad (1.9.13)$$

This gives an equivalent set of four conditions that define the canonical transformation. We can see that the type-2 generating function is a Legendre transformation of our type-1 function with respect to the new coordinates and momenta. A “type-3 generating function” is defined by Legendre transforming our type-1 function with respect to the old coordinates and momenta:

$$F_3(t', Q', t, P) \stackrel{\text{def}}{=} F(t', Q', t, Q) + Q^a P_a \quad (1.9.14)$$

$$\implies \frac{\partial F_3}{\partial t'} = -\mathcal{H}', \quad \frac{\partial F_3}{\partial Q'^a} = P'_a, \quad \frac{\partial F_3}{\partial t} = \mathcal{H}, \quad \frac{\partial F_3}{\partial P_a} = Q^a. \quad (1.9.15)$$

A “type-4 generating function” is defined by Legendre transforming our type-1 function with respect to both the old coordinates and momenta and the new coordinates and momenta:

$$F_4(t', P', t, P) \stackrel{\text{def}}{=} F(t', Q', t, Q) - Q'^a P'_a + Q^a P_a \quad (1.9.16)$$

$$\implies \frac{\partial F_4}{\partial t'} = -\mathcal{H}', \quad \frac{\partial F_4}{\partial P'_a} = -Q'^a, \quad \frac{\partial F_4}{\partial t} = \mathcal{H}, \quad \frac{\partial F_4}{\partial P_a} = Q^a. \quad (1.9.17)$$

While these four types of generating function are common and useful, they are not exhaustive. It is also possible to Legendre transform between the times and Hamiltonians or between some of the coordinates and momenta but not all of them. One can Legendre transform independently for the untransformed and

transformed time/Hamiltonian and each coordinate/momentum. If there are d coordinates Q^a then this means there are 4^{d+1} possible Legendre transforms to make on the generating function! The reason one might care about ever making such a transformation is that if you only know some of the transformation functions that relate $t', Q', P', \mathcal{H}'$ to $t, Q, P, \mathcal{H}$, the functions you do know imply some information about the derivatives of the generating function and it may be easier or harder to integrate those derivatives to identify what the generating function is depending on which generating function you choose to use. Ultimately, all these variously transformed generating functions are calculation tools to aid in performing a canonical transformation.

1.9.1 Time Reversal

We made a seemingly quite reasonable assumption in deriving (1.9.11); we assumed that the canonical transformation did not reverse the direction of time. It will turn out to be useful later on to consider canonical transformations which do reverse the direction of time and so we will consider that case here as well. Time reversal may seem very esoteric but it turns out to be both theoretically and experimentally interesting. Let us return to (1.9.4) and now assume that the transformation *is* time reversing so that $\frac{dt'}{dt} < 0$. Then, the final time t'_f depends on the *initial* data t_0, Q_0, P_0 and vice versa because which end of the path is identified as the start and which as the end is different between the transformed and untransformed variables. With this, the integrals written both as integrals over t become:

$$\int_{t_f}^{t_0} \left(P'_a(t') \frac{d}{dt} Q'^a(t') - \mathcal{H}'(t', Q', P') \frac{dt'}{dt} \right) dt = \int_{t_0}^{t_f} \left(P_a \frac{dQ^a}{dt} - \mathcal{H}(t, Q, P) + \frac{dF}{dt} \right) dt. \quad (1.9.18)$$

Again this holds for all t_f and t_0 and so the integrands must match, but this time up to a minus sign due to the opposite order of integration:

$$-P'_a \frac{dQ'^a}{dt} + \mathcal{H}' \frac{dt'}{dt} = P_a \frac{dQ^a}{dt} - \mathcal{H} + \frac{\partial F}{\partial t'} \frac{dt'}{dt} + \frac{\partial F}{\partial Q'^a} \frac{dQ'^a}{dt} + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial Q^a} \frac{dQ^a}{dt} \quad (1.9.19)$$

Performing the same matching we did in the case that time was not reversed we have that for any time reversing canonical transformation there exists a function $F(t', Q', t, Q)$ so that:

$$\frac{\partial F}{\partial t'} = \mathcal{H}', \quad \frac{\partial F}{\partial Q'^a} = -P'^a, \quad \frac{\partial F}{\partial t} = \mathcal{H}, \quad \frac{\partial F}{\partial Q^a} = -P_a. \quad (1.9.20)$$

Suppose we have a canonical transformation in which time is reversed so that $\frac{dt'}{dt} < 0$. If we compose it with another canonical transformation in which time is reversed so that the new new time t'' satisfies $\frac{dt''}{dt'} < 0$ then the relationship between the untransformed time t and the new new time satisfies $\frac{dt''}{dt} > 0$ because it is the product of $\frac{dt''}{dt'}$ and $\frac{dt'}{dt}$. Suppose we have a single time reversing transformation that we know how to write down; call it “simple time reversal”. Then, suppose we have another time reversing transformation of interest. Their composition is then not time reversing and so is described by the generating function formalism we already covered. We can then get back the time reversing transformation of interest by applying to this composed transformation the inverse of the simple time reversal. Therefore, if we know how to do a single time reversing transformation, we can write any other time reversing transformation as a composition of the inverse of that simple time reversal and a canonical transformation in which time is not reversed. So, let us consider the “simple time reversal” in which:

$$t' = -t, \quad Q'^a = Q^a. \quad (1.9.21)$$

This may or may not be the actual time reversal transformation of theoretical or experimental interest in applications, but as we explained any such transformation can be written as this transformation composed with a canonical transformation which does not reverse time. This simple time reversal defines how the time and coordinates are changed but does not specify how the Hamiltonian or momenta should be changed. We can find how they must change by using a generating function. In particular, because we know Q'^a and t' and they can be written in terms of Q^a and t , it is nice to use a generating function which has Q'^a and t' as derivatives and which depends on Q^a and t . The appropriate Legendre transform is then:

$$G(\mathcal{H}', P', t, Q) = F(t', Q', t, Q) - t' \mathcal{H}' + Q'^a P'_a \quad (1.9.22)$$

$$\implies \frac{\partial G}{\partial \mathcal{H}'} = -t', \quad \frac{\partial G}{\partial P'_a} = Q'^a, \quad \frac{\partial G}{\partial t} = \mathcal{H}, \quad \frac{\partial G}{\partial Q^a} = -P_a. \quad (1.9.23)$$

Using that $t' = -t$:

$$\frac{\partial G}{\partial \mathcal{H}'} = -t' \stackrel{!}{=} t \implies G = \mathcal{H}'t + g(t, Q, P') \quad (1.9.24)$$

for some function $g(t, Q, P')$. Now using that $Q'^a = Q^a$:

$$\frac{\partial G}{\partial P'_a} = Q'^a \stackrel{!}{=} Q^a \implies \frac{\partial g}{\partial P'_a} = Q^a \implies g(t, Q, P) = P'_a Q^a + h(t, Q) \quad (1.9.25)$$

for some function $h(t, Q)$. Then, we have:

$$G = \mathcal{H}'t + P'_a Q^a + h(t, Q) \quad (1.9.26)$$

and the remaining two conditions become:

$$\frac{\partial G}{\partial t} = \mathcal{H}' + \frac{\partial h}{\partial t} \stackrel{!}{=} \mathcal{H} \implies \mathcal{H}' = \mathcal{H} - \frac{\partial h}{\partial t} \quad (1.9.27)$$

$$\frac{\partial G}{\partial Q^a} = P'_a + \frac{\partial h}{\partial Q^a} \stackrel{!}{=} -P_a \implies P'_a = -\left(P_a + \frac{\partial h}{\partial Q^a}\right). \quad (1.9.28)$$

The function h is not determined by any of these conditions and because we only need a single representative time reversal transformation to make all the others, we make the choice for simple time reversal that $h = 0$. Then, we have that the transformation:

$$t' = -t, \quad Q'^a = Q^a, \quad P'_a = -P_a, \quad \mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P) \quad (1.9.29)$$

is a valid canonical transformation in which time is reversed. It is also automatically its own inverse. So, all other time reversing canonical transformations are given by the composition of this transformation and a time nonreversing canonical transformation.

1.9.2 Preservation of the Poisson Bracket

Suppose we have a time nonreversing canonical transformation with generating function $F(t', Q', t, Q)$. The fancy word people use for a transformation that doesn't reverse time is "orthochronous". Ortho means right/correct, chronous means time, and so orthochronous means time is alright (as opposed to topsy turvy). The derivatives of this F implicitly define $t' = t'(t, Q, P)$ and $Q'^a = Q'^a(t, Q, P)$. Define the function $f(t, Q, P)$ by:

$$f(t, Q, P) = F(t'(t, Q, P), Q'(t, Q, P), t, Q). \quad (1.9.30)$$

From (1.9.3) we can see that the surface term added to the action under the canonical transformation then can be equivalently written:

$$S'[Q', P'] = S[Q, P] + f(t_f, Q_f, P_f) - f(t_0, Q_0, P_0). \quad (1.9.31)$$

So, we will call f the surface function of the canonical transformation. As explained in section 1.8, the surface term added to the action cannot depend on the initial and final momenta if the time and coordinate Q^a are untransformed. Here the Q^a are allowed to be transformed and this is why it is okay for the surface term to depend on the initial and final momenta when written this way. Recall that the left hand side here is not required to be independent of the initial and final untransformed momenta; it is required to be independent of the initial and final transformed momenta because it is the action of the transformed variables. If we now rewrite the actions as integrals over t in the same way we did in (1.9.5) we have:

$$\int_{t_0}^{t_f} \left(P'_a \frac{dQ'^a}{dt} - \mathcal{H}' \frac{dt'}{dt} \right) dt = \int_{t_0}^{t_f} \left(P_a \frac{dQ^a}{dt} - \mathcal{H} + \frac{df}{dt} \right) dt. \quad (1.9.32)$$

Again this must hold at each t_f and t_0 , but now we have applied directly the relationships between t' , Q'^a and our untransformed quantities and so expanding their derivatives using the chain rule:

$$P'_a \frac{\partial Q'^a}{\partial t} + P'_a \frac{\partial Q'^a}{\partial Q^b} \dot{Q}^b + P'_a \frac{\partial Q'^a}{\partial P_b} \dot{P}_b - \mathcal{H}' \frac{\partial t'}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial Q^a} \dot{Q}^a - \mathcal{H}' \frac{\partial t'}{\partial P_a} \dot{P}_a = P_a \dot{Q}^a - \mathcal{H} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \dot{Q}^a + \frac{\partial f}{\partial P_a} \dot{P}_a. \quad (1.9.33)$$

While this used how t' and Q' relate to t and Q , it did not use the equations of motion. So, this still must hold for all $\dot{Q}^a$ and $\dot{P}_a$. Matching the $\dot{P}_a$ terms gives:

$$P'_b \frac{\partial Q'^b}{\partial P_a} - \mathcal{H}' \frac{\partial t'}{\partial P_a} = \frac{\partial f}{\partial P_a}. \quad (1.9.34)$$

Then, matching the $\dot{Q}^a$ terms gives:

$$P'_b \frac{\partial Q'^b}{\partial Q^a} - \mathcal{H}' \frac{\partial t'}{\partial Q^a} = P_a + \frac{\partial f}{\partial Q^a}. \quad (1.9.35)$$

Finally, matching the remaining terms with no time derivatives gives:

$$P'_a \frac{\partial Q'^a}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial t} = -\mathcal{H} + \frac{\partial f}{\partial t}. \quad (1.9.36)$$

Then, (1.9.34), (1.9.35), and (1.9.36) provide an equivalent set of conditions $t', \mathcal{H}', Q', P'$ must satisfy in order to be orthochronous canonical. If there exists a function $f(t, Q, P)$ so that these are all true, then the transformation is orthochronous canonical. If there does not, the transformation is not orthochronous canonical.

The three conditions (1.9.34), (1.9.35), (1.9.36) can only be satisfied if it is possible to integrate them to find the function $f(t, Q, P)$. If transformation functions for $t', \mathcal{H}', Q', P'$ in terms of $t, \mathcal{H}, Q, P$ are known and one would like to check if they are orthochronous canonical, then these three conditions give the derivatives of f in terms of t, Q, P and we can wonder under what conditions does an f with these derivatives exist. We essentially are given functions which are to be the gradient of f with respect to t, Q, P and we would like to know when an f exists with that gradient. We know from vector calculus that a vector field with components $A_a(x)$ can be written as a gradient if²⁰ and only if all of its components of its curl are zero, that is $\frac{\partial A_a}{\partial x^b} = \frac{\partial A_b}{\partial x^a}$ (this is known as the Poincare lemma). Equivalently, this means we need all of the mixed partial derivatives of f to match between the two possible ways of computing them. From equation (1.9.34), take its second derivative with respect to P_b :

$$\frac{\partial P'_c}{\partial P_b} \frac{\partial Q'^c}{\partial P_a} + P'_c \frac{\partial^2 Q'^c}{\partial P_a \partial P_b} - \frac{\partial \mathcal{H}'}{\partial P_b} \frac{\partial t'}{\partial P_a} - \mathcal{H}' \frac{\partial^2 t'}{\partial P_a \partial P_b} = \frac{\partial^2 f}{\partial P_a \partial P_b}. \quad (1.9.37)$$

The right hand side is necessarily symmetric under interchanging a and b . So, if we subtract the a, b swapped version of this equation from the unswapped equation the result must be 0:

$$\frac{\partial Q'^c}{\partial P_a} \frac{\partial P'_c}{\partial P_b} - \frac{\partial Q'^c}{\partial P_b} \frac{\partial P'_c}{\partial P_a} + \frac{\partial \mathcal{H}'}{\partial P_a} \frac{\partial t'}{\partial P_b} - \frac{\partial \mathcal{H}'}{\partial P_b} \frac{\partial t'}{\partial P_a} = 0. \quad (1.9.38)$$

The partial derivatives of $\mathcal{H}'$ with respect to the unprimed quantities don't have much of an obvious interpretation but we know that the partial derivatives of $\mathcal{H}'$ with respect to primed quantities will give the equations of motion. So, now will use the equations of motion for the primed quantities (but not assume the equations of motion for the unprimed quantities) and use the chain rule:

$$\frac{\partial \mathcal{H}'}{\partial P_a} = \frac{\partial \mathcal{H}'}{\partial t'} \frac{\partial t'}{\partial P_a} + \frac{\partial \mathcal{H}'}{\partial Q'^b} \frac{\partial Q'^b}{\partial P_a} + \frac{\partial \mathcal{H}'}{\partial P'_b} \frac{\partial P'_b}{\partial P_a} = \frac{\partial \mathcal{H}'}{\partial t'} \frac{\partial t'}{\partial P_a} - \frac{dP'_b}{dt'} \frac{\partial Q'^b}{\partial P_a} + \frac{dQ'^b}{dt'} \frac{\partial P'_b}{\partial P_a}. \quad (1.9.39)$$

Returning this to (1.9.38) and doing just a little algebra:

$$\left(\frac{\partial Q'^c}{\partial P_a} - \frac{dQ'^c}{dt'} \frac{\partial t'}{\partial P_a} \right) \left(\frac{\partial P'_c}{\partial P_b} - \frac{dP'_c}{dt'} \frac{\partial t'}{\partial P_b} \right) - \left(\frac{\partial Q'^c}{\partial P_b} - \frac{dQ'^c}{dt'} \frac{\partial t'}{\partial P_b} \right) \left(\frac{\partial P'_c}{\partial P_a} - \frac{dP'_c}{dt'} \frac{\partial t'}{\partial P_a} \right) = 0. \quad (1.9.40)$$

The structures appearing here can be cleaned up nicely by introducing new partial derivatives with respect to t, Q, P which are taken at fixed t' . That is, define:

$$\frac{\partial}{\partial t} \Big|_{t'} \stackrel{\text{def}}{=} \frac{\partial}{\partial t} - \frac{\partial t'}{\partial t} \frac{d}{dt'}, \quad \frac{\partial}{\partial Q^a} \Big|_{t'} \stackrel{\text{def}}{=} \frac{\partial}{\partial Q^a} - \frac{\partial t'}{\partial Q^a} \frac{d}{dt'}, \quad \frac{\partial}{\partial P_a} \Big|_{t'} \stackrel{\text{def}}{=} \frac{\partial}{\partial P_a} - \frac{\partial t'}{\partial P_a} \frac{d}{dt'}. \quad (1.9.41)$$

These have the property that automatically:

$$\frac{\partial t'}{\partial t} \Big|_{t'} = 0, \quad \frac{\partial t'}{\partial Q^a} \Big|_{t'} = 0, \quad \frac{\partial t'}{\partial P_a} \Big|_{t'} = 0. \quad (1.9.42)$$

This justifies the interpretation of these as partial derivatives taken at fixed t' . As well, for any function $g(t, Q, P)$ it follows that:

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial g}{\partial P_a} \frac{dP_a}{dt} \quad (1.9.43)$$

$$= \frac{\partial g}{\partial t} \Big|_{t'} + \frac{\partial t'}{\partial t} \frac{dg}{dt'} + \frac{\partial g}{\partial Q^a} \Big|_{t'} \dot{Q}^a + \frac{\partial t'}{\partial Q^a} \frac{dg}{dt'} \dot{Q}^a + \frac{\partial g}{\partial P_a} \Big|_{t'} \dot{P}_a + \frac{\partial t'}{\partial P_a} \frac{dg}{dt'} \dot{P}_a \quad (1.9.44)$$

²⁰Here we will need to assume the phase space is contractible, but this is perfectly reasonable for our purposes.

$$= \frac{\partial g}{\partial t} \Big|_{t'} + \frac{dt'}{dt} \frac{dg}{dt'} + \frac{\partial g}{\partial Q^a} \Big|_{t'} \dot{Q}^a + \frac{\partial g}{\partial P_a} \Big|_{t'} \dot{P}_a \quad (1.9.45)$$

$$\Rightarrow \frac{\partial g}{\partial t} \Big|_{t'} + \frac{\partial g}{\partial Q^a} \Big|_{t'} \dot{Q}^a + \frac{\partial g}{\partial P_a} \Big|_{t'} \dot{P}_a = 0. \quad (1.9.46)$$

Therefore these three derivatives are not all independent and we can use this to always eliminate the t derivatives taken at fixed t' . With these derivative structures, (1.9.40) becomes:

$$\frac{\partial Q'^c}{\partial P_a} \Big|_{t'} \frac{\partial P'_c}{\partial P_b} \Big|_{t'} - \frac{\partial Q'^c}{\partial P_b} \Big|_{t'} \frac{\partial P'_c}{\partial P_a} \Big|_{t'} = 0. \quad (1.9.47)$$

This is the second derivative condition implied by (1.9.34) alone. We could also take a Q derivative of that equation and match it against a P derivative of (1.9.35) because both ways allow us to compute the mixed partial $\frac{\partial^2 f}{\partial Q^a \partial P_b}$. Doing so and matching the second derivatives in the same way and following the same steps from equations (1.9.37) to (1.9.47) gives:

$$\frac{\partial Q'^c}{\partial Q^a} \Big|_{t'} \frac{\partial P'_c}{\partial P_b} \Big|_{t'} - \frac{\partial Q'^c}{\partial P_b} \Big|_{t'} \frac{\partial P'_c}{\partial Q^a} \Big|_{t'} = \delta_a^b. \quad (1.9.48)$$

Similarly, we could take a t derivative of (1.9.34) and compare it against a P derivative of (1.9.36) as they both give a way to compute the mixed partial $\frac{\partial^2 f}{\partial t \partial P_a}$. Doing so again following equations (1.9.37) to (1.9.47) gives:

$$\frac{\partial Q'^c}{\partial P_a} \Big|_{t'} \frac{\partial P'_c}{\partial t} \Big|_{t'} - \frac{\partial Q'^c}{\partial t} \Big|_{t'} \frac{\partial P'_c}{\partial P_a} \Big|_{t'} = \frac{\partial \mathcal{H}}{\partial P_a}. \quad (1.9.49)$$

These are the only second derivative conditions we can find using (1.9.34). We can still use (1.9.35) and take a second Q derivative to compute the mixed partial $\frac{\partial^2 f}{\partial Q^a \partial Q^b}$ and require it to be symmetric under interchanging a and b . Doing so following (1.9.37) to (1.9.47) gives:

$$\frac{\partial Q'^c}{\partial Q^a} \Big|_{t'} \frac{\partial P'_c}{\partial Q^b} \Big|_{t'} - \frac{\partial Q'^c}{\partial Q^b} \Big|_{t'} \frac{\partial P'_c}{\partial Q^a} \Big|_{t'} = 0. \quad (1.9.50)$$

The final second derivative condition we can derive comes from the mixed partial $\frac{\partial^2 f}{\partial t \partial Q^a}$ gotten from differentiating (1.9.35) with respect to t and (1.9.36) with respect to Q :

$$\frac{\partial Q'^b}{\partial Q^a} \Big|_{t'} \frac{\partial P'_b}{\partial t} \Big|_{t'} - \frac{\partial Q'^b}{\partial t} \Big|_{t'} \frac{\partial P'_b}{\partial Q^a} \Big|_{t'} = \frac{\partial \mathcal{H}}{\partial Q^a}. \quad (1.9.51)$$

These are all the second derivative conditions that can be formed. Thus, by the Poincare lemma, equations (1.9.47)-(1.9.51) give the full set of conditions necessary for there to be an f that solves (1.9.34)-(1.9.36) and thus the transformation is orthochronous canonical if and only if these conditions are satisfied.

If we use (1.9.46) to eliminate the partial derivatives with respect to t at fixed t' , we can rewrite (1.9.49) and (1.9.51) as:

$$\left(\frac{\partial Q'^c}{\partial Q^b} \Big|_{t'} \frac{\partial P'_c}{\partial P_a} \Big|_{t'} - \frac{\partial Q'^c}{\partial P_a} \Big|_{t'} \frac{\partial P'_c}{\partial Q^b} \Big|_{t'} \right) \dot{Q}^b + \left(\frac{\partial Q'^c}{\partial P_b} \Big|_{t'} \frac{\partial P'_c}{\partial P_a} \Big|_{t'} - \frac{\partial Q'^c}{\partial P_a} \Big|_{t'} \frac{\partial P'_c}{\partial P_b} \Big|_{t'} \right) \dot{P}_b = \frac{\partial \mathcal{H}}{\partial P_a} \quad (1.9.52)$$

$$(1.9.53)$$

$$\left(\frac{\partial Q'^c}{\partial Q^b} \Big|_{t'} \frac{\partial P'_c}{\partial Q^a} \Big|_{t'} - \frac{\partial Q'^c}{\partial Q^a} \Big|_{t'} \frac{\partial P'_c}{\partial Q^b} \Big|_{t'} \right) \dot{Q}^b - \left(\frac{\partial Q'^c}{\partial Q^a} \Big|_{t'} \frac{\partial P'_c}{\partial P_b} \Big|_{t'} - \frac{\partial Q'^c}{\partial P_b} \Big|_{t'} \frac{\partial P'_c}{\partial Q^a} \Big|_{t'} \right) \dot{P}_b = \frac{\partial \mathcal{H}}{\partial Q^a}, \quad (1.9.54)$$

If we now apply equations (1.9.47), (1.9.48), and (1.9.50) to these we see that they simply become Hamilton's equations for the unprimed variables:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a} \quad (1.9.55)$$

which we never actually assumed. We assumed the equations of motion for the primed variables and we see that the consistency conditions guarantee they imply the equations of motion for the unprimed variables. This is exactly how we want canonical transformations to work! Thus, the transformation preserves Hamilton's equations in the change of coordinates and is orthochronous canonical if and only if the remaining three conditions hold, meaning (1.9.47), (1.9.48), (1.9.50). Those equations look so much like the Poisson bracket but just aren't quite it. They are clearly related somehow, which we will establish next.

We can clean up our remaining three conditions by defining the matrices $\left. \frac{\partial Q'}{\partial Q} \right|_{t'}$, $\left. \frac{\partial Q'}{\partial P} \right|_{t'}$, $\left. \frac{\partial P'}{\partial Q} \right|_{t'}$, $\left. \frac{\partial P'}{\partial P} \right|_{t'}$ as the matrices with components given by these partial derivatives when appropriate indices are added. In particular, when we write the matrix $\frac{\partial F}{\partial x}$ for vector quantities F and x we mean the matrix where each row is the list of the partial derivatives of the same component of the vector F . This way, if δx is a column vector, the first order change in F as a column vector is given by the matrix multiplication $\frac{\partial F}{\partial x} \delta x$. We use the superscript T to indicate the matrix transpose. With this notation, equations (1.9.47), (1.9.48), and (1.9.50) are given by:

$$\left(\left. \frac{\partial Q'}{\partial P} \right|_{t'} \right)^T \left. \frac{\partial P'}{\partial P} \right|_{t'} - \left(\left. \frac{\partial P'}{\partial P} \right|_{t'} \right)^T \left. \frac{\partial Q'}{\partial P} \right|_{t'} = 0 \quad (1.9.56)$$

$$\left(\left. \frac{\partial Q'}{\partial Q} \right|_{t'} \right)^T \left. \frac{\partial P'}{\partial P} \right|_{t'} - \left(\left. \frac{\partial P'}{\partial Q} \right|_{t'} \right)^T \left. \frac{\partial Q'}{\partial P} \right|_{t'} = \mathbb{1} \quad (1.9.57)$$

$$\left(\left. \frac{\partial Q'}{\partial Q} \right|_{t'} \right)^T \left. \frac{\partial P'}{\partial Q} \right|_{t'} - \left(\left. \frac{\partial P'}{\partial Q} \right|_{t'} \right)^T \left. \frac{\partial Q'}{\partial Q} \right|_{t'} = 0. \quad (1.9.58)$$

These can be unified by using block matrix notation:

$$\begin{pmatrix} \left. \frac{\partial Q'}{\partial Q} \right|_{t'} & \left. \frac{\partial Q'}{\partial P} \right|_{t'} \\ \left. \frac{\partial P'}{\partial Q} \right|_{t'} & \left. \frac{\partial P'}{\partial P} \right|_{t'} \end{pmatrix}^T \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \left. \frac{\partial Q'}{\partial Q} \right|_{t'} & \left. \frac{\partial Q'}{\partial P} \right|_{t'} \\ \left. \frac{\partial P'}{\partial Q} \right|_{t'} & \left. \frac{\partial P'}{\partial P} \right|_{t'} \end{pmatrix} = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \quad (1.9.59)$$

The constant matrix appearing here has fundamental importance in the canonical formalism; it is called the symplectic form $\mathbb{J}$:

$$\mathbb{J} = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \quad (1.9.60)$$

This matrix $\mathbb{J}$ appears in Hamilton's equations immediately if we write Hamilton's equations in this block matrix form. Define $\Phi(t)$ as the column vector:

$$\Phi(t) = \begin{pmatrix} Q(t) \\ P(t) \end{pmatrix}. \quad (1.9.61)$$

The derivative $\frac{\partial}{\partial Q}$ is generally written as a row vector (and similar so for $\frac{\partial}{\partial P}$) so we take the transpose to get the column vector of derivatives:

$$\frac{\partial}{\partial \Phi^T} = \begin{pmatrix} \frac{\partial}{\partial Q^T} \\ \frac{\partial}{\partial P^T} \end{pmatrix}. \quad (1.9.62)$$

Then, Hamilton's equations become:

$$\begin{aligned} \frac{dQ^a}{dt} &= \frac{\partial \mathcal{H}}{\partial P_a} \\ \frac{dP_a}{dt} &= -\frac{\partial \mathcal{H}}{\partial Q^a} \end{aligned} \implies \frac{d}{dt} \begin{pmatrix} Q \\ P \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial Q^T} \\ \frac{\partial \mathcal{H}}{\partial P^T} \end{pmatrix} \quad (1.9.63)$$

$$\implies \boxed{\mathbb{J} \frac{d\Phi}{dt} = \frac{\partial \mathcal{H}}{\partial \Phi^T}}. \quad (1.9.64)$$

Any matrix $\hat{S}$ satisfying:

$$\hat{S}^T \mathbb{J} \hat{S} = \mathbb{J} \quad (1.9.65)$$

is called a symplectic matrix. We see that the condition for orthochronous canonical transformation is that the matrix of derivatives in (1.9.59) be symplectic. Notice that if a matrix $\hat{S}$ is symplectic then its determinant is necessarily ± 1 by taking the determinant of both sides (and using that the determinant of a product is the product of determinants and that the transpose does not change the determinant):

$$\det \hat{S} \det \mathbb{J} \det \hat{S} = \det \mathbb{J} \implies (\det \hat{S})^2 = 1 \implies \det \hat{S} = \pm 1. \quad (1.9.66)$$

It is actually the case that every symplectic matrix has determinant $+1$ and never -1 , but we will not prove it or need it. Because $\det \hat{S} \neq 0$, every symplectic matrix is invertible. The inverse of a symplectic matrix is automatically symplectic:

$$\hat{S}^{-T} \hat{S}^T \mathbb{J} \hat{S} \hat{S}^{-1} = \hat{S}^{-T} \mathbb{J} \hat{S}^{-1} \implies \hat{S}^{-T} \mathbb{J} \hat{S}^{-1} = \mathbb{J} \quad (1.9.67)$$

where the exponent $-T$ indicates the transpose of the inverse of a matrix (which is the same as the inverse of the transpose). Because $\mathbb{J}^2 = -\mathbb{1}$ it immediately follows that the transpose of a symplectic matrix is

symplectic as well:

$$\hat{S}^T \mathbb{J} \hat{S} = \mathbb{J} \implies \hat{S} \mathbb{J} \hat{S}^T \mathbb{J} \hat{S} = \hat{S} \mathbb{J}^2 = -\hat{S} \implies \hat{S} \mathbb{J} \hat{S}^T \mathbb{J} = -\mathbb{1} = \mathbb{J}^2 \implies \hat{S} \mathbb{J} \hat{S}^T = \mathbb{J}. \quad (1.9.68)$$

It is instructive to consider the inverse of the matrix of derivatives in (1.9.59). By the chain rule (and using that the partial Q' and P' derivatives are always taken at fixed t'):

$$\begin{pmatrix} \frac{\partial Q'}{\partial Q} \Big|_{t'} & \frac{\partial Q'}{\partial P} \Big|_{t'} \\ \frac{\partial P'}{\partial Q} \Big|_{t'} & \frac{\partial P'}{\partial P} \Big|_{t'} \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial Q'} & \frac{\partial Q}{\partial P'} \\ \frac{\partial P}{\partial Q'} & \frac{\partial P}{\partial P'} \end{pmatrix} = \begin{pmatrix} \frac{\partial Q'}{\partial Q'} & \frac{\partial Q'}{\partial P'} \\ \frac{\partial P'}{\partial Q'} & \frac{\partial P'}{\partial P'} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}. \quad (1.9.69)$$

Therefore:

$$\begin{pmatrix} \frac{\partial Q'}{\partial Q} \Big|_{t'} & \frac{\partial Q'}{\partial P} \Big|_{t'} \\ \frac{\partial P'}{\partial Q} \Big|_{t'} & \frac{\partial P'}{\partial P} \Big|_{t'} \end{pmatrix}^{-1} = \begin{pmatrix} \frac{\partial Q}{\partial Q'} & \frac{\partial Q}{\partial P'} \\ \frac{\partial P}{\partial Q'} & \frac{\partial P}{\partial P'} \end{pmatrix} \quad (1.9.70)$$

This matrix as well as its transpose are then automatically symplectic. In particular, for the transpose we have in components:

$$\begin{pmatrix} \frac{\partial Q}{\partial Q'} & \frac{\partial Q}{\partial P'} \\ \frac{\partial P}{\partial Q'} & \frac{\partial P}{\partial P'} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial Q'} & \frac{\partial Q}{\partial P'} \\ \frac{\partial P}{\partial Q'} & \frac{\partial P}{\partial P'} \end{pmatrix}^T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (1.9.71)$$

$$\implies \frac{\partial Q^a}{\partial Q'^c} \frac{\partial Q^b}{\partial P'_c} - \frac{\partial Q^a}{\partial P'_c} \frac{\partial Q^b}{\partial Q'^c} = 0, \quad (1.9.72)$$

$$\frac{\partial Q^a}{\partial Q'^c} \frac{\partial P_b}{\partial P'_c} - \frac{\partial Q^a}{\partial P'_c} \frac{\partial P_b}{\partial Q'^c} = \delta_b^a, \quad (1.9.73)$$

$$\frac{\partial P_a}{\partial Q'^c} \frac{\partial P_b}{\partial P'_c} - \frac{\partial P_a}{\partial P'_c} \frac{\partial P_b}{\partial Q'^c} = 0. \quad (1.9.74)$$

These precisely say that we must have the canonical Poisson brackets of the old variables when using the Poisson bracket of the new coordinates! That is, if we let $\{f, g\}'$ denote:

$$\{f, g\}' = \frac{\partial f}{\partial Q'^a} \frac{\partial g}{\partial P'_a} - \frac{\partial f}{\partial P'_a} \frac{\partial g}{\partial Q'^a}. \quad (1.9.75)$$

Then:

$$\{Q^a, Q^b\}' = 0, \quad \{Q^a, P_b\}' = \delta_b^a, \quad \{P_a, P_b\}' = 0. \quad (1.9.76)$$

Here all the partial derivatives in the primed Poisson brackets are taken at fixed t' . Equivalently, we could have considered the inverse of this canonical transformation and in doing so we would have found the same requirement with the roles of the unprimed and primed variables swapped:

$$\{Q'^a, Q'^b\} = 0, \quad \{Q'^a, P'_b\} = \delta_b^a, \quad \{P'_a, P'_b\} = 0. \quad (1.9.77)$$

Here all the partial derivatives in the unprimed Poisson brackets are taken at fixed t . Because (1.9.70) is symplectic, if we interchange the roles of the primed and unprimed coordinates in this way it reveals that the matrix of derivatives of the primed coordinates with respect to the unprimed coordinates at fixed t is also symplectic. We can then use the canonical brackets to automatically check that Q', P' are allowed without even knowing t' or $\mathcal{H}'$. Once $t'(t, Q, P)$ is supplied we can then (nearly) compute the transformed Hamiltonian by using that the unprimed and primed equations of motion imply each other. Consequently:

$$\frac{\partial \mathcal{H}'}{\partial P'_a} = \frac{dQ'^a}{dt'} = \frac{\left(\frac{dQ'^a}{dt}\right)}{\left(\frac{dt'}{dt}\right)} = \frac{\frac{\partial Q'^a}{\partial t} + \{Q'^a, \mathcal{H}\}}{\frac{\partial t'}{\partial t} + \{t', \mathcal{H}\}}. \quad (1.9.78)$$

Similarly:

$$\frac{\partial \mathcal{H}'}{\partial Q'^a} = -\frac{dP'_a}{dt'} = -\frac{\left(\frac{dP'_a}{dt}\right)}{\left(\frac{dt'}{dt}\right)} = -\frac{\frac{\partial P'_a}{\partial t} + \{P'_a, \mathcal{H}\}}{\frac{\partial t'}{\partial t} + \{t', \mathcal{H}\}}. \quad (1.9.79)$$

These two conditions determine the transformed Hamiltonian up to adding an arbitrary function of t' . Such a function does not affect the equations of motion and so it doesn't matter what choice of function is made (because the choice does not affect the dynamics of the system it does not affect the physical predictions).

Ultimately then we have three different equivalent ways of considering orthochronous canonical trans-

formations. A transformation is orthochronous canonical if and only if there exists a function $F(t', Q', t, Q)$ so that (1.9.11) holds; equivalently there exists a function $f(t, Q, P)$ so that (1.9.34), (1.9.35), (1.9.36) hold; equivalently $Q'(t, Q, P)$ and $P'(t, Q, P)$ must satisfy the canonical brackets in terms of the untransformed coordinates and the transformed Hamiltonian must satisfy (1.9.78) and (1.9.79).

As always we can tack on time reversing transformations at the end by just considering simple time reversal. Under simple time reversal it is quick to compute how the Poisson brackets are changed:

$$\{Q'^a, Q'^b\} = \{Q^a, Q^b\} = 0, \quad \{Q'^a, P'_b\} = \{Q^a, -P_b\} = -\delta_b^a, \quad \{P'_a, P'_b\} = \{-P_a, -P_b\} = 0. \quad (1.9.80)$$

As well, we already identified that the transformed Hamiltonian can be taken to satisfy $\mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P)$. Because the Poisson bracket is unchanged by any orthochronous canonical transformation, we see that under any time reversing canonical transformation the Poisson bracket of the transformed variables is the negative of the usual canonical brackets.

By definition, if a canonical transformation $t'(t, Q, P), Q'(t, Q, P), P'(t, Q, P)$ is a symmetry the transformed variables must evolve in the same way in terms of each other that the unprimed variables did (this is just a repeat of (1.2.9)). That is, for a symmetry the equation of motion functions for Q' and P' must be the same functions as the equation of motion functions for Q and P , just evaluated now at the transformed variables. These functions determine the Q' and P' derivatives of the transformed Hamiltonian and so determine $\mathcal{H}'$ up to adding a function of t' . Thus, if $\mathcal{H} = h(t, Q, P)$ for some particular function h then a symmetry requires that $\mathcal{H}' = h(t', Q', P') + g(t')$ for that same function h and some arbitrary function g . We explained before that identifying the transformed Hamiltonian from t', Q', P' is not unique and that the choice of g is arbitrary. Hence, we can take $g = 0$ by definition and say **a canonical transformation is a symmetry of the system if and only if the transformed and untransformed Hamiltonians are the same function, just evaluated at their appropriate respective variables**. All together, these results give us:

Theorem 1.8: Canonical Transformations

A canonical transformation is any transformation $t' = t'(t, Q, P)$, $Q' = Q'(t, Q, P)$, $P' = P'(t, Q, P)$, $\mathcal{H}' = \mathcal{H}'(t, Q', P')$ so that Hamilton's equations are satisfied by the primed variables using the primed Hamiltonian $\mathcal{H}'$ whenever Hamilton's equations are satisfied by the unprimed variables using the unprimed Hamiltonian $\mathcal{H}(t, Q, P)$.

A transformation which is time nonreversing ($\frac{dt'}{dt} > 0$, called orthochronous) is canonical if and only if there exists a function $F(t', Q', t, Q)$, called the generating function of the transformation, so that without using the equations of motion the actions for the primed and unprimed variables are related by:

$$S'[Q', P'] = S[Q, P] + F(t'_f, Q'_f, t_f, Q_f) - F(t'_0, Q'_0, t_0, Q_0). \quad (1.9.81)$$

Equivalently, that function F satisfies:

$$\frac{\partial F}{\partial t'} = -\mathcal{H}', \quad \frac{\partial F}{\partial Q'^a} = P'_a, \quad \frac{\partial F}{\partial t} = \mathcal{H}, \quad \frac{\partial F}{\partial Q^a} = -P_a. \quad (1.9.82)$$

If we let $f(t, Q, P) = F(t'(t, Q, P), Q'(t, Q, P), t, Q)$ be called the surface function then the existence of F above is equivalent to the existence of f so that:

$$\frac{\partial f}{\partial t} = \mathcal{H} + P'_a \frac{\partial Q'^a}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial t} \quad (1.9.83)$$

$$\frac{\partial f}{\partial Q^a} = -P_a + P'_b \frac{\partial Q'^b}{\partial Q^a} - \mathcal{H}' \frac{\partial t'}{\partial Q^a} \quad (1.9.84)$$

$$\frac{\partial f}{\partial P_a} = P'_b \frac{\partial Q'^b}{\partial P_a} - \mathcal{H}' \frac{\partial t'}{\partial P_a}. \quad (1.9.85)$$

Such an f exists if and only if Q' and P' satisfy the canonical brackets with respect to the unprimed coordinates:

$$\{Q'^a, Q'^b\} = 0, \quad \{Q'^a, P'_b\} = \delta_b^a, \quad \{P'_a, P'_b\} = 0 \quad (1.9.86)$$

and the transformed Hamiltonian satisfies:

$$\frac{\partial \mathcal{H}'}{\partial P'_a} = \frac{\frac{\partial Q'^a}{\partial t} + \{Q'^a, \mathcal{H}\}}{\frac{\partial t'}{\partial t} + \{t', \mathcal{H}\}} \quad (1.9.87)$$

$$\frac{\partial \mathcal{H}'}{\partial Q'^a} = -\frac{\frac{\partial P'_a}{\partial t} + \{P'_a, \mathcal{H}\}}{\frac{\partial t'}{\partial t} + \{t', \mathcal{H}\}}. \quad (1.9.88)$$

Q' and P' satisfy the canonical brackets if and only if the matrix of their derivatives with respect to the untransformed coordinates is symplectic:

$$\hat{S} = \begin{pmatrix} \frac{\partial Q'}{\partial Q} & \frac{\partial Q'}{\partial P} \\ \frac{\partial P'}{\partial Q} & \frac{\partial P'}{\partial P} \end{pmatrix}, \quad \mathbb{J} = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \quad \hat{S}^T \mathbb{J} \hat{S} = \mathbb{J}. \quad (1.9.89)$$

A general time reversing canonical transformation is given by first performing the “simple time reversal”:

$$t' = -t, \quad Q'^a = Q^a, \quad P'_a = P_a, \quad \mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P) \quad (1.9.90)$$

and then performing an orthochronous canonical transformation. Under a time reversing canonical transformation, the Poisson brackets of the transformed variables with respect to the untransformed variables are given by the negative of the usual canonical brackets in (1.9.86).

A canonical transformation is a symmetry of the system if and only if the transformed and untransformed Hamiltonian are the same function.

1.9.3 Common Subsets of Transformations

There are some very common subclasses of canonical transformations which are helpful to consider and for which we can simplify our general structure of canonical transformations a bit. Here we will consider the structure of action gauge transformations, extended point transformations, time preserving canonical transformations, and time independent canonical transformations. We will summarize the results in a diagram at the end.

Action Gauge Transformations

We found in theorem 1.6 that action gauge transformations represent the extent to which the definition of the action (and consequently, Lagrangian, Hamiltonian, and momentum) is nonunique. For functions $f(t, Q)$ we found that transformations of the form:

$$t' = t, \quad Q'^a = Q^a, \quad P'_a = P_a + \frac{\partial f}{\partial Q^a}, \quad \mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P) - \frac{\partial f}{\partial t} \quad (1.9.91)$$

correspond to the most general transformation that always does not affect the evolution of the coordinates Q^a . Equivalently, this transformation identifies that the Lagrangians $\mathcal{L}$ and $\mathcal{L}'$ related by:

$$\mathcal{L}'(t, Q, \dot{Q}) = \mathcal{L}(t, Q, \dot{Q}) + \frac{d}{dt} f(t, Q) \quad (1.9.92)$$

are physically equivalent for all functions f .

Extended Point Transformations

Extended point transformations are canonical transformations in which $t' = t'(t, Q)$ and $Q' = Q'(t, Q)$. The set of such transformations includes simple time reversal and just like before we can consider any extended point transformation which reverses time as an orthochronous extended point transformation composed with simple time reversal. It will be helpful to invert these transformation functions to have $t = t(t', Q')$ and $Q = Q(t', Q')$. For studying orthochronous extended point transformations we use the generating function G defined by:

$$G(t', Q', \mathcal{H}, P) = F(t', Q', t, Q) - t\mathcal{H} + Q^a P_a \quad (1.9.93)$$

$$\implies \frac{\partial G}{\partial t'} = -\mathcal{H}', \quad \frac{\partial G}{\partial Q'^a} = P'_a, \quad \frac{\partial G}{\partial \mathcal{H}} = -t, \quad \frac{\partial G}{\partial P_a} = Q^a. \quad (1.9.94)$$

Using the third of these conditions:

$$\frac{\partial G}{\partial \mathcal{H}}(t', Q', \mathcal{H}, P) = -t(t', Q') \implies G(t', Q', \mathcal{H}, P) = -t(t', Q')\mathcal{H} + g(t', Q', P) \quad (1.9.95)$$

for some function $g(t', Q', P)$. Using the fourth condition:

$$\frac{\partial G}{\partial P_a}(t', Q', \mathcal{H}, P) = Q^a(t', Q') \implies \frac{\partial g}{\partial P_a} = Q^a(t', Q') \implies g(t', Q', P) = Q^a(t', Q')P_a + h(t', Q') \quad (1.9.96)$$

for some function $h(t', Q')$. We can see that automatically $h(t', Q')$ is equal to the surface function $f(t, Q)$:

$$f(t, Q) = F(t'(t, Q), Q'(t, Q), t, Q) = G(t'(t, Q), Q'(t, Q), \mathcal{H}, P) + t\mathcal{H} - Q^a P_a \quad (1.9.97)$$

$$= -t\mathcal{H} + Q^a P_a + h(t', Q') + t\mathcal{H} - Q^a P_a = h(t', Q'). \quad (1.9.98)$$

So for some function $f(t, Q)$ we have:

$$G(t', Q', \mathcal{H}, P) = -t(t', Q')\mathcal{H} + Q^a(t', Q')P_a + f(t(t', Q'), Q(t', Q')). \quad (1.9.99)$$

Then, the first and second conditions on G just give how the momentum and Hamiltonian transform:

$$\mathcal{H}' = \frac{\partial t}{\partial t'}\mathcal{H} - \frac{\partial Q^a}{\partial t'}P_a - \frac{\partial f}{\partial t'} \quad (1.9.100)$$

$$P'_a = \frac{\partial Q^b}{\partial Q'^a}P_b - \frac{\partial t}{\partial Q'^a}P_a + \frac{\partial f}{\partial Q'^b}. \quad (1.9.101)$$

At the level of the Lagrangian, these can nicely be combined as:

$$\mathcal{L}'(t', Q', \dot{Q}') = P'_a \dot{Q}'^a - \mathcal{H}'(t', Q', P') = \left(\frac{\partial Q^b}{\partial Q'^a}P_b - \frac{\partial t}{\partial Q'^a}P_a + \frac{\partial f}{\partial Q'^b} \right) \frac{dQ'^a}{dt'} - \frac{\partial t}{\partial t'}\mathcal{H} + \frac{\partial Q^a}{\partial t'}P_a + \frac{\partial f}{\partial t'} \quad (1.9.102)$$

$$= \left(\frac{\partial Q^a}{\partial t'} + \frac{\partial Q^a}{\partial Q'^b} \frac{dQ'^b}{dt'} \right) P_a - \left(\frac{\partial t}{\partial t'} + \frac{\partial t}{\partial Q'^a} \frac{dQ'^a}{dt'} \right) \mathcal{H} + \frac{\partial f}{\partial t'} + \frac{\partial f}{\partial Q'^a} \frac{dQ'^a}{dt'} \quad (1.9.103)$$

$$= \frac{dQ^a}{dt'}P_a - \frac{dt}{dt'}\mathcal{H} + \frac{d}{dt'}f(t, Q) = \frac{dt}{dt'} \left(P_a \dot{Q}^a - \mathcal{H} \right) + \frac{d}{dt'}f(t, Q) \quad (1.9.104)$$

$$\implies \mathcal{L}'(t', Q', \dot{Q}') = \frac{dt}{dt'}\mathcal{L}(t, Q, \dot{Q}) + \frac{d}{dt'}f(t, Q). \quad (1.9.105)$$

Thus, an orthochronous extended point transformation changes the Lagrangian only by a factor for changing the time and by adding a surface term. The Lagrangian perspective is nice here because both the transformation rules for P'_a and $\mathcal{H}'$ can be derived from this single transformation rule for the Lagrangian.

Another reason the Lagrangian perspective is useful here is because it is easy to include the case of time reversal, in which case we saw that the primed integrand picks up an additional minus sign in equation (1.9.19) versus (1.9.6). Because the Lagrangian is the integrand of the action it follows that for a time reversing extended point transformation:

$$-\mathcal{L}'(t', Q', \dot{Q}') = \frac{dt'}{dt} \mathcal{L}(t, Q, \dot{Q}) + \frac{d}{dt'}f(t, Q). \quad (1.9.106)$$

Both the time reversing and non time reversing case are then covered by:

$$\boxed{\mathcal{L}'(t', Q', \dot{Q}') = \left| \frac{dt}{dt'} \right| \left(\mathcal{L}(t, Q, \dot{Q}) + \frac{d}{dt}f(t, Q) \right)}. \quad (1.9.107)$$

We will often study symmetries under extended point transformations. If the extended point transformation is a symmetry then because the transformed Hamiltonian will be the same function as the untransformed Hamiltonian, the transformed Lagrangian will be the same function as the untransformed Lagrangian due to its functional form being determined by the Hamiltonian through the Legendre transformation. Thus:

$$\boxed{t' = t'(t, Q), \quad Q' = Q'(t, Q) \text{ is a symmetry} \iff \mathcal{L}'(t', Q', \dot{Q}') = \mathcal{L}(t', Q', \dot{Q}')} \quad (1.9.108)$$

Looking at the $\frac{df}{dt}$ term in (1.9.107), we can see that any extended point transformation consists of an action gauge transformation of adding $\frac{df}{dt}$ to the Lagrangian followed by a “simple” extended point transformation in which the new Lagrangian is equal to the old Lagrangian times $\left| \frac{dt}{dt'} \right|$. In general, we will

find that a class of transformations of interest will always carry this gauge term and so when we say “simple” in front of a transformation we mean with the gauge term $\left(\frac{df}{dt}\right)$ excluded. A very common subset of interest of extended point transformations is the set of point transformations, which are the special case $t' = t$ and $Q' = Q'(Q)$.

Time Preserving Canonical Transformations

Time preserving canonical transformations are transformations in which $t' = t$, $Q' = Q'(t, Q, P)$, $P' = P'(t, Q, P)$. This is the most general family of canonical transformations considered by most sources (such as [37]), but as we have seen it is possible (and later it will be useful) to be more general. Nonetheless, this subclass is very commonly useful. Consider the generating function:

$$G(\mathcal{H}', Q', t, Q) = F(t', Q', t, Q) + t'\mathcal{H}' \quad (1.9.109)$$

$$\implies \frac{\partial G}{\partial \mathcal{H}'} = t', \quad \frac{\partial G}{\partial Q'^a} = P'_a, \quad \frac{\partial G}{\partial t} = \mathcal{H}, \quad \frac{\partial G}{\partial Q^a} = -P_a. \quad (1.9.110)$$

Then, using the first condition:

$$\frac{\partial G}{\partial \mathcal{H}'} = t'(t) = t \implies G = t\mathcal{H}' + F_1(t, Q, Q') \quad (1.9.111)$$

for some function $F_1(t, Q, Q')$. We can see that $F_1(t, Q, Q')$ is actually equal to $F(t', Q', t, Q)$ when the relationship between t' and t is used:

$$F_1(t, Q, Q') = G - t\mathcal{H}' = F(t, Q', t, Q) + t\mathcal{H}' - t\mathcal{H}' = F(t, Q', t, Q). \quad (1.9.112)$$

As well, the remaining three conditions on G give that F_1 satisfies:

$$\frac{\partial F_1}{\partial t} = \mathcal{H} - \mathcal{H}', \quad \frac{\partial F_1}{\partial Q^a} = -P_a, \quad \frac{\partial F_1}{\partial Q'^a} = P'_a. \quad (1.9.113)$$

Thus, for a time preserving canonical transformation one can use F_1 as the effective generating function for the transformation with these conditions.

Time Independent Canonical Transformations

A time independent canonical transformation does what it says on the tin. It is a transformation of the form:

$$t' = t, \quad Q' = Q'(Q, P), \quad P' = P'(Q, P). \quad (1.9.114)$$

This is clearly a subset of time preserving canonical transformations. So, we can use the effective generating function $F_1(t, Q, Q')$ when considering them. F_1 by definition satisfies:

$$\frac{\partial F_1}{\partial Q'^a} = P'_a(Q, P) = P'_a(Q, P(Q, Q')). \quad (1.9.115)$$

Here we have used $Q'(Q, P)$ to solve for P in terms of Q and Q' . The right hand side must be the derivative of some function with respect to Q'^a by the left hand side but because the right hand side does not depend explicitly on t it further follows that there must be a function $g(Q, Q')$ so that:

$$\frac{\partial g}{\partial Q'^a} = P'_a(Q, P(Q, Q')). \quad (1.9.116)$$

Then, $F_1 - g$ has vanishing derivative with respect to Q'^a and so the function F_1 must satisfy:

$$F_1(t, Q, Q') = g(Q, Q') + h(t, Q) \quad (1.9.117)$$

for some function $h(t, Q)$. The Q^a derivative of F_1 then gives:

$$\frac{\partial F_1}{\partial Q^a} = -\frac{\partial g}{\partial Q^a} - \frac{\partial h}{\partial Q^a} = -P_a(Q, Q') \implies \frac{\partial h}{\partial Q^a} = -\frac{\partial g}{\partial Q^a} + P_a(Q, Q'). \quad (1.9.118)$$

Again the right hand side does not depend explicitly on time and so because it must be the derivative of some function with respect to Q^a there must be some function $i(Q, Q')$ so that:

$$\frac{\partial i}{\partial Q^a} = -\frac{\partial g}{\partial Q^a} + P_a(Q, Q'). \quad (1.9.119)$$

Then, $h - i$ has vanishing Q^a derivative and so the function h must satisfy:

$$h(t, Q) = i(Q) + j(t) \quad (1.9.120)$$

for some function $j(t)$. Returning these results to F_1 :

$$F_1(t, Q, Q') = g(Q, Q') + i(Q) + j(t). \quad (1.9.121)$$

The final condition on F_1 requires:

$$\frac{\partial F_1}{\partial t} = \frac{\partial j}{\partial t} = \mathcal{H} - \mathcal{H}' \implies \mathcal{H}' = \mathcal{H} - \frac{\partial j}{\partial t}. \quad (1.9.122)$$

As we've already established, the transformed Hamiltonian is only defined up to a choice of a function of time only by the transformations of t', Q', P' and this function of time only drops out of all dynamics. So, we can add a function of time only to $\mathcal{H}'$ so that $j = 0$ by definition (just choose $\frac{\partial j}{\partial t}$). Then, we have that for a time independent canonical transformation we can take the generating function to itself be independent of time and $\mathcal{H}' = \mathcal{H}$:

$$F_1 = F_1(Q, Q'), \quad \frac{\partial F_1}{\partial Q^a} = -P_a, \quad \frac{\partial F_1}{\partial Q'^a} = P'_a, \quad \mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P). \quad (1.9.123)$$

The relationships between the different subclasses of canonical transformations can be summarized in the Venn diagram 1.2.

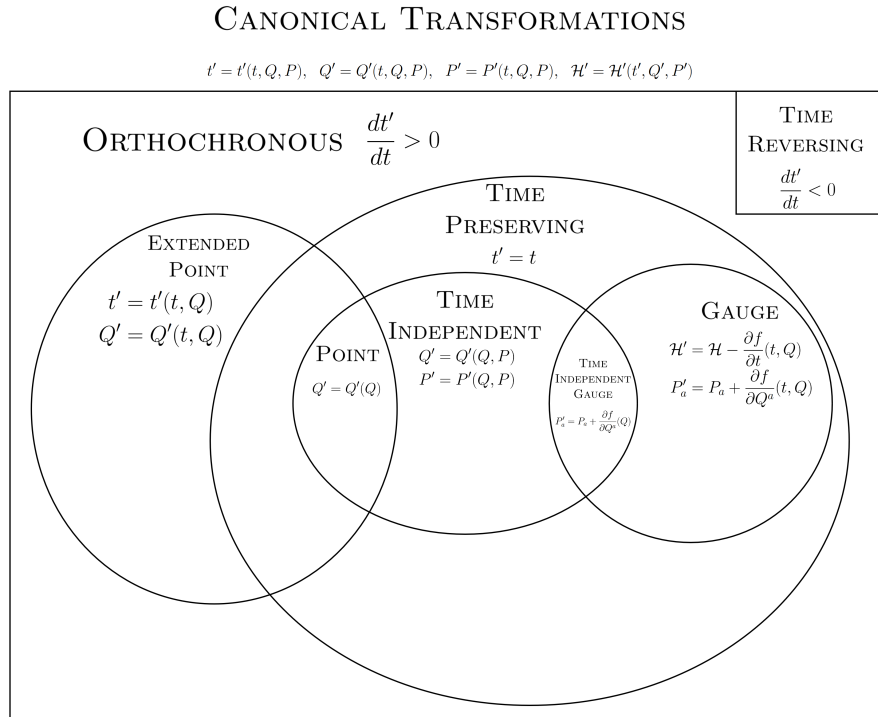


Figure 1.2: Some of the different classes of Canonical Transformations. One should note this diagram does not reflect the relative size of each set; the regions are not drawn “to scale”. The hierarchy of largest to smallest sets of transformations is: Canonical > Orthochronous = Time Reversing > Time-Preserving Canonical > Time Independent > Extended Point > Point > Gauge > Time Independent Gauge.

Exercises

Problem 1.26: Generate! Show that each of the following transformations are canonical by finding generating functions for them. In all examples in this question take $t' = t$ and $\mathcal{H}' = \mathcal{H}$.

- (a) $Q' = \frac{Q+P}{\sqrt{2}}, \quad P' = \frac{P-Q}{\sqrt{2}}$
- (b) $Q' = \frac{Q+iP}{\sqrt{2}}, \quad P' = \frac{P+iQ}{\sqrt{2}}$
- (c) $Q' = P, \quad P' = -Q$

$$(d) \quad Q' = \sqrt{2Q} \cos P, \quad P' = \sqrt{2Q} \sin P.$$

Problem 1.27: Checking consistency. For the transformations in Problem 1.26, compute their Jacobian matrices $\hat{S}$ and show by explicit calculation that for each of them that $\hat{S}$ is symplectic: $\hat{S}\mathbb{J}\hat{S}^T = \mathbb{J}$.

Problem 1.28: ★ Scaling Properties. The whole canonical formalism carries with it the ability to rescale variables in three specific ways.

- Show that if we make the transformation $Q' = \alpha Q$ and $P' = \frac{1}{\alpha}P$ while keeping t and $\mathcal{H}$ unchanged, then Hamilton's equations are still satisfied by Q' and P' . Conceptually, rescaling Q changes what state of the variable Q you identify with having a value of 1. This is precisely the choice of a “reference unit” as defined in section 1.2. Thus, the units of conjugate momentum are inversely proportional to the units of the coordinate. This should not be surprising as in section 1.3, we started in our operator formalism with $\hat{P}_a = \frac{\partial}{\partial Q^a}$.
- Show that if we make the transformation $t' = \alpha t$ and $\mathcal{H}' = \frac{1}{\alpha}\mathcal{H}$ while keeping Q and P unchanged, then Hamilton's equations are still satisfied by Q and P under the new t' and $\mathcal{H}'$. Conceptually, rescaling t changes what length of time you identify with having a value of 1. This is precisely the choice of a “reference unit” for time. Thus, the units of the Hamiltonian are inversely proportional to the units of time. This should not be surprising as because the Hamiltonian is the generator of time evolution, in our operator formalism we have $\hat{H} = \frac{d}{dt}$.
- Show that if we make the transformation of the action $S' = \alpha S$ then the stationary variation of the action S' gives the same dynamics as S (the equations of motion will be scaled by α). Then, show that the Lagrangian corresponding to S' is $\mathcal{L}' = \alpha\mathcal{L}$ and that the Hamiltonian and momenta are $\mathcal{H}' = \alpha\mathcal{H}$, $P' = \alpha P$. Conceptually, rescaling S is again a choice of units as to what value corresponds to 1. Thus, units of the Hamiltonian, Lagrangian, and momenta are all proportional to the units of the action. If this scaling is done, it has to be done self consistently with any terms that are later added to the action. If you only scale some terms but not others, the equations of motion will not be equivalent.
- Let square brackets around a quantity denote “units of” that quantity. Using the previous results, conclude that one must choose units of time, coordinates, and the action and that once one has done so, all the remaining canonical quantities have units given by:

$$[\mathcal{L}] = [\mathcal{H}] = \frac{[S]}{[t]}, \quad [P] = \frac{[S]}{[Q]}.$$

Determining the units of quantities by scaling properties is called **dimensional analysis**.

1.10 Noether's Theorem (Version 1)

The machinery of analytical mechanics gives an incredible relationship between the continuous symmetries of a theory and quantities which are **conserved** in that theory. A continuous symmetry, as defined in section 1.3, is a symmetry under a continuous transformation. A continuous transformation is a transformation which depends smoothly on a real-valued parameter (translations in time or space or rotations for example). A conserved quantity is a quantity whose value remains constant under the dynamics of a system; as time changes, a conserved quantity does not.

Consider a continuous canonical transformation. That is, there will be some parameter ε (by convention we define ε so that $\varepsilon = 0$ corresponds to the identity transformation) so that for real ε there are functions $t'(\varepsilon, t, Q, P)$, $Q'(\varepsilon, t, Q, P)$, $P'(\varepsilon, t, Q, P)$, $\mathcal{H}'(\varepsilon, t', Q', P')$ which make a canonical transformation and which depend smoothly on ε . We define the symbol $\mathcal{D}$ to indicate total differentiation with respect to ε at $\varepsilon = 0$. This defines the functions $\mathcal{D}t$, $\mathcal{D}Q^a$, $\mathcal{D}P_a$, which are functions of (t, Q, P) :

$$\mathcal{D}t \stackrel{\text{def}}{=} \left. \frac{\partial t'(\varepsilon, t, Q, P)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}Q^a \stackrel{\text{def}}{=} \left. \frac{\partial Q'^a(\varepsilon, t, Q, P)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}P_a \stackrel{\text{def}}{=} \left. \frac{\partial P'_a(\varepsilon, t, Q, P)}{\partial \varepsilon} \right|_{\varepsilon=0}. \quad (1.10.1)$$

The transformed Hamiltonian $\mathcal{H}'$ depends on ε in a nontrivial way in general in that $\mathcal{H}'(t', Q', P')$ will generally change its form as a function as ε is changed. So, we write $\mathcal{H}'(\varepsilon, t', Q', P')$ to indicate that $\mathcal{H}'$ changes directly with ε (as its functional form changes) and indirectly with ε (through the ε dependence of t', Q', P'). We will use the notation $\delta\mathcal{H}$ to indicate the change in the form of $\mathcal{H}'$ as a function as ε is changed near the identity. That is, we define:

$$\delta\mathcal{H} \stackrel{\text{def}}{=} \left. \frac{\partial}{\partial \varepsilon} \mathcal{H}'(\varepsilon, t', Q', P') \right|_{\varepsilon=0}. \quad (1.10.2)$$

The partial ε derivative of $\mathcal{H}'$ is taken at fixed t', Q', P' . The total ε derivative of $\mathcal{H}'$ gives:

$$\frac{d\mathcal{H}'}{d\varepsilon} = \frac{\partial \mathcal{H}'}{\partial \varepsilon} + \frac{\partial \mathcal{H}'}{\partial t'} \frac{\partial t'}{\partial \varepsilon} + \frac{\partial \mathcal{H}'}{\partial Q'^a} \frac{\partial Q'^a}{\partial \varepsilon} + \frac{\partial \mathcal{H}'}{\partial P'_a} \frac{\partial P'_a}{\partial \varepsilon}. \quad (1.10.3)$$

At $\varepsilon = 0$ then:

$$\mathcal{D}\mathcal{H} = \delta\mathcal{H} + \frac{\partial \mathcal{H}}{\partial t} \mathcal{D}t + \frac{\partial \mathcal{H}}{\partial Q^a} \mathcal{D}Q^a + \frac{\partial \mathcal{H}}{\partial P_a} \mathcal{D}P_a. \quad (1.10.4)$$

Because a canonical transformation is a symmetry if and only if the form of the Hamiltonian as a function does not change, we have symmetry whenever $\delta\mathcal{H} = 0$.

Let us hold off on requiring the transformation to be a symmetry and see what can be said in general. At $\varepsilon = 0$ the transformation is the identity transformation and so time is not changed and for $\varepsilon \neq 0$ the transformation is continuously connected to the identity. Time evolution is not defined if one crosses through $\frac{dt'}{dt} = 0$ and so a continuous transformation cannot continuously pass from $\frac{dt'}{dt} > 0$ to $\frac{dt'}{dt} < 0$. Consequently, no continuous transformation can reverse time. Then, any continuous canonical transformation will have some generating function $F(\varepsilon, t', Q', t, Q)$ (where we have written explicit ε dependence because the form of F has a function of its other variables will generally depend on ε). That generating function will satisfy (1.9.82). If we again adopt the notation that $f(\varepsilon, t, Q, P)$ is the surface term added to the action by the canonical transformation we have:

$$f(\varepsilon, t, Q, P) = F(\varepsilon, t'(\varepsilon, t, Q, P), Q'(\varepsilon, t, Q, P), t, Q) \quad (1.10.5)$$

$$\implies \frac{df}{d\varepsilon} = \frac{\partial F}{\partial \varepsilon} + \frac{\partial F}{\partial t'} \frac{\partial t'}{\partial \varepsilon} + \frac{\partial F}{\partial Q'^a} \frac{\partial Q'^a}{\partial \varepsilon} = \frac{\partial F}{\partial \varepsilon} - \mathcal{H}' \frac{\partial t'}{\partial \varepsilon} + P'_a \frac{\partial Q'^a}{\partial \varepsilon} \quad (1.10.6)$$

where we have used (1.9.82). If we now evaluate this at $\varepsilon = 0$ and use that at $\varepsilon = 0$ all of the primed quantities reduce to the unprimed ones:

$$\mathcal{D}f = \delta F - \mathcal{H}\mathcal{D}t + P_a \mathcal{D}Q^a. \quad (1.10.7)$$

Here we have adopted the same δ notation used for $\mathcal{H}'$ to indicate that δF represents the partial derivative of F with respect to ε keeping its variable dependence (t', Q', t, Q) fixed. Thus, this ε derivative captures how the form of F as a function of its other variables changes under the transformation.

Because the continuous transformation is canonical, the surface function f must satisfy (1.9.83), (1.9.84), (1.9.85). Let us see what these equations require when we differentiate with respect to ε (recall that the

unprimed t, Q, P do not change with ε):

$$\frac{\partial f}{\partial t} = \mathcal{H} + P'_a \frac{\partial Q'^a}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial t} \implies \frac{\partial}{\partial t} \frac{df}{d\varepsilon} = 0 + \frac{dP'_a}{d\varepsilon} \frac{\partial Q'^a}{\partial t} + P'_a \frac{\partial}{\partial t} \frac{dQ'^a}{d\varepsilon} - \frac{d\mathcal{H}'}{d\varepsilon} \frac{\partial t'}{\partial t} - \mathcal{H}' \frac{\partial}{\partial t} \frac{dt'}{d\varepsilon} \quad (1.10.8)$$

$$\frac{\partial f}{\partial Q^a} = -P_a + P'_b \frac{\partial Q'^b}{\partial Q^a} - \mathcal{H}' \frac{\partial t'}{\partial Q^a} \implies \frac{\partial}{\partial Q^a} \frac{df}{d\varepsilon} = 0 + \frac{dP'_b}{d\varepsilon} \frac{\partial Q'^b}{\partial Q^a} + P'_b \frac{\partial}{\partial Q^a} \frac{dQ'^b}{d\varepsilon} - \frac{d\mathcal{H}'}{d\varepsilon} \frac{\partial t'}{\partial Q^a} - \mathcal{H}' \frac{\partial}{\partial Q^a} \frac{dt'}{d\varepsilon} \quad (1.10.9)$$

$$\frac{\partial f}{\partial P_a} = P'_b \frac{\partial Q'^b}{\partial P_a} - \mathcal{H}' \frac{\partial t'}{\partial P_a} \implies \frac{\partial}{\partial P_a} \frac{df}{d\varepsilon} = \frac{dP'_b}{d\varepsilon} \frac{\partial Q'^b}{\partial P_a} + P'_b \frac{\partial}{\partial P_a} \frac{dQ'^b}{d\varepsilon} - \frac{d\mathcal{H}'}{d\varepsilon} \frac{\partial t'}{\partial P_a} - \mathcal{H}' \frac{\partial}{\partial P_a} \frac{dt'}{d\varepsilon}. \quad (1.10.10)$$

If we now evaluate these at $\varepsilon = 0$ we have:

$$\frac{\partial \mathcal{D}f}{\partial t} = P_a \frac{\partial \mathcal{D}Q^a}{\partial t} - \mathcal{H} \frac{\partial \mathcal{D}t}{\partial t} - \mathcal{D}\mathcal{H} \quad (1.10.11)$$

$$\frac{\partial \mathcal{D}f}{\partial Q^a} = \mathcal{D}P_a + P_b \frac{\partial \mathcal{D}Q^b}{\partial Q^a} - \mathcal{H} \frac{\partial \mathcal{D}t}{\partial Q^a} \quad (1.10.12)$$

$$\frac{\partial \mathcal{D}f}{\partial P_a} = P_b \frac{\partial \mathcal{D}Q^b}{\partial P_a} - \mathcal{H} \frac{\partial \mathcal{D}t}{\partial P_a}. \quad (1.10.13)$$

The derivatives on the right hand side are reminiscent of the structures appearing on the right hand side of (1.10.7) so let's rewrite $\mathcal{D}f$ using (1.10.7) in these equations:

$$\frac{\partial \delta F}{\partial t} = -\mathcal{D}\mathcal{H} + \frac{\partial \mathcal{H}}{\partial t} \mathcal{D}t \quad (1.10.14)$$

$$\frac{\partial \delta F}{\partial Q^a} = \mathcal{D}P_a + \frac{\partial \mathcal{H}}{\partial Q^a} \mathcal{D}t \quad (1.10.15)$$

$$\frac{\partial \delta F}{\partial P_a} = -\mathcal{D}Q^a + \frac{\partial \mathcal{H}}{\partial P_a} \mathcal{D}t. \quad (1.10.16)$$

The canonical transformation conditions are certainly simpler in terms of δF . We can give δF a very nice interpretation by introducing a new notion of differentiation. We define the total ε derivative minus the contribution from how it changes the time so that for any function $A(t', Q', P')$:

$$\mathcal{D}A|_t = \mathcal{D}A - \mathcal{D}t \frac{dA(t, Q, P)}{dt}. \quad (1.10.17)$$

The first term is the total change in A and the second term explicitly subtracts the change in A due to time changing with ε . Using Hamilton's equations we have:

$$\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial t} + \frac{\partial \mathcal{H}}{\partial Q^a} \dot{Q}^a + \frac{\partial \mathcal{H}}{\partial P_a} \dot{P}_a = \frac{\partial \mathcal{H}}{\partial t} + \frac{\partial \mathcal{H}}{\partial Q^a} \frac{\partial \mathcal{H}}{\partial P_a} - \frac{\partial \mathcal{H}}{\partial P_a} \frac{\partial \mathcal{H}}{\partial Q^a} = \frac{\partial \mathcal{H}}{\partial t} \quad (1.10.18)$$

$$\implies \mathcal{D}\mathcal{H}|_t = \mathcal{D}\mathcal{H} - \mathcal{D}t \frac{d\mathcal{H}}{dt} = \mathcal{D}\mathcal{H} - \mathcal{D}t \frac{\partial \mathcal{H}}{\partial t}. \quad (1.10.19)$$

Then, we can rewrite (1.10.14), (1.10.15), (1.10.16) as:

$$\frac{\partial \delta F}{\partial t} = -\mathcal{D}\mathcal{H}|_t, \quad \frac{\partial \delta F}{\partial Q^a} = \mathcal{D}P_a|_t, \quad \frac{\partial \delta F}{\partial P_a} = -\mathcal{D}Q^a|_t. \quad (1.10.20)$$

Using these, consider how a general function $A(t', Q', P')$ changes under the transformation at fixed time:

$$\mathcal{D}A|_t = \mathcal{D}A - \mathcal{D}t \frac{dA}{dt} = \frac{\partial A}{\partial t} \mathcal{D}t + \frac{\partial A}{\partial Q^a} \mathcal{D}Q^a + \frac{\partial A}{\partial P_a} \mathcal{D}P_a - \frac{\partial A}{\partial t} \mathcal{D}t - \frac{\partial A}{\partial Q^a} \dot{Q}^a \mathcal{D}t - \frac{\partial A}{\partial P_a} \dot{P}_a \mathcal{D}t \quad (1.10.21)$$

$$= \frac{\partial A}{\partial Q^a} \mathcal{D}Q^a|_t + \frac{\partial A}{\partial P_a} \mathcal{D}P_a|_t = -\frac{\partial A}{\partial Q^a} \frac{\partial \delta F}{\partial P_a} + \frac{\partial A}{\partial P_a} \frac{\partial \delta F}{\partial Q^a} \quad (1.10.22)$$

$$= \{A, -\delta F\}. \quad (1.10.23)$$

Therefore, the Poisson bracket of a function with $-\delta F$ gives how that function changes at the present time under the continuous transformation. This is precisely (1.4.1) where we identify $-\delta F$ as the generator of the transformation. That is, the generator G of a continuous canonical transformation is given by:

$$\boxed{G = -\delta F = P_a \mathcal{D}Q^a - \mathcal{H} \mathcal{D}t - \mathcal{D}f.} \quad (1.10.24)$$

This is the fundamental relationship between the generator G of a continuous transformation and the canonical function F of that transformation.

The identification of $G = -\delta F$ only used the last two conditions in (1.10.20). To see the meaning of the first condition it is nicer to look at the total time derivative rather than the partial time derivative and to use (1.10.4):

$$\frac{dG}{dt} = -\frac{\partial \delta F}{\partial t} - \frac{\partial \delta F}{\partial Q^a} \dot{Q}^a - \frac{\partial \delta F}{\partial P_a} \dot{P}_a = \mathcal{H}|_t - \frac{\partial \mathcal{H}}{\partial P_a} \mathcal{D}P_a|_t - \frac{\partial \mathcal{H}}{\partial Q^a} \mathcal{D}Q^a|_t \quad (1.10.25)$$

$$= \delta \mathcal{H} + \frac{\partial \mathcal{H}}{\partial t} \mathcal{D}t + \frac{\partial \mathcal{H}}{\partial Q^a} \mathcal{D}Q^a + \frac{\partial \mathcal{H}}{\partial P_a} \mathcal{D}P_a - \frac{d\mathcal{H}}{dt} \mathcal{D}t - \frac{\partial \mathcal{H}}{\partial P_a} \left(\mathcal{D}P_a - \frac{\partial \mathcal{H}}{\partial Q^a} \mathcal{D}t \right) - \frac{\partial \mathcal{H}}{\partial Q^a} \left(\mathcal{D}Q^a + \frac{\partial \mathcal{H}}{\partial P_a} \mathcal{D}t \right) \quad (1.10.26)$$

$$\Rightarrow \boxed{\frac{dG}{dt} = \delta \mathcal{H}}. \quad (1.10.27)$$

This is all true regardless of whether the transformation is a symmetry.

Now consider the special case that our continuous transformation generated by G is a symmetry of the system. Then, by theorem 1.8, the transformed and untransformed Hamiltonians are the same function (just evaluated at the appropriate transformed or untransformed arguments) and so $\delta \mathcal{H} = 0$. Consequently, we immediately have that the generator G is conserved. Alternatively, if the generator G is conserved for all points in phase space, then $\delta \mathcal{H} = 0$ and so the transformation is a symmetry. **Whenever the theory has a continuous symmetry the generator of that transformation is conserved.** This result is known as Noether's theorem²¹.

The symmetry condition that the Hamiltonian does not change form as a function immediately implies that the action of the transformed variables is the same functional as the action of the untransformed variables, just evaluated at Q', P' instead of Q, P . They will be the same functional, not literally equal numerically. We already found that regardless of whether the transformation is a symmetry they differ by the surface term $f(t, Q, P)$. So, the symmetry condition is equivalently stated as requiring the untransformed action evaluated at the transformed variables $S[Q', P']$ to be numerically equal to $S[Q, P]$ up to a surface term $f(t, Q, P)$.

It is interesting for many applications to consider the special case that the continuous transformation is an extended point transformation. Because the formula for the generator was completely general, it is unchanged. However, for an extended point transformation we know the Lagrangian very nicely satisfies (1.9.107) and in the case of symmetry satisfies (1.9.108). Because $\frac{dt'}{dt}$ we can combine these as:

$$\frac{dt'}{dt} \mathcal{L}(t', Q', \dot{Q}') = \mathcal{L}(t, Q, \dot{Q}) + \frac{df}{dt} \quad (1.10.28)$$

$$\Rightarrow \frac{d}{d\varepsilon} \left(\frac{dt'}{dt} \mathcal{L}(t', Q', \dot{Q}') \right) \Big|_{\varepsilon=0} = \frac{d\mathcal{D}f(t, Q)}{dt}. \quad (1.10.29)$$

Therefore, an extended point transformation is a symmetry if and only if when the left hand side is computed there exists a function $\mathcal{D}f(t, Q)$ so that that left hand side is its total time derivative without using the equation of motion.

Theorem 1.9: Noether's Theorem - Global Conservation

For a continuous transformation $t' = t'(\varepsilon, t, Q, P)$, $Q' = Q'(\varepsilon, t, Q, P)$, $P' = P'(\varepsilon, t, Q, P)$ (with parameter ε defined so that $\varepsilon = 0$ corresponds to the identity transformation) with generating function $F(\varepsilon, t', Q', t, Q)$, the generator $G(t, Q, P)$ of that transformation is given by:

$$G(t, Q, P) = - \frac{\partial}{\partial \varepsilon} F(\varepsilon, t', Q', t, Q) \Big|_{\varepsilon=0} = P_a \mathcal{D}Q^a - \mathcal{H} \mathcal{D}t - \mathcal{D}f \quad (1.10.30)$$

²¹ Emmy Noether (1882-1935) was described upon her death by Einstein in a letter to the New York Times: "In the judgment of the most competent living mathematicians, Fräulein Noether was the most significant creative mathematical genius thus far produced since the higher education of women began." [77]. Carefully note that according to Einstein she was the most mathematically brilliant person of any gender to have existed since women were allowed access to higher education.

where:

$$\mathcal{D}t(t, Q, P) = \left. \frac{\partial t'}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}Q^a(t, Q, P) = \left. \frac{\partial Q'^a}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}f(t, Q, P) = \left. \frac{d}{d\varepsilon} F(\varepsilon, t', Q', t, Q) \right|_{\varepsilon=0}. \quad (1.10.31)$$

The generator G generates the change in any function $A(t', Q', P')$ on the phase space as the continuous transformation is applied at fixed time:

$$\left. \frac{dA}{d\varepsilon} \right|_{\varepsilon=0, t \text{ fixed}} = \{A, G\}. \quad (1.10.32)$$

The Hamiltonian will change both due to t', Q', P' changing and due to its form as a function changing with ε . The time derivative of the generator is related to the change in the form of the Hamiltonian function as the transformation is applied:

$$\frac{dG}{dt} = \left. \frac{\partial \mathcal{H}'(\varepsilon, t', Q', P')}{\partial \varepsilon} \right|_{\varepsilon=0}. \quad (1.10.33)$$

The generator is conserved if the system has symmetry under the continuous transformation it generates (and so the Hamiltonian does not change form under the transformation). Conversely, if the system has a conserved quantity (also called a Noether charge), the continuous transformation generated by using that conserved quantity as the generator is a symmetry of the system. Equivalently, a continuous transformation is a symmetry if and only if when the untransformed Hamiltonian action functional S is evaluated at the transformed variables $S[Q', P']$, the result differs from $S[Q, P]$ only by a surface term $f(t, Q, P)$.

In the case that the continuous transformation of interest is an extended point transformation the symmetry condition is equivalent to requiring the existence of a function $\mathcal{D}f(t, Q)$ so that:

$$\left. \frac{d}{d\varepsilon} \left(\frac{dt'}{dt} \mathcal{L}(t', Q', \dot{Q}') \right) \right|_{\varepsilon=0} = \frac{d\mathcal{D}f(t, Q)}{dt}. \quad (1.10.34)$$

Equivalently, a continuous extended point transformation is a symmetry if and only if when the untransformed Lagrangian action functional S is evaluated at the transformed variables $S[Q']$, the result differs from $S[Q]$ only by a surface term $f(t, Q)$.

Exercises

Problem 1.29: Length scale symmetry. Consider the Lagrangian $\mathcal{L} = \frac{\dot{x}^2}{2x^2}$.

- Find and solve the Euler-Lagrange equation of motion for this Lagrangian.
- Define the scaling transformation $x' = e^\varepsilon x$ which just multiplies x by a constant while keeping t fixed, $t' = t$. Show that the action and/or Lagrangian for this system has symmetry under this scale transformation.
- Find the generator of this scale transformation and compute its time derivative explicitly using the Euler-Lagrange equation. Compare your result with the conclusion of Noether's Theorem.

Problem 1.30: Length and time scale symmetry. Consider the Lagrangian $\mathcal{L} = \frac{\dot{x}^2}{2x}$.

- Find and solve the Euler-Lagrange equation of motion for this Lagrangian.
- Define the scaling transformation $x' = e^\varepsilon x$, $t' = e^\varepsilon t$ in which x and t are scaled together. Show that the action for this system has symmetry under this scale transformation. Notice that the action is unchanged but the Lagrangian transforms because $t' \neq t$.
- Find the generator of this scale transformation and compute its time derivative explicitly using the Euler-Lagrange equation. Compare your result with the conclusion of Noether's Theorem.

Problem 1.31: Rotational symmetry. Consider the Lagrangian $\mathcal{L} = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\dot{y}^2 - U(x^2 + y^2)$ where U is a continuously differentiable function.

- Consider the rotation transformation $x' = x \cos \alpha - y \sin \alpha$, $y' = x \sin \alpha + y \cos \alpha$. Show that the action and/or Lagrangian for this system has symmetry under this transformation.

- (b) Find the generator of this transformation and compute its time derivative explicitly using the Euler-Lagrange equations. Compare your result with the conclusion of Noether's Theorem.
- (c) Make the point transformation $(x, y) \rightarrow (r, \varphi)$ by $x = r \cos \varphi$, $y = r \sin \varphi$ and reexpress the Lagrangian in terms of these coordinates. Find the Euler-Lagrange equations in these coordinates and show that symmetry under rotation in these coordinates is implied by $\frac{\partial \mathcal{L}}{\partial \varphi} = 0$.

1.11 Lie Algebras and Lie Groups

We will typically consider more than one kind of transformation within any given system. For example, we may consider rotations and translations together. These transformations will map the extended phase space (t, Q, P) invertibly into itself (one can undo a translation or rotation). As well, we can compose rotations and translations. And, there is of course an identity transformation of simply not rotating and not translating. Thus, the set of translations and rotations satisfies the mathematical definition of a **group**:

A group G is a set which has some notion of multiplication where multiplication just means a map that takes two elements of G and from them produces a new element in a way which satisfies the following properties:

1. Multiplication is closed – the product of any two elements in the group is in the group.
2. Multiplication is associative – for all f, g, h in the group, $f(gh) = (fg)h$.
3. An identity element exists – there is an element $\mathbb{1}$ in the group so that for all g in the group, $\mathbb{1}g = g\mathbb{1} = g$.
4. Each element has an inverse – for each g in the group there is an element g^{-1} in the group so that $g^{-1}g = gg^{-1} = \mathbb{1}$.

The group multiplication generally has nothing to do with ordinary numerical multiplication. Some classic groups are the integers under the operation of addition and the rationals (excluding 0) under the operation of regular multiplication. In the case of transformations, the multiplication operation which forms a group is the composition of transformations. Consider for example rotations in the plane. If R_θ is a rotation by θ then rotating by θ_1 and then by θ_2 is given by $R_{\theta_2}R_{\theta_1}$. When applied to a vector v this notation means $R_{\theta_2}(R_{\theta_1}(v))$. This is equivalent to a single rotation $R_{\theta_1+\theta_2}$. Because the composition of rotations is a rotation, the set of rotations satisfies the closure property. A sequence of three rotations is a single rotation with angle $\theta_1 + \theta_2 + \theta_3$ and so the associativity property is satisfied because $(\theta_1 + \theta_2) + \theta_3 = \theta_1 + (\theta_2 + \theta_3)$. A rotation by $\theta = 0$ is obviously the identity and a rotation of $-\theta$ is the inverse of a rotation by θ . Thus, the group definition is satisfied for rotations in the plane. The transformations considered in physics very often satisfy the group definition.

Not only are the transformations used in physics generally groups, they are in particular typically a special kind of group called a **Lie group**. A group is a Lie group when in addition to the above requirements, there are real parameters which we can smoothly differentiate the elements of the group with respect to. We will not go into full depth on Lie groups in this book, but we will outline a few properties which will be important for us to know. First, let us consider a Lie group with potentially many parameters but for which at the moment we will only change 1 parameter ε (such as translations by the parameter $\varepsilon = x$). We will study this using our generic Lie bracket formalism from before. Then, we know the transformation $T(\varepsilon)$ has some generator τ . From section 1.3 we have that any other operator u on which that transformation acts evolves with ε as (suppressing the hats above operators):

$$\frac{du}{d\varepsilon} = u\angle\tau. \quad (1.11.1)$$

By differentiating a second time with respect to ε we find:

$$\frac{d^2u}{d\varepsilon^2} = \frac{d}{d\varepsilon}(u\angle\tau) = (u\angle\tau)\angle\tau. \quad (1.11.2)$$

It is useful to define the notation of the Lie bracket acting as a linear operator on u :

$$(\cdot\angle\tau)u \stackrel{\text{def}}{=} u\angle\tau. \quad (1.11.3)$$

Then we can write this self composition of $\cdot\angle\tau$ as:

$$(u\angle\tau)\angle\tau = (\cdot\angle\tau)^2u. \quad (1.11.4)$$

By differentiating u n times with respect to ε we have:

$$\frac{d^n u}{d\varepsilon^n} = (\cdot\angle\tau)^n u. \quad (1.11.5)$$

Now assuming u changes analytically with ε , we can write u after transformation by ε as a Taylor series in ε :

$$u(\varepsilon) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} u^{(n)}(0) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} (\cdot\angle\tau)^n u(0) = e^{\varepsilon(\cdot\angle\tau)} u(0). \quad (1.11.6)$$

This last jump is made by identifying that the series is the Taylor expansion of the exponential and this series

is taken as the definition of what it means to raise e to an operator. Hence we can write the transformed $u(\varepsilon)$ as this linear operator that is the operator exponential acting on the untransformed $u(0)$. With this we can write the transformation operator $T(\varepsilon)$ as:

$$u(\varepsilon) = T(\varepsilon)u(0) \implies T(\varepsilon) = e^{\varepsilon(\cdot\angle\tau)}. \quad (1.11.7)$$

If we take this solution and differentiate at the identity we find:

$$\frac{dT}{d\varepsilon} = (\cdot\angle\tau)T, \quad T(0) = \mathbb{1} \quad (1.11.8)$$

$$\implies T'(0) = (\cdot\angle\tau)\mathbb{1} = (\cdot\angle\tau) \quad (1.11.9)$$

$$\implies T(\varepsilon) = e^{\varepsilon T'(0)}. \quad (1.11.10)$$

So, the full continuous transformation for finite values of the parameter can be recovered just from the derivative at the identity by this exponential. This reveals to us a very important tool. If we study how a continuous transformation behaves in the neighborhood of the identity transformation, meaning we find an expression for $T'(0)$, we can use that together with the operator exponential to recover the full continuous transformation. This is why when studying continuous transformations in deriving Noether's theorem we only needed to study their behavior near $\varepsilon = 0$.

Now let us consider a second family of transformations in our group so that we have two families of continuous transformations, $T(\alpha)$ and $S(\beta)$ (with generators f and g respectively). From our reasoning in section 1.2, specifically our commutative diagram (1.2.2), one transformation has symmetry under another if composing them in different orders gives the same result. That is:

$$T(\alpha)S(\beta) = S(\beta)T(\alpha) \iff T \text{ and } S \text{ are symmetric under each other.} \quad (1.11.11)$$

From our exponential form (1.11.10), we can see that $T(-\alpha)$ is the inverse of $T(\alpha)$. Hence:

$$T(\alpha)S(\beta) = S(\beta)T(\alpha) \iff S(-\beta)T(-\alpha)S(\beta)T(\alpha) = \mathbb{1}. \quad (1.11.12)$$

This product is itself a continuous transformation. Now that we know we only need to study continuous transformations for small parameters to be able to recover the full transformation by exponentiation, let us expand this product acting on an arbitrary u (without assuming these two transformations have symmetry with respect to each other):

$$S(-\beta)T(-\alpha)S(\beta)T(\alpha)u = (1 - \beta(\cdot\angle g))(1 - \alpha(\cdot\angle f))(1 + \beta(\cdot\angle g))(1 + \alpha(\cdot\angle f))u + \text{Higher Order Terms} \quad (1.11.13)$$

$$= (1 - \beta(\cdot\angle g))(1 - \alpha(\cdot\angle f))(1 + \beta(\cdot\angle g))(u + \alpha u \angle f) + \text{H.O.T.} \quad (1.11.14)$$

$$= (1 - \beta(\cdot\angle g))(1 - \alpha(\cdot\angle f))(u + \alpha u \angle f + \beta u \angle g + \alpha \beta (u \angle f) \angle g) + \text{H.O.T.} \quad (1.11.15)$$

$$= (1 - \beta(\cdot\angle g))(u + \alpha u \angle f + \beta u \angle g + \alpha \beta (u \angle f) \angle g - \alpha u \angle f - \alpha \beta (u \angle g) \angle f) + \text{H.O.T.} \quad (1.11.16)$$

$$= u + \beta u \angle g + \alpha \beta (u \angle f) \angle g - \alpha \beta (u \angle g) \angle f - \beta u \angle g + \text{H.O.T.} \quad (1.11.17)$$

$$= u + \alpha \beta ((u \angle f) \angle g - (g \angle u) \angle f) + \text{H.O.T.} \quad (1.11.18)$$

Using the Jacobi property (equation (1.3.27)):

$$(u \angle f) \angle g + (g \angle u) \angle f + (f \angle g) \angle u = 0 \quad (1.11.19)$$

$$\implies (u \angle f) \angle g + (g \angle u) \angle f = -(f \angle g) \angle u = u \angle (f \angle g). \quad (1.11.20)$$

Thus simplifying our calculation to:

$$S(-\beta)T(-\alpha)S(\beta)T(\alpha)u = (1 + \alpha \beta (\cdot\angle (f \angle g)))u + \text{H.O.T.} \quad (1.11.21)$$

Hence the deviation from the identity can be written to lowest order as the bracket of the bracket of the generators acting on the object being transformed. Given the transformations this gives us a way to compute the bracket of their generators by simply taking equation (1.11.21) and differentiating:

$$u \angle (f \angle g) = \frac{d}{d\alpha} \frac{d}{d\beta} S(-\beta)T(-\alpha)S(\beta)T(\alpha)u|_{(\alpha,\beta)=(0,0)}. \quad (1.11.22)$$

We can make this calculation for any u which then defines the bracket $f \angle g$ up to a term whose bracket with all u is 0. If a generator has vanishing bracket with everything, it is necessarily a constant (if it depended on any variables then its bracket with the generator of translations of that variable would be non zero). Hence, equation (1.11.22) can be used to compute brackets up to an additive constant. As well, this means that if two transformations commute then the bracket of their generators must be a constant.

When S and T do not have symmetry under each other, $S(-\beta)T(-\alpha)S(\beta)T(\alpha)$ will not be the identity.

However, from our definition of Lie groups, the composition of transformations in the group must also be in the group. Therefore, $S(-\beta)T(-\alpha)S(\beta)T(\alpha)$ must also be in the group. For fixed β , by (1.11.21), near the identity this combination is as if it were a continuous transformation with parameter α and generator $\beta f \angle g$. Because this is true for each β we see that closure requires that if f and g are allowed generators to use for defining a transformation then $f \angle g$ is also an allowed generator for defining a transformation.

From our definition of the space of generators, we were able to consider the linear combinations of different generators and so we can consider the vector space of all allowed generators. For a given Lie group, that vector space is called its **Lie algebra**. Because it is a vector space, we can consider a basis²² for the space τ_a . That is, any generator f can be written as a linear combination for some coefficients c^a , $f = c^a \tau_a$. This space is a special vector space equipped with this Lie bracket structure we have defined. We found that closure of the group requires that if f and g are in the algebra then $f \angle g$ is in the algebra. Hence, the Lie bracket of our basis generators $\tau_a \angle \tau_b$ must be in the vector space and so there must exist coefficients f_{ab}^c so that $\tau_a \angle \tau_b$ can be written as the linear combination of basis vector τ_c :

$$\tau_a \angle \tau_b = f_{ab}^c \tau_c. \quad (1.11.23)$$

These f_{ab}^c constants are called the **structure constants** of the algebra. Clearly they depend on the choice of basis for algebra. Two Lie algebras are said to be equivalent if they have the same structure constants (or if there exists a change of basis of generators τ_a so that in the appropriate bases they have the same structure constants). Putting all of these results together we have:

Theorem 1.10: Lie Algebra Theorem

For a continuous transformation $T(\alpha)$ with generator f :

$$T(\alpha) = e^{\alpha T'(0)} = e^{\alpha(\cdot \angle f)}. \quad (1.11.24)$$

For another continuous transformation $S(\beta)$ with generator g :

$$u \angle (f \angle g) = \frac{d}{d\alpha} \frac{d}{d\beta} S(-\beta)T(-\alpha)S(\beta)T(\alpha)u|_{(\alpha,\beta)=(0,0)}. \quad (1.11.25)$$

If the transformations $T(\alpha)$ and $S(\beta)$ commute, then the Lie bracket $f \angle g$ of their generators must be a constant.

For a given Lie group of transformations, the space of generators of those transformations forms a Lie algebra which is a vector space with some basis generators τ_a satisfying for some constants f_{ab}^c :

$$\tau_a \angle \tau_b = f_{ab}^c \tau_c. \quad (1.11.26)$$

We have found that from a Lie group, we can form a Lie algebra describing the generators of continuous transformations in the group. The Lie algebra is determined by the behavior of the group near the identity by (1.11.24). We might wonder if that exponential in (1.11.24) could be used to recover the full Lie group. It is not generally quite so simple. A single exponential $e^{\alpha(\cdot \angle f)}$ gives essentially a “straight” path through the group, viewed as a function of α . It is a theorem of finite dimensional Lie groups that within a neighborhood of finite size of the identity transformation, every element of the group can be written as the exponential of an element of the algebra. Therefore, these straight paths are enough nearby to the identity. However, one may have elements in a group of transformation of interest that cannot be reached by a single exponential. Define the connected component of a Lie group as the subgroup that can be connected to the identity transformation by a continuous path within the group (meaning changing the group parameters continuously). It is a theorem of finite dimensional Lie groups that every element of the connected component can be reached by composing a finite number of continuous transformations (meaning something of the form $e^{\cdot \angle f_1} e^{\cdot \angle f_2} \dots e^{\cdot \angle f_N}$). Therefore, through the exponential of the Lie algebra and compositions, one can reach any point in the connected component of the Lie group. General Lie groups can also contain discrete transformations which cannot be connected to the identity and these cannot be reached by the exponential of the Lie algebra with any number of compositions. The relationship between the algebra and the group is only invertible when the group is connected.

²²Wary mathematicians will say that this requires the axiom of choice, but for the cases we will use a basis can be constructed rather than required by postulate.

As usual, this Lie formalism is quite abstract but we can get more insight with a representation. If we have a representation of the generators and of the bracket, then by definition the representation bracket of the generator representation is the same as the representation of the bracket of the generators (1.3.47). If we apply this to (1.11.26):

$$R(\tau_a \angle \tau_b) = R(f_{ab}^c \tau_c) \quad (1.11.27)$$

$$\implies R(\tau_a) \angle_R R(\tau_b) = f_{ab}^c R(\tau_c). \quad (1.11.28)$$

Therefore, the structure constants are the same in all representations. Because of this, once we have one representation of the algebra which allows us to compute the structure constants then we have the full information about the abstract definition of the algebra.

It will be useful for us to study a special case of Lie algebras. Consider a continuous point transformation: $Q' = Q'(\varepsilon, Q)$ in the Poisson representation. Then, $\mathcal{D}Q^a$ will only be a function of Q^a . By (1.9.100) and (1.9.101) using that $t' = t$:

$$\mathcal{H}' = \mathcal{H} - \frac{\partial f(t, Q'(Q))}{\partial t}, \quad P'_a = \frac{\partial Q^b}{\partial Q'^a} P_b + \frac{\partial f}{\partial Q'^a} = \frac{\partial Q^b}{\partial Q'^a} \left(P_b + \frac{\partial f(t, Q'(Q))}{\partial Q^b} \right). \quad (1.11.29)$$

This transformation is time independent and so we can take the surface function to be time independent by (1.9.123). Consequently:

$$\mathcal{H}' = \mathcal{H}. \quad (1.11.30)$$

The remaining transformation is equivalent to an action gauge transformation by $f(Q)$ followed by the transformation:

$$\mathcal{H}' = \mathcal{H}, \quad P'_a = \frac{\partial Q^b}{\partial Q'^a} P_b. \quad (1.11.31)$$

The gauge transformation contribution may be desirable for symmetry considerations but this simpler transformation will often be of interest. So, we define a “simple point transformation” as the transformation:

$$t' = t, \quad Q'^a = Q'^a(Q), \quad P'_a = \frac{\partial Q^b}{\partial Q'^a} P_b, \quad \mathcal{H}'(t', Q', P') = \mathcal{H}(t, Q, P). \quad (1.11.32)$$

Then, by (1.10.30) the generator of this transformation is:

$$G = P_a \mathcal{D}Q^a. \quad (1.11.33)$$

A particularly convenient case for our purposes will be linear point transformations. That is, point transformations which depend linearly on Q and hence are of the form:

$$\mathcal{D}Q^a = A^a_b Q^b \quad (1.11.34)$$

for some matrix of coefficients A^a_b . Then, the generator f is:

$$G = P_a A^a_b Q^b. \quad (1.11.35)$$

Now if we consider the Poisson bracket of two such generators $G_1 = P_a A^a_b Q^b$ and $G_2 = P_a B^a_b Q^b$, we come to quite a nice conclusion:

$$\{G_1, G_2\} = \{P_a A^a_b Q^b, P_c B^c_d Q^d\} \quad (1.11.36)$$

$$= \frac{\partial}{\partial Q^e} (P_a A^a_b Q^b) \frac{\partial}{\partial P_e} (P_c B^c_d Q^d) - \frac{\partial}{\partial P_e} (P_a A^a_b Q^b) \frac{\partial}{\partial Q^e} (P_c B^c_d Q^d) \quad (1.11.37)$$

$$= P_a A^a_b \delta^b_e \delta^e_c B^c_d Q^d - \delta^e_a A^a_b Q^b P_c B^c_d \delta^d_e \quad (1.11.38)$$

$$= P_a (A^a_c B^c_b - B^a_c A^c_b) Q^b. \quad (1.11.39)$$

Define the matrix $\hat{A}$ as the matrix with components A^a_b and $\hat{B}$ as the matrix with components B^a_b . Then, this expression in (1.11.39) is the expression for the components of the matrix $\hat{A}\hat{B} - \hat{B}\hat{A}$. Therefore:

$$\{G_1, G_2\} = P_a [\hat{A}, \hat{B}]^a_b Q^b. \quad (1.11.40)$$

Hence, if we have some generators τ_a of a Lie algebra which generate simple linear point transformations and thus have associated matrices $\hat{T}_a$, those matrices must form a representation of the algebra with the matrix commutator acting as the representation of the Lie bracket:

$$\tau_a = P_b (\hat{T}_a)^b_c Q^c, \quad \{\tau_a, \tau_b\} = f_{ab}^c \tau_c \quad (1.11.41)$$

$$\implies \{\tau_a, \tau_b\} = P_m [\hat{T}_a, \hat{T}_b]^m_n Q^n = f_{ab}^c P_m (\hat{T}_c)^m_n Q^n \quad (1.11.42)$$

$$\implies [\hat{\mathcal{T}}_a, \hat{\mathcal{T}}_b] = f_{ab}{}^c \hat{\mathcal{T}}_c. \quad (1.11.43)$$

Therefore for simple linear point transformations we can determine the structure coefficients by computing commutators of the transformation matrices. Equation (1.11.43) is exactly the same as (1.11.26) with the matrix commutator acting as the representation of the Lie bracket and the matrices acting as a representation of the generators. A representation of a Lie algebra by matrices in which the bracket is the matrix commutator is called a matrix representation of the Lie algebra. Hence we have:

Theorem 1.11: Linear Point Transformation Theorem

If τ_a are generators of simple linear point transformations which form a Lie algebra:

$$\tau_a \angle \tau_b = f_{ab}{}^c \tau_c \quad (1.11.44)$$

then in the Poisson representation there exist matrices $\hat{\mathcal{T}}_a$ so that:

$$\tau_a = P \cdot \hat{\mathcal{T}}_a \cdot Q, \quad [\hat{\mathcal{T}}_a, \hat{\mathcal{T}}_b] = f_{ab}{}^c \hat{\mathcal{T}}_c \quad (1.11.45)$$

and hence the $\hat{\mathcal{T}}_a$ matrices form a matrix representation of the Lie algebra with the matrix commutator as the Lie bracket.

Exercises

Problem 1.32: ★ The adjoint representation. The goal of this problem is to show that every finite dimensional Lie algebra has a matrix representation.

- Use (1.11.44) and the antisymmetry of the Lie bracket to show that for any Lie algebra the structure constants satisfy: $f_{ab}{}^c = -f_{ba}{}^c$.
- Compute the left hand side of the Jacobi-Identity using τ_a, τ_b, τ_c . Because this left hand side must automatically be 0, conclude from your calculation that for any Lie algebra the structure constants must satisfy:

$$f_{ad}{}^e f_{bc}{}^d + f_{bd}{}^e f_{ca}{}^d + f_{cd}{}^e f_{ab}{}^d = 0.$$

- Define the matrices $\mathcal{T}_a$ which have components $(\mathcal{T}_a)^c{}_b = f_{ab}{}^c$. Show that the condition on the structure constants found in (b) restated in terms of these matrices is:

$$\mathcal{T}_a \mathcal{T}_b - \mathcal{T}_b \mathcal{T}_a - f_{ab}{}^c \mathcal{T}_c = 0.$$

- From the conclusion of (c), explain how this shows that the vector space spanned by $\mathcal{T}_a$ is a representation of the Lie algebra we started with with the bracket represented by the matrix commutator. This representation is called the “adjoint representation”. It exists for infinite dimensional Lie algebras as well but the idea of a matrix has to be properly generalized to the idea of a linear operator when in infinite dimensions.

Problem 1.33: The Affine Group. Consider the two transformations of translation $x(\alpha) = T(\alpha, x_0) = x_0 + \alpha$ and scaling $x(\beta) = S(\beta, x_0) = e^\beta x_0$ acting on a single real variable x_0 .

- Differentiate these two transformations to show that $\frac{dx}{d\alpha} = 1$ and $\frac{dx}{d\beta} = x$. From these, use (1.3.3) and (1.3.6) to show that the generator of T is written as $\hat{F} = \partial_x$ and that the generator of S is written as $\hat{G} = x\partial_x$ in this representation.
- Using the expressions for $\hat{F}$ and $\hat{G}$ found in (a) and the expression for the bracket in this representation (1.3.22), show that $\hat{F} \angle \hat{G} = -\hat{F}$.
- Considering $\tau_1 = \hat{F}$ and $\tau_2 = \hat{G}$, we have a two-dimensional Lie algebra with the structure constants given by the conclusion of (b). Compute those structure constants explicitly from the answer to (b).
- Using the structure constants in (c) and the method of Problem 1.32(c), explicitly construct the 2x2 matrices $\mathcal{T}_1$ and $\mathcal{T}_2$ which are the adjoint representation of this two dimensional Lie algebra. Explicitly calculate the matrix commutator of these two matrices to see that they do have the right structure constants.
- Compute the matrix exponentials $\mathcal{M}(\alpha) = e^{\alpha \mathcal{T}_1}$ and $\mathcal{N}(\beta) = e^{\beta \mathcal{T}_2}$ explicitly.
- Show this matrix equation holds for any real number x :

$$\mathcal{M}(\alpha)\mathcal{N}(\beta) \begin{pmatrix} x \\ -1 \end{pmatrix} = \begin{pmatrix} e^\beta x + \alpha \\ -1 \end{pmatrix}.$$

Explain how this exactly recovers our original definition of the transformations.

1.12 (2nd Pass) Incorporating Higher Derivatives

So far we have only considered Lagrangians which depend on the first time derivative of Q but we know we can formulate variational calculations up to arbitrary order of differentiation from Theorem 1.3. We have only had to consider Lagrangians up to first derivative in Q by construction from our original dynamical system and so in principle this should be sufficient. However, it could be the case that the configuration space Q can be written as $Q = (q, \dot{q}, \ddot{q}, \dots, \overset{N}{q})$ for some variable q . That is, some of the Q^a could be time derivatives of the others in principle (this can be done by choosing some of the V^a in (1.1.6) to be equal to some of the coordinates). This is just a special case of the formalism we have done so far and so it is entirely consistent with it. This point is important: **higher derivative Lagrangians are not a generalization of our analysis so far; they are a special case of it.** However, it does allow for a nice reduction of the Lagrangian so that it appears instead as $\mathcal{L}(t, q, \dot{q}, \dots, \overset{N}{q})$, which is now a Lagrangian with higher than first time derivative dependence of q (although the reduced coordinate q is not the full configuration Q). Thus, higher derivative Lagrangians are fully allowed. But, one should not mistake the q appearing in them as the configuration Q . For notation, let $q^{(n)}$ be the n^{th} time derivative of q . Because each $q^{(n)}$ is an independent coordinate of the configuration for $n < N$, each one has a corresponding conjugate momenta p_n and the dynamics of the theory are given by Hamilton's equations:

$$\dot{q}^{(n)} = \frac{\partial \mathcal{H}}{\partial p_n}, \quad \dot{p}_n = -\frac{\partial \mathcal{H}}{\partial q^{(n)}}. \quad (1.12.1)$$

Here we have $\mathcal{H} = \mathcal{H}(t, q^{(0)}, p_0, \dots, q^{(N-1)}, p_{N-1})$ because as always we have a momentum conjugate to each variable in the configuration. The requirement that $\dot{q}^{(n)} = q^{(n+1)}$ then puts strict constraints on the form of the Hamiltonian. For $0 \leq n < N - 1$:

$$\dot{q}^{(n)} = q^{(n+1)} = \frac{\partial \mathcal{H}}{\partial p_n}(t, q^{(0)}, p_0, \dots, q^{(N-1)}, p_{N-1}) \quad (1.12.2)$$

$$\implies \mathcal{H} = \sum_{n=0}^{N-2} q^{(n+1)} p_n + h(t, q^{(0)}, \dots, q^{(N-1)}, p_{N-1}). \quad (1.12.3)$$

And so, the Hamiltonian can be reduced to this form in terms of the unknown function h which depends on far fewer variables. This h is called the reduced Hamiltonian and we see that the only momentum it depends on is the one of highest order. The second of Hamilton's equations gives us for $0 < n \leq N - 1$:

$$\dot{p}_n = -\frac{\partial \mathcal{H}}{\partial q^{(n)}} = -p_{n-1} - \frac{\partial h}{\partial q^{(n)}}. \quad (1.12.4)$$

From Hamilton's equations we can perform the Legendre transformation:

$$\mathcal{L} = \sum_{n=0}^{N-1} \dot{q}^{(n)} p_n - \mathcal{H} = \sum_{n=0}^{N-1} q^{(n+1)} p_n - \sum_{n=0}^{N-2} q^{(n+1)} p_n - h(t, q^{(0)}, \dots, q^{(N-1)}, p_{N-1}) \quad (1.12.5)$$

$$= \dot{q}^{(N-1)} p_N - h(t, q^{(0)}, \dots, q^{(N-1)}, p_{N-1}) = q^{(N)} p_N - h(t, q^{(0)}, \dots, q^{(N-1)}, p_{N-1}). \quad (1.12.6)$$

The first of Hamilton's equations with $n = N - 1$ completes the Legendre transform (assuming the map is invertible):

$$q^{(N)} = \frac{\partial \mathcal{H}}{\partial p_{N-1}} = \frac{\partial h}{\partial p_{N-1}} \implies p_{N-1} = p_{N-1}(t, q^{(0)}, \dots, q^{(N)}). \quad (1.12.7)$$

Now we can compute the equations of motion in terms of the Lagrangian. For $0 \leq n < N$:

$$\frac{\partial \mathcal{L}}{\partial q^{(n)}} = q^{(N)} \frac{\partial p_{N-1}}{\partial q^{(n)}} - \frac{\partial h}{\partial q^{(n)}} - \frac{\partial h}{\partial p_{N-1}} \frac{\partial p_{N-1}}{\partial q^{(n)}} \quad (1.12.8)$$

$$= q^{(N)} \frac{\partial p_{N-1}}{\partial q^{(n)}} - \frac{\partial h}{\partial q^{(n)}} - \dot{q}^{(N-1)} \frac{\partial p_{N-1}}{\partial q^{(n)}} \quad (1.12.9)$$

$$= -\frac{\partial h}{\partial q^{(n)}} \quad (1.12.10)$$

$$\implies \frac{\partial \mathcal{L}}{\partial q^{(0)}} = \dot{p}_0, \quad \frac{\partial \mathcal{L}}{\partial q^{(n)}} = \dot{p}_n + p_{n-1} \quad (0 < n < N). \quad (1.12.11)$$

For $n = N$:

$$\frac{\partial \mathcal{L}}{\partial q^{(N)}} = p_{N-1}. \quad (1.12.12)$$

Equation (1.12.11) gives a recursion relation defining the momenta and (1.12.12) gives an initial condition for that recursion relation, therefore giving the unique solution for $0 < n \leq N$ by iterating (1.12.11):

$$p_{n-1} = \frac{\partial \mathcal{L}}{\partial q^{(n)}} - \frac{d}{dt} p_n \quad (1.12.13)$$

$$= \frac{\partial \mathcal{L}}{\partial q^{(n)}} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q^{(n+1)}} - \frac{d}{dt} \left(\dots \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q^{(N)}} \right) \right) \right) \quad (1.12.14)$$

$$= \frac{\partial \mathcal{L}}{\partial q^{(n)}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q^{(n+1)}} + \dots + (-1)^{N-n} \left(\frac{d}{dt} \right)^{N-n} \frac{\partial \mathcal{L}}{\partial q^{(N)}}. \quad (1.12.15)$$

We know from (1.7.12) that the canonical momenta should be the derivative of the Lagrangian with respect to the time derivative of the coordinate. Although it may not look like it at first, (1.12.15) is consistent with this. The canonical momenta should be the derivative of the Lagrangian with respect to the time derivative of the coordinate keeping the other coordinates and their time derivatives fixed. Once we make the coordinates to be time derivatives of each other, when we vary one, we vary those made from that one's derivatives and so have to cancel the effects of that variation to get what the derivative would have been if we had held them fixed. That is where the “extra” terms in (1.12.15) come from. Another way to understand this is that the operations of differentiating with respect to $\dot{Q}$ and setting some of the coordinates to be time derivatives of the others do not commute which is no surprise because evaluating a function and differentiating a function usually don't commute. $P = \frac{\partial \mathcal{L}}{\partial \dot{Q}}$ would hold in the usual form with no extra terms if we differentiated first and then evaluated the appropriate Q 's as being time derivatives of the others but in (1.12.13) we did the evaluation first and then differentiated, and so the extra terms come up simply to cancel this fact. If we now take the first part of equation (1.12.11), we get our full equation of motion:

$$\frac{\partial \mathcal{L}}{\partial q^{(0)}} = \dot{p}_0 = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial q^{(1)}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q^{(2)}} + \dots + (-1)^{N-1} \left(\frac{d}{dt} \right)^{N-1} \frac{\partial \mathcal{L}}{\partial q^{(N)}} \right) \quad (1.12.16)$$

$$\implies \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} + \dots + (-1)^N \left(\frac{d}{dt} \right)^N \frac{\partial \mathcal{L}}{\partial \dot{q}^{(N)}} = 0. \quad (1.12.17)$$

Hence the full equation of motion for q alone is given by equation (1.12.17). We see from Theorem 1.3 that this is equivalent to the stationary variation of the action in which we just apply that some of the coordinates are derivatives of others:

$$S[q] = \int_{t_0}^{t_f} \mathcal{L}(t, q, \dot{q}, \dots, \dot{q}^{(N)}) dt \quad (1.12.18)$$

$$\frac{\delta S}{\delta q(t)} = \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} + \dots + (-1)^N \left(\frac{d}{dt} \right)^N \frac{\partial \mathcal{L}}{\partial \dot{q}^{(N)}} = 0. \quad (1.12.19)$$

In order to derive this Euler-Lagrange equation from the action we have to assume that the boundary conditions which are held fixed in the variation are the initial and final values of $q, \dot{q}, \dots, q^{(N-1)}$. This is exactly what we would expect because the configuration $Q = (q^{(0)}, q^{(1)}, \dots, q^{(N-1)})$. Therefore, these are the usual boundary conditions in which the initial and final values of Q are held fixed in the variation. And so, the analytical formalism is completely capable of handling higher derivatives:

Theorem 1.12: Higher Derivative Theorem

The stationary variation of the action:

$$S[q] = \int_{t_0}^{t_f} \mathcal{L}(t, q, \dot{q}, \dots, \dot{q}^{(N)}) dt \quad (1.12.20)$$

(with initial and final values of q and all of its derivatives up to order $N - 1$ fixed) gives equations of motion for q equivalent to the Hamiltonian with configuration space $Q = (q, \dot{q}, \dots, q^{(N-1)})$ and phase

space (Q, P) :

$$\mathcal{H}(t, q^{(0)}, p_0, \dots, q^{(N-1)}, p_{N-1}) = \sum_{n=0}^{N-1} \dot{q}^{(n)} p_n - \mathcal{L}(t, q, \dot{q}, \dots, \overset{\cdot N}{q}) \quad (1.12.21)$$

where the canonical momenta are given by:

$$p_{n-1} = \frac{\partial \mathcal{L}}{\partial q^{(n)}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q^{(n+1)}} + \dots + (-1)^{N-n} \left(\frac{d}{dt} \right)^{N-n} \frac{\partial \mathcal{L}}{\partial q^{(N)}}. \quad (1.12.22)$$

Exercises

Problem 1.34: Wiggling free particle. For the Lagrangian $\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}\alpha\ddot{x}^2$ with m and α positive:

- Compute the Euler-Lagrange equation of motion and solve it.
- Compute the conjugate momenta and Hamiltonian.
- Compute Hamilton's equations of motion and verify that they reproduce the Euler-Lagrange equations.

Problem 1.35: Ostrogradsky's Theorem. From (1.12.3), show that the Hamiltonian of any higher-derivative theory is neither bounded from below nor from above; there exist points in phase space where the Hamiltonian takes any real number you desire as its value. This result is known as Ostrogradsky's Theorem. This fact has implications in thermodynamics where it is necessary for the Hamiltonian to be either bounded below or above for a notion of thermodynamic equilibrium to exist for that system. Theories for which such a notion does not exist are called “thermodynamically unstable”²³.

²³It should be noted that being thermodynamically unstable does not mean that that system is mechanically unstable when isolated. Being a higher derivative theory automatically entails having a Hamiltonian which is not bounded above or below but this does not imply that the solutions to the equations of motion of that Hamiltonian runaway in any way (consider the previous wiggling free particle with an additional term in the Lagrangian $-\frac{1}{2}kx^2$ and $0 < k < \frac{m^2}{4\alpha}$).

1.13 (2nd Pass) The Hamilton-Jacobi Equation

I mentioned previously that it is possible but not useful to undo our dimension doubling to the phase space. In this section we will see how to do it and along the way will find some interesting structure which has many applications, of which we will eventually see a few. We found in theorem 1.4 that the general variation of the action without any requirement on boundary conditions is:

$$\delta S = P_{fa}\delta Q_f^a - \mathcal{H}_f\delta t_f - P_{0a}\delta Q_0^a + \mathcal{H}_0\delta t_0 + \int_{t_0}^{t_f} \left(\left(\dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} \right) \delta P_a - \left(\dot{P}_a + \frac{\partial \mathcal{H}}{\partial Q^a} \right) \delta Q^a \right) dt. \quad (1.13.1)$$

Let us consider the action which results from requiring its variation with respect to the paths $Q(t)$ and $P(t)$ to vanish. The value of the action taken along that path is called the classical action or canonical action S_c . That is, if $Q_c(t)$ and $P_c(t)$ solve the equations of motion:

$$S_c = S[Q_c, P_c]. \quad (1.13.2)$$

Because we have evaluated the path dependence, S_c is now only a function of the boundary conditions t_f, Q_f, t_0, Q_0 . Then, the variation of S_c is simply the variation of S when considered along the equations of motion and we have:

$$\delta S_c = P_{fa}\delta Q_f^a - \mathcal{H}_f\delta t_f - P_{0a}\delta Q_0^a + \mathcal{H}_0\delta t_0. \quad (1.13.3)$$

For the final quantities we will drop the subscript f , so that $t, Q, P, \mathcal{H}$ are the final values of those quantities. For an ordinary function like S_c , the variation δS_c is just the differential dS_c and so we have:

$$dS_c = P_a dQ^a - \mathcal{H} dt - P_{0a} dQ_0^a + \mathcal{H}_0 dt_0 \quad (1.13.4)$$

$$\Rightarrow P_a = \frac{\partial S_c}{\partial Q^a}, \quad \mathcal{H} = -\frac{\partial S_c}{\partial t}, \quad P_{0a} = -\frac{\partial S_c}{\partial Q_0^a}, \quad \mathcal{H}_0 = \frac{\partial S_c}{\partial t}. \quad (1.13.5)$$

These are known as the Hamilton-Jacobi conditions. By comparing to (1.9.82), we can see that these are exactly the conditions for S_c to be the generating function of a canonical transformation with the untransformed variables being the initial values and the transformed variables being the final values. In this way, S_c is **exactly the generating function for time evolution as a canonical transformation**. By comparing $\mathcal{H} = -\frac{\partial S_c}{\partial t}$ to (1.10.30) taking t as the transformation parameter ε and S_c as the generating function F , we see that when time evolution is treated as a continuous canonical transformation, the Hamiltonian is precisely the generator of that transformation. This is exactly how we originally defined the Hamiltonian, and so it is nice to see it explicitly reproduced from our general formula for a generator.

The first of the Hamilton-Jacobi conditions defines $P_a(t, Q, t_0, Q_0)$. Because the Hamiltonian is a known function $\mathcal{H}(t, Q, P)$ we can insert this first solution equation as the solution for P into the Hamiltonian to get that the second equation states:

$$\frac{\partial S_c}{\partial t} + \mathcal{H}(t, Q, \frac{\partial S_c}{\partial Q}) = 0. \quad (1.13.6)$$

This equation is called the Hamilton-Jacobi equation. We see that S_c satisfies a nonlinear partial differential equation. In principle, this equation has solutions²⁴. We will see the Hamilton-Jacobi equation appear in a few different contexts later on.

For now instead of solving the Hamilton-Jacobi equation directly, it will be useful to study a closely related function. To make fully undoubled equations of motion, we want to find an expression for $\frac{dQ^a}{dt}$ which depends on t and $Q(t)$ but not on the initial conditions Q_0 . To remove the direct t_0, Q_0 dependence from our equations, let us use the Legendre Transformation of S_c by defining:

$$W(t, Q, \mathcal{H}_0, P_0) \stackrel{\text{def}}{=} S_c(t, Q, t_0, Q_0) + P_{0a}Q_0^a - \mathcal{H}_0 t_0. \quad (1.13.7)$$

Of course, as is always the case with the Legendre transformation, this requires that the relationship between the variable being transformed and its transformed partner, in this case Q_0 and P_0 , be invertible. It is typically safe to assume this is true and can be checked directly for any particular system of interest. Then, using the Legendre transformation, we see that this W function satisfies:

$$\frac{\partial W}{\partial t} = -\mathcal{H}, \quad \frac{\partial W}{\partial Q^a} = P_a, \quad \frac{\partial W}{\partial \mathcal{H}_0} = -t_0, \quad \frac{\partial W}{\partial P_{0a}} = Q_0^a. \quad (1.13.8)$$

We can see that W also satisfies the Hamilton-Jacobi equation by using the first and second conditions

²⁴This is often a hard claim to prove.

together:

$$\frac{\partial W}{\partial t} + \mathcal{H}(t, Q, \frac{\partial W}{\partial Q}) = 0. \quad (1.13.9)$$

Though typically impractical, theoretically one can solve this differential equation to find the function $W(t, Q, \mathcal{H}_0, P_0)$. Then, we can use the first of Hamilton's equations and insert the solved for W to get a first order equation of motion for Q :

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}(t, Q, P) = \frac{\partial \mathcal{H}}{\partial P_a}(t, Q, \frac{\partial W}{\partial Q}(t, Q, \mathcal{H}_0, P_0)). \quad (1.13.10)$$

Hence (1.13.10) is exactly of the form of (1.1.6) as promised with the phase space replaced by the configuration space (the constants $\mathcal{H}_0, P_0$ are precisely that – constants during the motion as well as independent of the initial conditions t_0, Q_0). However, to actually compute the right hand side we essentially have to solve a nonlinear partial differential equation in general which is practically speaking an impossibility. Hence while this form exists it is almost always useless. There are many other uses for the Hamilton-Jacobi equation we will see later on.

Exercises

Problem 1.36: A free particle at first order. For the Hamiltonian $\mathcal{H}(x, p) = \frac{p^2}{2m}$ with m a constant for a coordinate x and its conjugate momentum p :

- Compute and solve the equations of motion.
- Insert the solved equations of motion into the action integral to compute W .
- Use the procedure of this section to rewrite the equation of motion for x as a first order equation of motion.
- Solve the equation of motion found in part (c).

1.14 (2nd Pass) Adiabatic Invariants and Integrable Systems

The arguments of this section are generally based on [2] and [60]. Some systems are especially nice and simple in a way which makes them “integrable”. We call a Hamiltonian system of phase space dimension $2N$ integrable if it has a time independent Hamiltonian $\mathcal{H}(Q, P)$ and N “independent” conserved quantities on phase space $G_1(Q, P), \dots, G_N(Q, P)$ which all have vanishing Poisson brackets with each other. The conserved quantities are called independent if none of them can be written purely as functions of the others. Because these quantities are conserved:

$$0 = \frac{dG_a}{dt} = \{G_a, \mathcal{H}\} \quad (1.14.1)$$

and so they all Poisson-commute with the Hamiltonian (two quantities are said to Poisson-commute if their Poisson bracket with each other is 0). As well, by requirement they Poisson commute with each other:

$$\{G_a, G_b\} = 0. \quad (1.14.2)$$

By the canonical brackets the N coordinates Q Poisson-commute with each other and the N momenta also Poisson-commute with each other but because each Q has an associated P it does not Poisson-commute with, there is no way to have more than N independent functions of the coordinates and momenta mutually Poisson-commute. Because these G_a all mutually Poisson-commute and there are an equal number of them to the number of momenta, we can make a time independent canonical transformation so that these G_a are our new canonical momenta with some associated canonical coordinates α^a . Actually finding and performing this time independent canonical transformation can be challenging. Assuming we have done so, Hamilton’s equations become:

$$\frac{d\alpha^a}{dt} = \frac{\partial \mathcal{H}}{\partial G_a}, \quad \frac{dG_a}{dt} = -\frac{\partial \mathcal{H}}{\partial \alpha^a} = 0. \quad (1.14.3)$$

Because these G_a are conserved, the Hamiltonian is not a function of the corresponding α^a . Thus, the Hamiltonian depends on the conserved G ’s only:

$$\mathcal{H} = \mathcal{H}(G). \quad (1.14.4)$$

Then, we see that $\dot{\alpha}^a$ depends only on conserved quantities and so is constant:

$$\frac{d\alpha^a}{dt} = \frac{\partial \mathcal{H}}{\partial G_a}(G) \implies \alpha^a(t) = \frac{\partial \mathcal{H}}{\partial G_a}(G)t + \alpha^a(0). \quad (1.14.5)$$

So, in these coordinates the dynamics are easily solved. Then, if one wants the time dependence of the original $Q^a(t)$ and $P_a(t)$, one need only invert the canonical transformation which got us here to begin with. These (α, G) coordinates are not unique as any of the G ’s could be defined among each other and the associated α ’s found to the new G ’s.

In these α, G coordinates, the Hamilton-Jacobi equation admits what are called “separable” solutions. That is, consider a canonical action of the form:

$$S_c(t, \alpha) = \sum_{a=1}^N S_a(t, \alpha^a) - E(t - t_0) \quad (1.14.6)$$

where each function S_a depends only on α^a with the same value of a and E is a constant. In fact, using the Hamilton-Jacobi conditions we can see that E is just given by the conserved energy of this system and the S_a are linear functions of G^a :

$$\frac{\partial S_c}{\partial t} + \mathcal{H}\left(\alpha, \frac{\partial S_c}{\partial \alpha}\right) = 0 \implies E = \mathcal{H}(G) \quad (1.14.7)$$

$$G_a = \frac{\partial S_c}{\partial \alpha^a} \implies S_a = G_a(\alpha^a - \alpha_0^a) \quad (1.14.8)$$

where the last conclusion only follows because each of the G_a are constant in time. Thus the canonical action in these coordinates is given by:

$$S_c(t, \alpha) = G_a(\alpha^a - \alpha_0^a) - \mathcal{H}(G)(t - t_0). \quad (1.14.9)$$

So, how do we actually find these coordinates and how do we identify if a system is integrable to begin with? I do not know of a simple or easy test to check if a system is integrable. The general theory of integrability is quite sophisticated but let us suppose instead we are able to get our canonical coordinates into a form so that the Hamilton-Jacobi equation is separable. That is, suppose we have coordinates (Q, P)

for which there exist solutions to the Hamilton-Jacobi equation of the form:

$$S_c(t, Q) = \sum_{a=1}^N S_a(Q^a) - E(t - t_0). \quad (1.14.10)$$

Supposing this is a solution, we have:

$$P_a = \frac{\partial S_a}{\partial Q^a}, \quad E = \mathcal{H}(Q, P). \quad (1.14.11)$$

The conservation of energy condition can be written more explicitly as:

$$E = \mathcal{H}\left(Q^1, \frac{\partial S_1}{\partial Q^1}, \dots, Q^N, \frac{\partial S_N}{\partial Q^N}\right). \quad (1.14.12)$$

This left hand side is not a function of any of the Q^a while the right hand side depends on each Q^a . Because each S_a (called the reduced action) only depends on the corresponding Q^a , in order for E to be a constant, the way $\mathcal{H}$ depends on Q^a explicitly and through $P_a = \frac{\partial S_a}{\partial Q^a}$ must conspire so that the result is independent of Q^a . That is, the Hamiltonian must depend only on each Q^a through some combination of Q^a and its corresponding P_a which is conserved. So, separability requires that there exist functions ψ_a and constants G_a so that:

$$\psi_a\left(Q^a, \frac{\partial S_a}{\partial Q^a}\right) = G_a \quad (1.14.13)$$

and that the Hamiltonian then only depends on these G_a :

$$\mathcal{H} = \mathcal{H}(G). \quad (1.14.14)$$

Because these G_a are made out of Q^a and P_a for a specific a only, they automatically Poisson-commute with each other for different a . Thus, if the Hamilton-Jacobi equation admits separable solutions in some particular coordinates then the system is integrable and we can immediately identify the N conserved quantities of the system by inserting the separated expression into the Hamilton-Jacobi equation. As well, because integrability implied the separability of the Hamilton-Jacobi equation and separability of the Hamilton-Jacobi equation here implied integrability, we see that a Hamiltonian system is integrable if and only if there exist coordinates in which the Hamilton-Jacobi equation is separable. Unfortunately, even if a system is separable it generally only is so in the right choice of canonical coordinates (Q, P) and so ultimately one does have to be smart about identifying the helpful coordinates for a given system. In practice, the smart coordinates to use for a system are the coordinates in which as many of the symmetries of the system as possible are as manifest as possible.

Now let us suppose that we have an integrable system and we have put it into canonical coordinates (Q, P) in which the Hamilton-Jacobi equation is separable. Further, let us suppose this system has surfaces of constant energy in phase space which are compact (meaning closed and bounded²⁵). Then, because each (Q^a, P_a) pair conserve a quantity G_a and the smooth curve in phase space of constant G_a lies on the surface of constant E , it is also compact and thus that curve has finite arclength. Then, because the motion of (Q^a, P_a) lies solely on that curve and moves on that curve at some finite rate, it will only take a finite time τ_a for those coordinates to explore that entire curve and return to a previously traversed point. Thus, the coordinates (Q^a, P_a) must be periodic in time with some period τ_a . Then, we can then define the integral:

$$J_a = \frac{1}{2\pi} \oint P_a dQ^a \quad (1.14.15)$$

where the closed path of integration is taken to be a single period of the motion of (Q^a, P_a) . This J_a is called the adiabatic invariant for the coordinate Q^a . Because this integral is taken over a full period of the motion, it does not depend on time and so must be conserved and thus a function of the constant G_a :

$$J_a = J_a(G_a). \quad (1.14.16)$$

In fact, we can simply take these adiabatic invariants as the set of G_a and will do so going forward. By viewing this integral as a line integral in the two dimensional sub-phase space of (Q^a, P_a) , we can use Stokes' theorem to rewrite this as an integral over the interior of the curve. The interior will be the area $\mathbb{A}_a$ in the two dimensional sub-phase space which has as its boundary the curve of constant G_a we have been integrating over. For many systems of interest the curve of constant G_a will run counterclockwise on the

²⁵We will not need to refer to the topological definition of compactness precisely.

actual motion. For such curves, the oriented area in Stokes' theorem is negative. By convention in this case we define the oriented area to be the opposite of the usual area in Stokes' theorem so that the area $\mathbb{A}_a$ is typically positive. Then, by Stokes' Theorem:

$$J_a = \frac{1}{2\pi} \oint P_a dQ^a = \frac{1}{2\pi} \oint (P_a, 0) \cdot (dQ^a, dP_a) \quad (1.14.17)$$

$$= -\frac{1}{2\pi} \int_{\mathbb{A}_a} \left(\frac{\partial}{\partial Q^a} 0 - \frac{\partial}{\partial P_a} P_a \right) dQ^a dP_a = \frac{1}{2\pi} \int_{\mathbb{A}_a} dQ^a dP_a = \frac{\mathbb{A}_a}{2\pi}. \quad (1.14.18)$$

Thus, the adiabatic invariant is really (up to 2π factors) the area in the two dimensional sub-phase space bounded by the (Q^a, P_a) orbit. If we treat this J_a as our G_a from before, we need to identify its canonically conjugate coordinate (as G_a we treated as our new canonical momentum after canonical transformation). Call θ^a the coordinate for which J_a is its canonical momentum. Then, $(Q^a, P_a) \rightarrow (\theta^a, J_a)$ is to be a time independent canonical transformation. Using 1.8, we can identify a type-2 generating function $F_2(Q, J)$ for this transformation. The generating function conditions are:

$$P_a = -\frac{\partial F_2}{\partial Q^a}, \quad \theta^a = -\frac{\partial F_2}{\partial J_a}. \quad (1.14.19)$$

Integrating this first condition gives (as an indefinite integral):

$$F_2(Q, J) = - \int_J P_a dQ^a. \quad (1.14.20)$$

The subscript on the integrand is to indicate that this integral is done at constant J . Because J being constant labels the actual motion taken by Q^a and P_a this is equivalently an integral done over a incomplete piece of the trajectory in phase space (incomplete in the sense of not necessarily being a full period for any of the coordinate pairs). Therefore, this is precisely the same integral one would get from integrating the momentum Hamilton-Jacobi condition in equation (1.14.11) (up to a minus sign). So, for this canonical transformation we can simply take:

$$F_2(Q, J) = - \sum_{a=1}^N S_a(Q^a). \quad (1.14.21)$$

$$\implies P_a = \frac{\partial S_a}{\partial Q^a}, \quad \theta^a = \frac{\partial S_a}{\partial J_a}. \quad (1.14.22)$$

Thus in order to find the canonical coordinate θ^a to which J_a is conjugate, one needs to complete the indefinite integral in equation (1.14.20) and then the partial derivative in equation (1.14.19). The combination of these gives:

$$\theta^a = \frac{\partial}{\partial J_a} \int_J P_b dQ^b. \quad (1.14.23)$$

After the canonical transformation, our Hamiltonian will be a function only of the adiabatic invariants, $\mathcal{H} = \mathcal{H}(J)$, and so:

$$\frac{d\theta^a}{dt} = \frac{\partial \mathcal{H}}{\partial J_a} \stackrel{\text{def}}{=} \omega^a = \text{Constant} \implies \theta^a(t) = \omega^a t + \theta^a(0). \quad (1.14.24)$$

Thus, $\theta^a(t)$ is a linear function of time. However, the motion is periodic in the (Q^a, P_a) phase space and so because they are periodic in t they must also be periodic in θ^a as θ^a is simply linear in t . Let $\Delta\theta^a$ be their period in θ^a :

$$Q^a(\theta^a + \Delta\theta^a, J_a) = Q^a(\theta^a, J_a) \quad (1.14.25)$$

$$P_a(\theta^a + \Delta\theta^a, J_a) = P_a(\theta^a, J_a). \quad (1.14.26)$$

The area element in phase space is preserved by canonical transformation:

$$d\theta^a dJ_a = \det \begin{pmatrix} \frac{\partial \theta^a}{\partial Q^a} & \frac{\partial \theta^a}{\partial P_a} \\ \frac{\partial J_a}{\partial Q^a} & \frac{\partial J_a}{\partial P_a} \end{pmatrix} dQ^a dP_a = \left(\frac{\partial \theta^a}{\partial Q^a} \frac{\partial J_a}{\partial P_a} - \frac{\partial \theta^a}{\partial P_a} \frac{\partial J_a}{\partial Q^a} \right) dQ^a dP_a \quad (1.14.27)$$

$$= \{\theta^a, J_a\} dQ^a dP_a = 1 dQ^a dP_a = dQ^a dP_a. \quad (1.14.28)$$

Then, the area integral in θ^a and J_a is automatically:

$$\mathbb{A}_a = \int dQ^a dP_a = \int d\theta^a dJ_a = \Delta\theta^a J_a = \Delta\theta^a \frac{\mathbb{A}_a}{2\pi} \quad (1.14.29)$$

$$\implies \Delta\theta^a = 2\pi. \quad (1.14.30)$$

Thus, Q^a and P_a are 2π periodic in θ and so we identify θ^a as a sort of angle in phase space. As well, from the definition of J_a , we can see that $2\pi J_a$ is the increase in the S_a component of the action over a full period of the orbit. Consequently, θ^a and J_a are called **Action-Angle variables** or also Angle-Area variables. Knowing now that the phase space is 2π periodic in θ , we have that θ^a must change by 2π over the course of a single period τ_a of the orbit:

$$\theta^a(t + \tau_a) = \theta^a + 2\pi \implies \omega^a t + \omega^a \tau_a + \theta^a(0) = \omega^a t + \theta^a(0) \implies \tau_a = \frac{2\pi}{\omega^a}. \quad (1.14.31)$$

Because of this, we can identify ω^a as the angular frequency of the motion and we can recover the period directly from the Hamiltonian as:

$$\omega^a = \frac{2\pi}{\tau_a} = \frac{\partial \mathcal{H}}{\partial J_a}. \quad (1.14.32)$$

The adiabatic invariants J_a are particularly physically important if we have a Hamiltonian which depends on some parameter λ which varies slowly in time. By “slowly” we mean that the change in λ over the course of one period of the motion is small compared to λ (small with respect to our experimental resolution). This is known as the adiabatic approximation. In the adiabatic approximation, we treat λ as essentially constant over a single period of the motion. Then, because the adiabatic invariants are defined over a full period of the motion and λ is to be treated as constant in that time interval, in the adiabatic approximation the adiabatic invariants J_a are approximately constant (which is why they are called adiabatic invariants). For the moment let us refrain from actually making any such approximation. For a fixed value of λ , there is some path followed by the coordinate Q^a and along that path we define the adiabatic invariant exactly as before. That path will of course depend on the value of λ . As well, that path was specified by the value of J_a which by being a conserved quantity on phase space (at least when λ is constant) is some function of Q^a , P_a , and λ (which is constant along the path of integration). So, the definition of the adiabatic invariant at fixed λ defines it as a function of Q^a , P_a , and λ :

$$\mathcal{H} = \mathcal{H}(Q, P; \lambda) \implies J_a|_{\lambda} = \frac{1}{2\pi} \oint_{\lambda \text{ constant}} P_a dQ^a = J_a(Q^a, P_a, \lambda) \quad (1.14.33)$$

where Q^a and P_a are any values of those two variables at the same point along the path of integration. As well, the angle variable θ^a by being the canonical coordinate for which J_a is the canonical momentum is also related to Q^a and P_a in a λ dependent way. That is:

$$\theta^a = \theta^a(Q^a, P_a, \lambda). \quad (1.14.34)$$

When λ is constant, the relationship between Q^a, P_a and θ^a, J_a is a time independent canonical transformation. When λ is time dependent this is still a canonical transformation but now it is only time preserving as described in 1.9. Thus, there still is some generating function of this transformation. In fact the derivatives from before in equation (1.14.19) are unchanged. All that is different is that now F_2 depends on time because the transformation does. Then, the new Hamiltonian is given by using the results of 1.9 with a time dependent generating function:

$$\mathcal{H}' = \mathcal{H} - \frac{\partial F_2}{\partial t} = \mathcal{H} + \sum_{a=1}^N \frac{\partial S_a}{\partial t} = \mathcal{H} + \sum_{a=1}^N \frac{\partial S_a}{\partial \lambda} \dot{\lambda}. \quad (1.14.35)$$

The new Hamiltonian needs to be expressed completely in terms of θ^a and J_a so let Λ be defined by:

$$\Lambda(\theta, J, \lambda) = \sum_{a=1}^N \frac{\partial S_a}{\partial \lambda} \quad (1.14.36)$$

expressed in terms of the new variables. Then our Hamiltonian after canonical transformation is:

$$\mathcal{H}'(\theta, J, \lambda) = \mathcal{H}(J, \lambda) + \Lambda(\theta, J, \lambda) \dot{\lambda} \quad (1.14.37)$$

and so our equations of motion are:

$$\frac{d\theta^a}{dt} = \frac{\partial \mathcal{H}'}{\partial J_a} = \frac{\partial \mathcal{H}}{\partial J_a} + \frac{\partial \Lambda}{\partial J_a} \dot{\lambda} = \omega_a + \frac{\partial \Lambda}{\partial J_a} \dot{\lambda} \quad (1.14.38)$$

$$\frac{dJ_a}{dt} = -\frac{\partial \mathcal{H}'}{\partial \theta^a} = -\frac{\partial \Lambda}{\partial \theta^a} \dot{\lambda}. \quad (1.14.39)$$

These equations of motion are exact so far. We can see that the adiabatic invariant only evolves due

to angular dependence of Λ at a rate proportional to $\dot{\lambda}$ and the angle coordinate evolves due to its period averaged angular frequency ω^a defined before plus a contribution proportional to $\dot{\lambda}$. Now let us make the adiabatic approximation and look at how much J_a changes over a single period of θ^a (that is θ^a incrementing by 2π). Exactly:

$$\Delta_1 J_a \stackrel{\text{def}}{=} \int_{t_0}^{t_f} \frac{dJ_a}{dt} dt = - \int_{t_0}^{t_f} \frac{\partial \Lambda}{\partial \theta^a} \dot{\lambda} dt. \quad (1.14.40)$$

We can rewrite the time integral as an integral over θ^a by making a change of variables and using the θ^a equation of motion:

$$\Delta_1 J_a = - \int_0^{2\pi} \frac{\partial \Lambda}{\partial \theta^a} \dot{\lambda} \frac{dt}{d\theta^a} d\theta^a = - \int_0^{2\pi} \frac{\partial \Lambda}{\partial \theta^a} \dot{\lambda} \frac{d\theta^a}{\dot{\theta}^a} \quad (1.14.41)$$

$$= - \int_0^{2\pi} \frac{\partial \Lambda}{\partial \theta^a} \dot{\lambda} \frac{1}{\omega^a + \frac{\partial \Lambda}{\partial J_a} \dot{\lambda}} d\theta^a. \quad (1.14.42)$$

In the adiabatic approximation $\dot{\lambda}$ is essentially constant over one period of the motion and is considered to be small. Thus:

$$\Delta_1 J_a = -\dot{\lambda} \int_0^{2\pi} \frac{\partial \Lambda}{\partial \theta^a} \frac{1}{\omega^a} d\theta^a + \mathcal{O}(\dot{\lambda}^2). \quad (1.14.43)$$

When λ was constant, ω^a was as well and therefore $\dot{\omega}^a = \mathcal{O}(\dot{\lambda})$. Thus:

$$\Delta_1 J_a = -\frac{\dot{\lambda}}{\omega^a} \int_0^{2\pi} \frac{\partial \Lambda}{\partial \theta^a} d\theta^a + \mathcal{O}(\dot{\lambda}^2) = -\frac{\dot{\lambda}}{\omega^a} (\Lambda(\theta + 2\pi, J, \lambda) - \Lambda(0, J, \lambda)) + \mathcal{O}(\dot{\lambda}^2). \quad (1.14.44)$$

Because the Hamiltonian is automatically a 2π periodic function of θ^a (as Q^a and P^a were so), Λ is 2π periodic in θ^a and so this difference is 0 giving:

$$\Delta_1 J_a = \mathcal{O}(\dot{\lambda}^2). \quad (1.14.45)$$

Thus, the change in the adiabatic invariant over the course of one period of the motion is suppressed by one higher power of $\dot{\lambda}$ than it had to be (a generic conserved quantity when λ is made time dependent would change as $\mathcal{O}(\dot{\lambda})$, such as the Hamiltonian). If we now define T as the characteristic time scale for the variation of λ by the time it would take λ to change its value by its initial amount:

$$\lambda = T\dot{\lambda} \implies T = \frac{\lambda}{\dot{\lambda}} \quad (1.14.46)$$

and we recall the natural period of the motion τ_a from before, we can exchange powers of $\dot{\lambda}$ for inverse powers of T and write our statement about the adiabatic invariant's time evolution over one period in a unitless way as:

$$\frac{\Delta_1 J_a}{J_a} = \mathcal{O}\left(\frac{\tau_a^2}{T^2}\right). \quad (1.14.47)$$

Then, if we look at how much the adiabatic invariant changes over the time interval T , that time interval is given by $\frac{T}{\tau_a}$ periods of the motion and so the order of the change in so many periods is given by multiplying the change in a single period by $\frac{T}{\tau_a}$:

$$\frac{\Delta J_a}{J_a} = \mathcal{O}\left(\frac{T}{\tau_a} \frac{\Delta_1 J_a}{J_a}\right) = \mathcal{O}\left(\frac{\tau_a}{T}\right). \quad (1.14.48)$$

So, if $\dot{\lambda}$ varies slowly compared to the period of our underlying motion then even on time scales so long that λ may change significantly the adiabatic invariant will only change by a small amount (it is suppressed by the ratio of time scales by an extra power than one would naively expect). This is why the adiabatic invariant is named how it is. Under adiabatic changes it is for all intents and purposes invariant, constant. Experimentally this property of the adiabatic invariants is very meaningful as many systems of interest have fast moving periodic parts compared to slower moving experimental probes. So, the effect of interacting with a system to measure it can be treated as an adiabatic perturbation of the system (meaning making some parameter of the system to be studied adiabatically time dependent) and the properties of that system which are stable under doing so are precisely its adiabatic invariants. These are the quantities we expect to be meaningfully measurable in experiment. (Quantities which are not adiabatically stable are prone to much faster changes than the experimental probe is capable to registering, resulting in noisy fluctuating

measurements.) Much has been studied about the behavior of the action variables after long times; more detailed and precise statements about their behavior can be made using Kolmogorov-Arnold-Misner (KAM) theory, but this is far beyond our scope and my expertise.

All of these results together give us:

Theorem 1.13: Adiabatic Invariance Theorem.

A Hamiltonian system with time independent Hamiltonian $\mathcal{H}(Q, P)$ on a $2N$ dimensional phase space is said to be integrable when it has N conserved quantities $G_a(Q, P)$ which cannot be written in terms of each other and which all have vanishing Poisson brackets with each other. Integrability is equivalent to the existence of a coordinate system (Q, P) for this system in which it is possible to solve the Hamilton-Jacobi equation with a “separated” solution of the form:

$$S(t, Q) = \sum_{a=1}^N S_a(Q^a) - Et. \quad (1.14.49)$$

If we have such an integrable system and the surfaces in phase space of constant energy of that system are closed and bounded then in those coordinates (Q, P) in which the Hamilton-Jacobi equation is separable, each pair of coordinates will follow its own periodic orbit with some period τ_a and which encloses an area $\mathbb{A}_a$ in the two dimensional sub-phase space (Q^a, P_a) . Then, we can define the new canonical coordinates called action-angle coordinates (θ, J) by for each pair Q^a, P_a defining the adiabatic invariant J_a as:

$$J_a = \frac{1}{2\pi} \oint P_a dQ^a = \frac{\mathbb{A}_a}{2\pi} \quad (1.14.50)$$

where this integral is taken over one period of the motion of that pair and then using the type-2 generating function $F_2(Q, J)$:

$$F_2(Q, J) = \int_J P_a dQ^a \quad (1.14.51)$$

where this integral is an indefinite integral taken along the path of the motion and so at fixed J (because each J_a is a conserved quantity). The phase space angle θ^a and old momentum P_a can be recovered by:

$$\theta^a = -\frac{\partial F_2}{\partial J_a}, \quad P_a = -\frac{\partial F_2}{\partial Q^a}. \quad (1.14.52)$$

In these coordinates, the Hamiltonian is simply a function of the J 's only: $\mathcal{H} = \mathcal{H}(J)$. Consequently, J_a is constant and $\theta^a(t) = \omega^a t + \theta^a(0)$ where the angular frequency ω^a is related to the period τ_a and Hamiltonian by:

$$\omega^a = \frac{2\pi}{\tau_a} = \frac{\partial \mathcal{H}}{\partial J_a}. \quad (1.14.53)$$

If an integrable system is perturbed by an external effect so that its Hamiltonian develops an explicit time dependence where T , the time scale on which that time dependence has an experimentally noticeable effect, is much larger than the natural periods τ_a of the system, then while the adiabatic invariants are no longer exactly conserved, the percent change in the adiabatic invariants after a time T is suppressed by an extra power of $\frac{\tau_a}{T}$ than a generic quantity would be:

$$\frac{\Delta J_a}{J_a} = \mathcal{O}\left(\frac{\tau_a}{T}\right). \quad (1.14.54)$$

Consequently, when a quickly evolving system is probed experimentally its adiabatic invariants are precisely the quantities which are stable enough in time to measure the values of without being overwhelmed by quick noisy fluctuations.

Exercises

Problem 1.37: Practicing separation of variables. For the Hamiltonian $\mathcal{H}(r, \varphi, p_r, p_\varphi) = \frac{p_r^2}{2m} + \frac{p_\varphi^2}{2mr^2}$ where m is a constant:

- (a) Write down the Hamilton-Jacobi equation for this system and show that it admits separable solutions:

$$S = S_r(r) + S_\varphi(\varphi) - Et.$$

Determine S_r and S_φ . Here φ is an angular variable so take all quantities to be 2π periodic in it.

- (b) Show that the corresponding Lagrangian to the above Hamiltonian is:

$$\mathcal{L} = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\varphi}^2.$$

- (c) Let $x = r \cos \varphi$ and $y = r \sin \varphi$ be new configuration coordinates. Show that the Lagrangian in these coordinates is:

$$\mathcal{L} = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2).$$

As well, show that in these coordinates the Hamiltonian becomes:

$$\mathcal{H} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m}.$$

- (d) Write down the Hamilton-Jacobi equation for this system in the (x, y) coordinates and show that it is also separable. Find those separated solutions and notice how much easier it is in these coordinates.
- (e) Let $u = xy$ and $v = \frac{y}{x}$ be new configuration coordinates. Find the Lagrangian and Hamiltonian in these coordinates and show that the Hamilton-Jacobi equation is not separable in these coordinates.

Problem 1.38: Stiffening oscillator. For the Hamiltonian $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2$:

- (a) Write down the Hamilton-Jacobi equation and show that it admits separable solutions:

$$S = S_x(x) - Et.$$

Solve the Hamilton-Jacobi equation and determine S_x . Explain how this system is integrable with the G conserved quantity identified with E .

- (b) Compute the adiabatic invariant J of this system and determine the canonical transformation which relates (x, p) and (θ, J) .
- (c) Find the equations of motion for θ and J if the parameter k is made time dependent.
- (d) Let the amplitude A be the maximum value attained by x during one period. If the parameter k varies slowly compared to the natural period of this oscillator, how does A depend on time?

1.15 (2nd Pass) The Theorem of Normal Modes

In multiple different contexts it will be useful for us to study systems which are close by to a linearly stable equilibrium state. Suppose our phase space has dimension $2d$ so that there are coordinates $Q^1, \dots, Q^d$ and canonical momenta $P_1, \dots, P_d$. Let the equilibrium position of the system in phase space be called (q, p) . (Here $q^1, \dots, q^d, p_1, \dots, p_d$ are constants.) By equilibrium position we mean that if the system starts at that point then it stays at that point for all time. Let $\epsilon > 0$ be called the “allowed deviation” from equilibrium. An equilibrium is called stable if for every ϵ there is a ball of nonzero radius (let that radius be called δ) around the equilibrium so that if we start in that ball we stay within a distance ϵ of the equilibrium for all time. That is, a stable equilibrium is one where if we start sufficiently close (within a distance δ) to it then we will remain close to it (within a distance ϵ) for all time. An equilibrium is linearly stable if the stability holds for the linearly approximated equations of motion near equilibrium²⁶. For simplicity, we will assume for this section that the Hamiltonian has no explicit dependence on time. Then, if we Taylor expand the Hamiltonian near equilibrium we have:

$$\begin{aligned} \mathcal{H}(Q, P) = & \mathcal{H}(q, p) + \frac{\partial \mathcal{H}}{\partial q^a}(q, p)(Q^a - q^a) + \frac{\partial \mathcal{H}}{\partial p_a}(P_a - p_a) + \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial q^a \partial q^b}(q, p)(Q^a - q^a)(Q^b - q^b) \\ & + \frac{\partial^2 \mathcal{H}}{\partial p_a \partial q^b}(q, p)(P_a - p_a)(Q^b - q^b) + \frac{1}{2} \frac{\partial^2 \mathcal{H}}{\partial p_a \partial p_b}(q, p)(P_a - p_a)(P_b - p_b) + \text{Higher Order Terms.} \end{aligned} \quad (1.15.1)$$

The constant $\mathcal{H}(q, p)$ does not affect the equations of motion and can be removed by gauge transformation through the surface term $f(t, Q) = \mathcal{H}(q, p)t$. Thus, we can equivalently just set $\mathcal{H}(q, p) = 0$ by definition. Let us now apply the condition that (q, p) should be an equilibrium of the system. By the definition of equilibrium, if the system is started at (q, p) it will stay there for all time. Thus, the time derivatives of Q and P should vanish when at (q, p) :

$$\left. \frac{dQ^a}{dt} \right|_{(Q, P)=(q, p)} = \frac{\partial \mathcal{H}}{\partial p_a}(q, p) \stackrel{!}{=} 0 \quad (1.15.2)$$

$$\left. \frac{dP_a}{dt} \right|_{(Q, P)=(q, p)} = -\frac{\partial \mathcal{H}}{\partial q^a}(q, p) \stackrel{!}{=} 0. \quad (1.15.3)$$

Thus the linear terms in the Hamiltonian must be 0 due to the equilibrium condition.

The quadratic terms in the Hamiltonian can be written more nicely too. Define the matrices $\hat{K}$, $\hat{\Gamma}$, and $\hat{W}$ with components:

$$K_{ab} = \frac{\partial^2 \mathcal{H}(q, p)}{\partial q^a \partial q^b}, \quad \Gamma^a_b = \frac{\partial^2 \mathcal{H}(q, p)}{\partial p_a \partial q^b}, \quad W^{ab} = \frac{\partial^2 \mathcal{H}(q, p)}{\partial p_a \partial p_b}. \quad (1.15.4)$$

From their definitions, the matrices $\hat{K}$ and $\hat{W}$ are symmetric:

$$K_{ba} = \frac{\partial^2 \mathcal{H}}{\partial q^a \partial q^b} \Big|_{(q, p)} = K_{ab} \implies \hat{K}^T = \hat{K} \quad (1.15.5)$$

$$W^{ba} = \frac{\partial^2 \mathcal{H}}{\partial p_a \partial p_b} \Big|_{(q, p)} = W^{ab} \implies \hat{W}^T = \hat{W}. \quad (1.15.6)$$

As well, we perform the canonical transformation $Q'^a = Q^a - q^a$, $P'_a = P_a - p_a$, $t' = t$, $\mathcal{H}' = \mathcal{H}$ so that in the new coordinates the equilibrium point is the origin by definition. We will assume going forward that the coordinates we write are these transformed coordinates. With all of these simplifications, the Hamiltonian becomes:

$$\mathcal{H} = \frac{1}{2} K_{ab} Q^a Q^b + \Gamma^a_b P_a Q^b + \frac{1}{2} W^{ab} P_a P_b + \text{H.O.T.} \quad (1.15.7)$$

$$\implies \dot{Q}^a = \frac{\partial \mathcal{H}}{\partial P_a} = W^{ab} P_b + \Gamma^a_b Q^b + \text{H.O.T.}, \quad \dot{P}_a = -\frac{\partial \mathcal{H}}{\partial Q^a} = -K_{ab} Q^b - \Gamma^b_a P_b + \text{H.O.T.} \quad (1.15.8)$$

²⁶Linear stability is generally safe to assume given stability for physics. Stability can only occur when linear stability fails for delicately chosen linearized equations of motion and unless there is a particular symmetry in the system which forces such a choice, we won't encounter this scenario. The reason this is safe is because if a system is stable but not linearly stable then there is an alternate system with equations of motion arbitrarily close to being the same as the original system which is both stable and linearly stable. Because we don't know exact equations of motion, it is safe to use these arbitrarily close equations of motion which are linearly stable unless there is a symmetry we believe in that prevents that modification from being possible.

Let Q and P be the vectors with components Q^a and P_a . Then, the Hamiltonian and equations of motion can be written:

$$\mathcal{H} = \frac{1}{2}Q^T \hat{K} Q + Q^T \hat{\Gamma} P + \frac{1}{2}P^T \hat{W} P + \text{H.O.T.} = \frac{1}{2} \begin{pmatrix} Q^T & P^T \end{pmatrix} \begin{pmatrix} \hat{K} & \hat{\Gamma} \\ \hat{\Gamma}^T & \hat{W} \end{pmatrix} \begin{pmatrix} Q \\ P \end{pmatrix} + \text{H.O.T.} \quad (1.15.9)$$

$$\implies \dot{Q} = \hat{W} P + \hat{\Gamma} Q + \text{H.O.T.}, \quad \dot{P} = -\hat{K} Q - \hat{\Gamma}^T P + \text{H.O.T.} \quad (1.15.10)$$

In our Φ notation from (1.9.61),

$$\Phi = \begin{pmatrix} Q \\ P \end{pmatrix}, \quad \hat{G} = \begin{pmatrix} \hat{K} & \hat{\Gamma} \\ \hat{\Gamma}^T & \hat{W} \end{pmatrix} = \hat{G}^T \quad (1.15.11)$$

$$\implies \mathcal{H} = \frac{1}{2}\Phi^T \hat{G} \Phi + \text{H.O.T.}, \quad \frac{d\Phi}{dt} = -\mathbb{J} \hat{G} \Phi + \text{H.O.T.} \quad (1.15.12)$$

1.15.1 Linear Stability Analysis

We have not yet used the condition that the equilibrium should be linearly stable. Linear stability requires that if one approximates the system near equilibrium by Taylor expanding the equations of motion then the associated linear system is stable. Here we see that the associated linear system to our generic Hamiltonian near equilibrium is:

$$\frac{d\Phi}{dt} = -\mathbb{J} \hat{G} \Phi \quad (1.15.13)$$

and linear stability requires that this be stable around the origin. Before applying linear stability directly to this equation of motion it is useful to study linear stability in general.

Suppose we have a dynamical system with coordinates $\vec{x}(t) = (x_1, \dots, x_d) \in \mathbb{R}^N$ and equations of motion:

$$\frac{d\vec{x}}{dt} = \hat{M} \vec{x} \quad (1.15.14)$$

for some constant matrix $\hat{M}$. We would like to understand the stability of this system for a given $\hat{M}$. Using an invertible matrix $\hat{C}$ we can define new coordinates $\vec{x}'(t) = (x'_1, \dots, x'_d)$ by:

$$\vec{x}' = \hat{C} \vec{x}. \quad (1.15.15)$$

Then, $\vec{x}'$ has the equations of motion:

$$\frac{d\vec{x}'}{dt} = \hat{C} \hat{M} \hat{C}^{-1} \vec{x}' = \hat{M}' \vec{x}' \quad (1.15.16)$$

where we have defined $\hat{M}' = \hat{C} \hat{M} \hat{C}^{-1}$. This type of transformation is called a change of basis.

It is a theorem of linear algebra [30] that through a change of basis any square matrix can be brought into Jordan Normal Form. In Jordan Normal Form, using block matrix notation, a matrix by definition takes the form:

$$\hat{C} \hat{M} \hat{C}^{-1} = \text{diag}(\hat{j}_1, \dots, \hat{j}_K) \quad (1.15.17)$$

where here $\text{diag}(\hat{j}_1, \dots, \hat{j}_K)$ means a diagonal block matrix with the matrices $\hat{j}_1, \dots, \hat{j}_K$ appearing along its diagonal and each $\hat{j}_k$ matrix is a Jordan Block. A Jordan Block by definition has components:

$$(\hat{j}_k)_a^b = \lambda_k \delta_a^b + \delta_{a+1}^b. \quad (1.15.18)$$

That is, it has some constant (potentially complex) λ_k (called its eigenvalue) down its diagonal, 1's entered along the "superdiagonal" of entries directly to the right of the diagonal, and 0's everywhere else. The different Jordan Blocks will generally be of different sizes and a matrix is diagonalizable if and only if its Jordan Blocks all have size 1x1.

Suppose we have performed a change of basis so that $\hat{M}'$ is in Jordan Normal Form. Then, because of the block diagonal structure of $\hat{M}'$, two coordinates in $\vec{x}'$ which correspond to different Jordan Blocks have equations of motion which don't depend on each other. That is, in Jordan Normal Form the coordinates from different Jordan Blocks don't interact. For each Jordan Block then we can define an independent dynamical system. Further it immediately follows that the total system is stable if and only if each of these independent systems are stable. Suppose we consider a Jordan Block of size $s \times s$ with eigenvalue λ and call the components of $\vec{x}'$ corresponding to this block $y_1, \dots, y_s$. Then, these $y_k(t)$ satisfy the equations of motion:

$$\frac{dy_a}{dt} = (\hat{j})_a^b y_b \implies \frac{dy_a}{dt} = \lambda y_a + y_{a+1} \quad (1 \leq a < s), \quad \frac{dy_s}{dt} = \lambda y_s. \quad (1.15.19)$$

These equations of motion can be simplified by defining:

$$z_a(t) = e^{-\lambda t} y_a(t) \quad (1.15.20)$$

$$\implies \frac{dz_a}{dt} = z_{a+1} \quad (1 \leq a < s), \quad \frac{dz_s}{dt} = 0. \quad (1.15.21)$$

Because $\dot{z}_s$ is 0, z_s is a constant. Then, $\dot{z}_{s-1} = z_s$ and so z_{s-1} is linear in time. Continuing iteratively, z_k is a polynomial of degree $s - k$ in time. Consequently, we have that for some constant vectors $\vec{\xi}_0, \dots, \vec{\xi}_{s-1}$:

$$\vec{y}(t) = e^{\lambda t} \left(\vec{\xi}_0 + t\vec{\xi}_1 + \dots + t^{s-1}\vec{\xi}_{s-1} \right). \quad (1.15.22)$$

If λ has negative real part then this function remains bounded for all $t > 0$ and decays to 0 with large t , thus giving stability. If λ has positive real part then this function grows exponentially, thus giving instability. If λ has real part 0 then the resulting imaginary exponential can be written as real sines and cosines. If λ has real part 0 and $s > 1$, these oscillations are multiplied by a nonconstant polynomial. Consequently, $\vec{y}(t)$ grows in magnitude with sufficiently long time (as any polynomial goes to $\pm\infty$ at large time), thus giving instability. If λ has real part 0 and $s = 1$ then the result is purely oscillatory and does not grow with time, thus giving stability.

So, our linear dynamical system is stable if and only if for each Jordan Block of the matrix $\hat{M}$ with size bigger than 1x1 the eigenvalue of that Jordan Block has real part less than zero and for each Jordan Block of the matrix $\hat{M}$ with size equal to 1x1 the eigenvalue of that Jordan Block has real part less than or equal to zero.

1.15.2 Hamiltonian Diagonalization

Returning to our Hamiltonian system, linear stability requires that:

$$\frac{d\Phi}{dt} = -\mathbb{J}\hat{G}\Phi = \hat{M}\Phi \quad (1.15.23)$$

be stable where we have defined $\hat{M} = -\mathbb{J}\hat{G}$ to keep the form of our previous notation. Again from linear algebra, the eigenvalues of $\hat{M}$ which appear in the Jordan Normal Form are precisely those λ which are the roots of the characteristic polynomial:

$$\wp(\lambda) = \det(-\mathbb{J}\hat{G} - \lambda\mathbb{1}) \quad (1.15.24)$$

$$\wp(\lambda) = 0 \iff \lambda \text{ an eigenvalue of } -\mathbb{J}\hat{G}. \quad (1.15.25)$$

The structure of Hamilton's equations imply that $\wp(\lambda)$ is an even function of λ . We can see this by using that $\hat{G}$ is symmetric, $\mathbb{J}$ is antisymmetric, $\mathbb{J}^2 = -1$, $\det \mathbb{J} = 1$, the determinant of a product is the product of determinants, and that the determinant of a matrix transpose is the same as the determinant of that matrix:

$$\wp(-\lambda) = \det(-\mathbb{J}\hat{G} + \lambda\mathbb{1}) = \det(-\hat{G}^T \mathbb{J}^T + \lambda\mathbb{1}^T) = \det(\hat{G}\mathbb{J} + \lambda\mathbb{1}) \quad (1.15.26)$$

$$= \det(-\mathbb{J}\hat{G}\mathbb{J} - \lambda\mathbb{J}\mathbb{J}) = \det(\mathbb{J}(-\mathbb{J}\hat{G} - \lambda\mathbb{1})\mathbb{J}) = \det(\mathbb{J})^2 \det(-\mathbb{J}\hat{G} - \lambda\mathbb{1}) = \wp(\lambda). \quad (1.15.27)$$

Therefore, if λ_1 is an eigenvalue of $-\mathbb{J}\hat{G}$ (meaning $\wp(\lambda_1) = 0$) then $-\lambda_1$ is also an eigenvalue of $-\mathbb{J}\hat{G}$. By stability, $-\mathbb{J}\hat{G}$ must have no eigenvalues with positive real part. But, if it has any eigenvalue with negative real part then the negative of that eigenvalue is also an eigenvalue but with positive real part. So, $-\mathbb{J}\hat{G}$ must have no eigenvalues with negative real part either. Together then all of the eigenvalues of $-\mathbb{J}\hat{G}$ must have real part of 0 (they are purely imaginary). Stability then requires that all of the Jordan Blocks of $-\mathbb{J}\hat{G}$ have size 1x1. Therefore, stability requires $-\mathbb{J}\hat{G}$ to be diagonalizable.

Because $-\mathbb{J}\hat{G}$ is diagonalizable, $(\mathbb{J}\hat{G})^2$ is diagonalizable. It is a theorem [21] of linear algebra that if $(\mathbb{J}\hat{G})^2$ is diagonalizable for a symmetric matrix $\hat{G}$ then there exists a symplectic matrix $\hat{S}$ so that $\hat{S}^T \hat{G} \hat{S}$ is diagonal. Let $\hat{S}$ be such a matrix and $\hat{D}$ be the corresponding diagonal matrix:

$$\hat{D} = \hat{S}^T \hat{G} \hat{S} = \text{diag}(a_1, \dots, a_d, b_1, \dots, b_d) \quad (1.15.28)$$

for some constants $a_1, \dots, a_d, b_1, \dots, b_d$. If we now perform the linear time independent canonical transformation:

$$\begin{pmatrix} Q' \\ P' \end{pmatrix} = \hat{S}^{-1} \begin{pmatrix} Q \\ P \end{pmatrix}, \quad t' = t, \quad \mathcal{H}' = \mathcal{H} \quad (1.15.29)$$

we have:

$$\Phi'^T \hat{D} \Phi' = \Phi^T \hat{S}^{-T} \hat{S}^T \hat{G} \hat{S} \hat{S}^{-1} \Phi = \Phi^T \hat{G} \Phi \quad (1.15.30)$$

and so the Hamiltonian in this coordinates becomes:

$$\mathcal{H} = \frac{1}{2} \Phi'^T \hat{D} \Phi' = \sum_{k=1}^d \left(\frac{a_k}{2} Q_k'^2 + \frac{b_k}{2} P_k'^2 \right). \quad (1.15.31)$$

Now the equation of motion for each Q_k' is much simpler:

$$\frac{d^2 Q_k'}{dt^2} = \frac{d}{dt} \frac{\partial \mathcal{H}}{\partial P_k'} = \frac{d}{dt} (b_k P_k') = -b_k \frac{\partial \mathcal{H}}{\partial Q_k'} = -a_k b_k Q_k'. \quad (1.15.32)$$

If $a_k b_k < 0$, this equation of motion has linearly independent solutions $e^{\pm t \sqrt{|a_k b_k|}}$ which due to the growing exponential violate stability. If $a_k b_k = 0$, this equation of motion has solutions $A + Bt$ which due to the unbounded growth of t violate stability. Therefore, stability requires $a_k b_k > 0$ in which case this is just a harmonic oscillator. This gives the theorem of normal modes: near a linearly stable equilibrium every Hamiltonian system is equivalent to a system of noninteracting harmonic oscillators.

Formally:

Theorem 1.14: Normal Mode Decomposition

For a Hamiltonian system with time independent Hamiltonian on phase space of dimension $2d$ with a linearly stable equilibrium at location (q, p) , there exists a gauge in which the Hamiltonian near (q, p) can be written in the form:

$$\mathcal{H}(Q, P) = \frac{1}{2} \begin{pmatrix} (Q - q)^T & (P - p)^T \end{pmatrix} \hat{G} \begin{pmatrix} Q - q \\ P - p \end{pmatrix} + \text{Higher Order Terms} \quad (1.15.33)$$

where $\hat{G}$ is a symmetric matrix for which there exists a symplectic matrix $\hat{S}$ so that for some constants $a_1, \dots, a_d, b_1, \dots, b_d$ with $a_k b_k > 0$:

$$\hat{S}^T \hat{G} \hat{S} = \text{diag}(a_1, \dots, a_d, b_1, \dots, b_d). \quad (1.15.34)$$

The time independent canonical transformation:

$$\begin{pmatrix} Q' \\ P' \end{pmatrix} = \hat{S}^{-1} \begin{pmatrix} Q - q \\ P - p \end{pmatrix}, \quad t' = t, \quad \mathcal{H}' = \mathcal{H} \quad (1.15.35)$$

explicitly transforms this system into d noninteracting simple harmonic oscillators:

$$\mathcal{H}'(Q', P') = \sum_{k=1}^d \left(\frac{a_k}{2} Q_k'^2 + \frac{b_k}{2} P_k'^2 \right) + \text{H.O.T.} \quad (1.15.36)$$

Thus, near a linearly stable equilibrium any Hamiltonian system is equivalent to a system of noninteracting harmonic oscillators. The pairs (Q_k', P_k') for each k are called the “normal modes” of the system.

1.16 (2nd Pass) General Coordinates on Phase Space

We have always formulated our equations of motion and variational principles using canonically conjugate coordinates Q^a and P_a , however there is no obstruction to using other coordinates, it just requires a little more effort in a couple places. Let $\Phi = (Q, P)$ be the list of all our coordinates when we are using canonically conjugate pairs. When we write the action, the integrand is $P_a \dot{Q}^a - \mathcal{H}$, which we integrate over time. So, we would like to understand how to nicely express $P_a dQ^a$ in general coordinates. The stationarity of the action is coordinate invariant, and so it is the easiest avenue for generalizing to arbitrary coordinates. We can express the combination $P_a dQ^a$ as:

$$P_a dQ^a = \begin{pmatrix} P & 0 \end{pmatrix} \begin{pmatrix} dQ \\ dP \end{pmatrix} = \theta_a d\Phi^a = \theta^T d\Phi \quad (1.16.1)$$

where we have defined the vector field on phase space θ by:

$$\theta = \begin{pmatrix} P & 0 \end{pmatrix} \quad (1.16.2)$$

when we are using canonically conjugate coordinates. The requirement that δQ_f and δQ_0 are 0 when we vary the path in the action can then be stated as requiring $\theta^T \delta\Phi$ to vanish at the endpoints of the path. This θ is called the canonical 1 form or the symplectic potential. Notice that the “curl” of θ gives the components of the standard symplectic matrix $\mathbb{J}$ defined by (1.9.60):

$$\frac{\partial \theta_b}{\partial \Phi^a} - \frac{\partial \theta_a}{\partial \Phi^b} = \mathbb{J}_{ab}. \quad (1.16.3)$$

As well, notice that the inverse matrix to $\mathbb{J}$, which we write as $\mathbb{J}^{-1}$ and which happens to be equal to $-\mathbb{J}$ is related to the Poisson bracket by:

$$\{f(\Phi), g(\Phi)\} = (\mathbb{J}^{-1})^{ab} \frac{\partial f}{\partial \Phi^a} \frac{\partial g}{\partial \Phi^b}. \quad (1.16.4)$$

With all of this, we can write the action as:

$$S[\Phi] = \int_{t_0}^{t_f} \left(\theta_a \frac{d\Phi^a}{dt} - \mathcal{H}(t, \Phi) \right) dt \quad (1.16.5)$$

and define our variational principle by requiring the stationarity of S with respect to variations of Φ that satisfy $\theta^T \delta\Phi = 0$ at the endpoints.

Suppose we were to use general coordinates on the phase space as well as possibly a new time variable $t' = t(t, \Phi)$. That is, we define new coordinates $\Phi' = \Phi'(t, \Phi)$ by some smooth invertible function of the old coordinates. We will not require these coordinates to be canonical. Then, we will not require the Φ' to split into a list of Q ’s and a list of P ’s which together satisfy the canonical Poisson brackets. Because the stationarity of the action is a coordinate invariant statement, we can reexpress the action for the Φ variables in terms of the Φ' and then take appropriate variations with respect to Φ' . As well, we can add a surface term if we like. Therefore, the action for Φ' can be taken to be:

$$S'[\Phi'] = S[\Phi] + f(t_f, \Phi_f) - f(t_0, \Phi_0) = \int_{t_0}^{t_f} \left(\theta_a \dot{\Phi}^a - \mathcal{H}(t, \Phi) + \frac{df}{dt} \right) dt \quad (1.16.6)$$

where we need to rewrite the right hand side as an integral over t' in terms of Φ' and its derivatives. The differential $d\Phi$ is transformed by the chain rule as:

$$d\Phi'^a = \frac{\partial \Phi'^a}{\partial t} dt + \frac{\partial \Phi'^a}{\partial \Phi^b} d\Phi^b. \quad (1.16.7)$$

Define the inverse of the matrix $\frac{\partial \Phi'}{\partial \Phi}$ at fixed t as:

$$\left. \frac{\partial \Phi^a}{\partial \Phi'^c} \right|_t \frac{\partial \Phi'^c}{\partial \Phi^b} = \delta_b^a. \quad (1.16.8)$$

Then:

$$\frac{d\Phi^a}{dt} = \left. \frac{\partial \Phi^a}{\partial \Phi'^b} \right|_t \left(\frac{d\Phi'^b}{dt} - \frac{\partial \Phi'^b}{\partial t} \right). \quad (1.16.9)$$

With this, the action can be expressed as:

$$S'[\Phi'] = \int_{t_0}^{t_f} \left(\left(\theta_b + \frac{\partial f}{\partial \Phi^b} \right) \left. \frac{\partial \Phi^b}{\partial \Phi'^a} \right|_t \frac{d\Phi'^a}{dt} - \left(\mathcal{H}(t, \Phi) - \frac{\partial f}{\partial t} + \theta_b \left. \frac{\partial \Phi^b}{\partial \Phi'^a} \right|_t \frac{\partial \Phi'^a}{\partial t} \right) \right) dt. \quad (1.16.10)$$

Let $\sigma = 1$ if the transformation $t' = t'(t, \Phi)$ is not time reversing and let $\sigma = -1$ if it is time reversing (equivalently let $\sigma = \text{sgn}\left(\frac{dt'}{dt}\right)$). Then, we can rewrite the above as:

$$S'[\Phi'] = \int_{t'_0}^{t'_f} \left(\sigma \left(\theta_b + \frac{\partial f}{\partial \theta^b} \right) \frac{\partial \Phi^b}{\partial \Phi'^a} \Big|_t \dot{\Phi}'^a - \sigma \frac{dt}{dt'} \left(\mathcal{H}(t, \Phi) - \frac{\partial f}{\partial t} + \theta_b \frac{\partial \Phi^b}{\partial \Phi'^a} \Big|_t \frac{\partial \Phi'^a}{\partial t} \right) \right) dt'. \quad (1.16.11)$$

Expanding out the total time derivative:

$$\frac{dt}{dt'} = \frac{\partial t}{\partial t'} + \frac{\partial t}{\partial \Phi'^a} \dot{\Phi}'^a \quad (1.16.12)$$

and returning this to the action, we find that the action for Φ' can be written as:

$$S'[\Phi'] = \int_{t'_0}^{t'_f} \left(\theta'_a(t', \Phi') \dot{\Phi}'^a - \mathcal{H}'(t', \Phi') \right) dt' \quad (1.16.13)$$

where the transformed symplectic potential and transformed Hamiltonian are defined by:

$$\boxed{\begin{aligned} \theta'_b \frac{\partial \Phi'^b}{\partial \Phi'^a} - \mathcal{H}' \frac{\partial t'}{\partial \Phi'^a} &= \sigma \theta_a + \sigma \frac{\partial f}{\partial \Phi^a} \\ \theta'_a \frac{\partial \Phi'^a}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial t} &= -\sigma \mathcal{H} + \sigma \frac{\partial f}{\partial t} \end{aligned}} \quad (1.16.14)$$

$$\theta'_a \frac{\partial \Phi'^a}{\partial t} - \mathcal{H}' \frac{\partial t'}{\partial t} = -\sigma \mathcal{H} + \sigma \frac{\partial f}{\partial t} \quad (1.16.15)$$

Thus, the form (1.16.13) is actually a valid action for our canonical system in any coordinates, even non canonical ones and the above provides the general transformation properties of the symplectic potential and the Hamiltonian between any coordinates, even non canonical ones. Canonical transformations are precisely the transformations which keep the symplectic potential in the form of (1.16.2), but we don't have to only use canonical coordinates if we like. In order for the above variational principle to give well defined equations of motion for Φ' , we need the boundary term under variation to be 0 and therefore we must consider variations of the path so that:

$$\theta'_a \delta \Phi'^a|_{t'_f} = \theta'_a \delta \Phi'^a|_{t'_0} = 0. \quad (1.16.16)$$

For the rest of this section then we will allow our coordinates Φ to be non canonical. Consequently, θ will not be given by (1.16.2). Then, our variational principle in general is to use the action:

$$S[\Phi] = \int_{t_0}^{t_f} \left(\theta_a(t, \Phi) \dot{\Phi}^a - \mathcal{H}(t, \Phi) \right) dt \quad (1.16.17)$$

subject to variations of Φ which satisfy:

$$\theta_a \delta \Phi^a|_{t_f} = \theta_a \delta \Phi^a|_{t_0} = 0. \quad (1.16.18)$$

Taking such a variation, we have:

$$\delta S = \int_{t_0}^{t_f} \left(\left(\frac{\partial \theta_b}{\partial \Phi^a} - \frac{\partial \theta_a}{\partial \Phi^b} \right) \dot{\Phi}^b - \frac{\partial \mathcal{H}}{\partial \Phi^a} \right) \delta \Phi^a dt \stackrel{!}{=} 0 \quad (1.16.19)$$

$$\implies \left(\frac{\partial \theta_b}{\partial \Phi^a} - \frac{\partial \theta_a}{\partial \Phi^b} \right) \dot{\Phi}^b - \frac{\partial \mathcal{H}}{\partial \Phi^a} = 0. \quad (1.16.20)$$

Define the symplectic form ω_{ab} :

$$\omega_{ab} = \frac{\partial \theta_b}{\partial \Phi^a} - \frac{\partial \theta_a}{\partial \Phi^b}. \quad (1.16.21)$$

When the coordinates are canonical, $\omega_{ab} = \mathbb{J}_{ab}$. In general, it is an antisymmetric matrix dependent on (t, Φ) . In order for the equations of motion to be determined by the variational principle, that matrix must be invertible by a matrix ω^{-1} with components ω^{-ab} so that:

$$\omega^{-ac} \omega_{cb} = \delta_b^a \quad (1.16.22)$$

$$\implies \frac{d\Phi^a}{dt} = \omega^{-ab} \frac{\partial \mathcal{H}}{\partial \Phi^b}. \quad (1.16.23)$$

These are Hamilton's equations in general coordinates. When one starts with canonical coordinates and uses the transformation to general coordinates, ω_{ab} can be related to $\mathbb{J}_{ab}$ by directly computing the symplectic potential and differentiating. Then, the invertibility of ω is guaranteed. The invertibility of ω is equivalent to the ability to perform the Legendre transformation.

In terms of the general coordinates, we have that the Poisson bracket is then determined by Hamilton's equations:

$$\frac{df(\Phi)}{dt} = \{f, \mathcal{H}\} = \frac{\partial f}{\partial \Phi^a} \frac{d\Phi^a}{dt} = \omega^{-ab} \frac{\partial f}{\partial \Phi^a} \frac{\partial \mathcal{H}}{\partial \Phi^b} \quad (1.16.24)$$

$$\implies \boxed{\{f(\Phi), g(\Phi)\} = \omega^{-ab} \frac{\partial f}{\partial \Phi^a} \frac{\partial g}{\partial \Phi^b}} \quad (1.16.25)$$

Therefore, in order to use the canonical formalism in general non-canonical coordinates we simply need a symplectic potential $\theta_a(t, \Phi)$ so that ω_{ab} defined by (1.16.21) is an invertible matrix and a Hamiltonian $\mathcal{H}(t, \Phi)$. Then, Hamilton's equations are given by (1.16.23) from the variational principle (1.16.17) with boundary conditions (1.16.18) and Poisson bracket (1.16.25). The transformation properties of the symplectic potential and the Hamiltonian under a general change of coordinates are given by (1.16.14) and (1.16.15). The space of points Φ is called a symplectic manifold. These conditions guarantee that locally (meaning in the neighborhood of any point in phase space) we can transform to canonical coordinates but for general symplectic potentials it may not be possible to do so globally. This quickly gets into the mathematics of symplectic geometry, which is the study of symplectic manifolds. We will not go into any depth on this, but see [2] for details.

1.17 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 1.11: Poisson bracket properties** proves the existence of the Poisson representation of mechanics.
- **Problem 1.15: Introduction to the Dirac delta** gives basic properties of the Dirac delta which we will use often going forward.
- **Problem 1.16: The Harmonic Oscillator** introduces the most important system in physics and shows that it is not in general a minimum of its action.
- **Problem 1.28: Scaling properties** introduces dimensional analysis and determines the units of various mechanical quantities.
- **Problem 1.32: The adjoint representation** proves that all finite dimensional Lie algebras have a matrix representation and introduces the adjoint representation of Lie algebras which we will use often going forward.

We have developed the core mathematical tools which underlie physics. We have not yet developed any specific theory of physics, simply laid the groundwork on which all theories will sit. This is the role played by Analytical Mechanics. In summary, section 1.1 introduced us to the idea of equations of motion and how they are used to make all predictions in physics. 1.2 described the application of the scientific method to physics and introduced several essential concepts such as units, symmetry, and approximation. 1.3 introduced us to the formalism behind continuous transformations and culminated with defining a Lie bracket and explaining how it is used to write any continuous transformation. 1.4 arrived at the core equations of physics, Hamilton's equations, and the Poisson bracket. 1.5 introduced functional differentiation and showed its relationship to the differentiation of vector calculus. 1.6 used functional differentiation to reproduce Hamilton's equations from an action by requiring that the action's functional derivative be 0. 1.7 established the Lagrangian giving us our three approaches to analytical mechanics (Hamiltonian, Action, Lagrangian). 1.8 explored the ambiguity of the action and corresponding ambiguity of the Lagrangian and Hamiltonian as well as introduced the idea of a gauge transformation. 1.9 derived the general theory of canonical transformations, the full set of transformations that preserve the form of Hamilton's equations. 1.10 showed Noether's beautiful theorem that for every continuous symmetry of a system there is a corresponding quantity conserved by that system. 1.11 introduced the idea of a Lie group and derived basic results about them. This was the end of the first pass content of the chapter.

For the second pass content, 1.12 showed that all of analytical mechanics can be directly applied to a theory containing any number of derivatives. 1.13 showed how the Hamilton-Jacobi equation can be used to recast Hamilton's equations in "undoubled" form in terms of the coordinates only. Section 1.14 introduced adiabatic invariants for integrable systems which give a set of quantities which are stable on experimentally relevant timescales even for quickly evolving systems. 1.15 proved the theorem of normal modes, that near a linearly stable equilibrium any Hamiltonian system is equivalent to a system of noninteracting harmonic oscillators. Finally, section 1.16 introduced the basic idea of a symplectic manifold and explained how to use general noncanonical coordinates in the canonical formalism.

This chapter is by no means a complete treatment of essential topics in Analytical Mechanics, merely an introduction to what we need for the rest of the book. There is much more to both the theory and applications of analytical mechanics than we will have time to talk about. For completeness sake, here is a list of important topics we have not covered in nearly the detail they are worth leaning about (in no particular order) with brief advertisements and places to read about them:

- Theory of Lie Groups. Lie groups are deeply involved in physics and will recur often for us. I strongly recommend [41].
- Symmetry methods for differential equations. Identifying what the symmetries of a differential equation are and using the identified symmetries to solve that equation. I recommend [48].
- The Hamilton-Jacobi equation. There is much more to this equation than we had time to discuss. It is useful for solving difficult classic problems (like motion of the planets) as well as special cases of fluid mechanics (non-rotational flow) and for understanding the relationship between classical and quantum mechanics. See chapter 9 of [2] and chapter 10 of [37].

- Symplectic Forms and Symplectic manifolds. The mathematics behind what analytical mechanics means geometrically. See chapters 7-9 of [2].
- Integrable systems and Action-Angle Variables. There is much more to them than we have had room to discuss. See chapter 10 of [2], sections 47-52 of [60], and chapters 10 and 12 of [37].
- Canonical Perturbation Theory. Most systems are not exactly solvable by pen or processor. This is how to approximately solve real systems by relating them to simpler exactly solvable systems. See chapter 10 and Appendices 7 and 8 of [2] and chapter 12 of [37].
- Chaos. Systems for which the perturbation theory fails to an embarrassing degree. See chapter 11 of [37] and the whole of [115].

Chapter 2

Nonrelativistic Classical Mechanics

*Give me a place to stand and with a lever
I will move the whole world.*
– Archimedes [124]

Now that you have eaten your vegetables, it is time to kill a fly with a machine gun. Let us try to describe the motion of matter and the stuff matter is made of. Whatever the basic constituents which make up a theory are, they are called **particles**. The simplest model of matter is that objects are made out of points of stuff which move around. That is, to assume that matter is made of point-particles. It is important for consistency of language to note that the word particle does **NOT** in general mean a moving point and that it is a specific model of particles to treat them as point-like. There are other possible models of particles; we will see several in the coming chapters¹. To make language perfectly clear, one would always say point-particle and not just particle when they mean a moving point. But, often in physics we are lazy about specifying what model of particle we are using because it is clear (to the experienced) from context. Particle physicists know very well when they say particle they mean something entirely different from a point particle, but the unfamiliar reader wouldn't. When we model matter as being made of moving points, we say we are doing **Classical Mechanics**². And so, whenever we are doing classical mechanics and we say particle, we mean point-particle.

We could take two perspectives in regards to point particles. We could think of them as fundamental ingredients of our theory (meaning we believe that microscopically stuff is really made of moving points) or we could think of them as effective (meaning we believe that microscopically more is going on inside stuff but for many macroscopic purposes nothing beyond where the bulk of the stuff is matters). The first of these was genuinely what physicists believed for centuries, but it has now been known for more than a century that point particles do not and cannot exist. There are foundational issues of mathematical inconsistency when making them interact which we will see in chapter 4. So, while we will “take point particles seriously” for the purpose of analysis, we are giving a spoiler that we will have to abandon them as fundamental eventually (why else would we need a Part II?). While they will not be fundamental, the effective theory of point particles is still useful to this very day for very many purposes. A spec of dust in the air has enormous internal dynamical structure, but for human purposes modeling it as a pure point like object is often good enough. It is important that you get into the habit of thinking of every theory we discuss as an effective theory only valid under appropriate circumstances.

By a point we mean something which has no internal structure and so is completely specified by its location. Thus for a theory of a moving point, we take our configuration space to be the space of possible locations in space: $Q(t) = \vec{x}(t)$ where the three real numbers $\vec{x}(t) = (x(t), y(t), z(t))$ give the coordinates of

¹For an easy example of another kind of particle, in a theory of modeling traffic flow on a highway the cars would be the particles as they are the smallest components of the theory. Cars are not singular points. If you have a visual association in your head of a particle and a point as being the same thing, this is a byproduct of some common abuses of language and a habit you should work to get rid of.

²Unfortunately, there are at least 3 competing uses of the word classical in physics. Some people say classical to mean Newtonian mechanics, which excludes magnetism and relativity, either special or general. We will never use the word classical in that sense. Classical can also mean a theory involving point particles. When we mean this we will say classical mechanics. Finally, classical can mean anything described using the Poisson representation introduced in section 1.4. When we mean this we will say classical physics. So, classical physics contains classical mechanics and classical mechanics contains Newton's mechanics.

our point particle in space.

Assumption :: GCMI: Matter is point-like

Matter consists of moving points. The points have no internal structure and so the configuration of each point is given by its position in space at the present time.

Notice that the above assumption is labeled “GCM” meaning it will only apply to Galilean Classical Mechanics, which is the type of mechanics we will be doing in this and the next chapter. We have taken the space of locations to be three dimensional because we seem to live in a smooth three dimensional space. We take this as an assumption that also applies to all physics:

Assumption :: PHSXII: Smoothness of space

Space is continuous, smooth, and three dimensional.

Certainly the objects of every day life are not points; they have size and seem continuous. However, we will see by the end of this chapter that a continuous body of matter can built up as an integral of point matter. Thus, we will be able to describe continuous bodies within this theory.

2.1 Galilean Boost Symmetry

Now that we know the configuration space of our system (and so have solved the “problem of interpretation”) we move on to the problem of dynamics. We need to find what the Lagrangian for our theory of points is. The way we generally do this is to find what Lagrangians are possible if we want them to have certain symmetries. For example, when you are sitting in a car on a smooth road going at a steady rate and you toss a ball into the air, it falls back into your hand just as it does when you are sitting on a bench outside. That is, two systems each of falling balls where the systems are moving at a constant relative velocity to each other evolve exactly the same way as each other (up to the relative velocity) and so there is a symmetry. This transformation of moving a whole system by a constant velocity is called a boost (because we “apply a boost” to one system so that it moves steadily relatively to the other) and symmetry under that boost is called boost symmetry. Assuming that time passes at the same rate in each of the two falling ball systems, then $t = t'$ where t is the time measured in the unboosted system and t' is the time measured in the boosted system. This assumption is taken by the prejudice of experience that if your well-made watch and your well-made house clock agree on the time in the morning then when you return to home after a long day of work, they still agree on the time when you get back and so time passed at the same rate for the watch as it did for the house clock regardless of the relative velocity between the two. By definition, the boost causes the position of the boosted system $\vec{x}'$ to move with a relative velocity $\vec{v}$ to the unboosted system $\vec{x}$:

$$t' = t, \quad \dot{\vec{x}}' = \dot{\vec{x}} + \vec{v}. \quad (2.1.1)$$

Integrating both sides with respect to t (using that $t' = t$) and defining t_b as the time at which the boost is applied (meaning the systems are at the same position at $t = t_b$):

$$\int_{t_b}^t \frac{d\vec{x}'}{dt'} dt = \int_{t_b}^t \left(\frac{d\vec{x}}{dt} + \vec{v} \right) dt \quad (2.1.2)$$

$$\implies \vec{x}'(t) - \vec{x}'(t_b) = \vec{x}(t) - \vec{x}(t_b) + \vec{v}(t - t_b) \quad (2.1.3)$$

$$\implies \vec{x}'(t) = \vec{x}(t) + \vec{v}(t - t_b). \quad (2.1.4)$$

Equation (2.1.4) is called a Galilean boost. Note that the position is boosted and the boosted and unboosted positions use the same time t . Often one calls the coordinate system $(t, \vec{x})$ here a “frame”. In this language, the Galilean boost gives a relationship between coordinates in different frames. Now, because we observe that the physics of our daily life has this boost symmetry, we take the assumption of this symmetry as part of our theory:

Assumption :: GCMII - Galilean Boost Symmetry

Isolated systems have symmetry under shifting the position of all objects at the same fixed rate (boosting by a constant velocity) while keeping time unchanged.

We want to find a Lagrangian for the particle which is consistent with this boost symmetry. By Noether's theorem 1.9, when we apply the boost to the variables in the Lagrangian, we need the new boosted Lagrangian to be related to the unboosted Lagrangian by an action gauge transformation. Define the boosted Lagrangian:

$$\mathcal{L}(t', \vec{x}', \dot{\vec{x}}') \stackrel{\text{def}}{=} \frac{dS}{dt'}[\vec{x}'] = \frac{dt}{dt'} \frac{dS}{dt}[\vec{x}'] = \mathcal{L}(t, \vec{x} + \vec{v}(t - t_b), \dot{\vec{x}} + \vec{v}). \quad (2.1.5)$$

When the boost is applied, we have at the same time and location two systems which differ only by a relative velocity $\vec{v}$. To have boost symmetry, the boosted and unboosted Lagrangians must be related by an action gauge transformation at the time the boost is applied. Therefore, there exists $f(\vec{v}, t_b, t, \vec{x})$ such that:

$$\mathcal{L}(t_b, \vec{x}', \dot{\vec{x}}') = \mathcal{L}(t_b, \vec{x}, \dot{\vec{x}}) + \left. \frac{df}{dt} \right|_{t=t_b} \quad (2.1.6)$$

Expanding the boosted Lagrangian at the time the boost is applied:

$$\mathcal{L}(t', \vec{x}', \dot{\vec{x}}') \Big|_{t=t_b} = \mathcal{L}(t, \vec{x}, \dot{\vec{x}} + \vec{v}) \Big|_{t=t_b} = \mathcal{L}(t_b, \vec{x}(t_b), \dot{\vec{x}}(t_b)) + \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \cdot \vec{v} + \mathcal{O}(v^2). \quad (2.1.7)$$

When no boost is applied, f is 0 by definition. So:

$$\vec{g}(t_b, t, \vec{x}) \stackrel{\text{def}}{=} \left. \frac{\partial f}{\partial \vec{v}} \right|_{\vec{v}=0} \implies f(t, \vec{x}, \vec{v}) = \vec{v} \cdot \vec{g}(t_b, t, \vec{x}) + \mathcal{O}(v^2). \quad (2.1.8)$$

Returning to equation (2.1.6) at the moment the boost is applied (using (2.1.7) on the left and (2.1.8) on the right):

$$\mathcal{L}(t_b, \vec{x}, \dot{\vec{x}}) + \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \cdot \vec{v} + \mathcal{O}(v^2) = \mathcal{L}(t_b, \vec{x}, \dot{\vec{x}}) + \left. \frac{d}{dt} (\vec{v} \cdot \vec{g}(t_b, t, \vec{x}) + \mathcal{O}(v^2)) \right|_{t=t_b} \quad (2.1.9)$$

$$\implies \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}}(t_b, \vec{x}, \dot{\vec{x}}) = \left. \frac{d\vec{g}}{dt} \right|_{t=t_b} = \frac{\partial \vec{g}}{\partial t}(t_b, t_b, \vec{x}) + \dot{\vec{x}} \cdot \nabla \vec{g}(t_b, t_b, \vec{x}). \quad (2.1.10)$$

The jump from equation (2.1.9) to (2.1.10) is gotten by matching the order $\vec{v}$ terms in equation (2.1.9) or equivalently, taking the derivative of both sides with respect to $\vec{v}$ and evaluating at $\vec{v} = 0$. Then, because equation (2.1.10) is only valid at the moment the boost is applied, $\frac{\partial \vec{g}}{\partial t}$ evaluated at the boost time and $\nabla \vec{g}$ evaluated at the boost time are completely independent functions. Define then $\vec{K}(t_b, \vec{x}) = \frac{\partial \vec{g}}{\partial t}(t_b, t_b, \vec{x})$ and $\hat{M}(t_b, t_b, \vec{x}) = \nabla \vec{g}(t_b, \vec{x})$. We could have applied the boost at any time and whenever we apply the boost we need this symmetry requirement. This then defines the functions $\vec{K}$ and $\hat{M}$ for all times, and means they have in principle unknown and unrelated time dependence. Therefore, for arbitrary boost time t :

$$\frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \vec{K}(t, \vec{x}) + \hat{M}(t, \vec{x}) \cdot \dot{\vec{x}}. \quad (2.1.11)$$

If we take a second $\dot{\vec{x}}$ derivative and look at this equation in components we see:

$$\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^a \partial \dot{x}^b} = M_{ab} \implies M_{ba} = \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^a \partial \dot{x}^b} = \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^b \partial \dot{x}^a} = M_{ab} \implies \hat{M}^T = \hat{M}.$$

The superscript of T when used on a matrix or vector will always mean the transpose of that quantity. We see $\hat{M}$ must be a symmetric matrix (meaning equal to its own transpose). Integrating (2.1.11) with respect to $\dot{\vec{x}}$, we get that a Galilean boost symmetric Lagrangian for a point object is (including the "constant" with respect to $\dot{\vec{x}}$ gotten from integration) must be of the form:

$$\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = \frac{1}{2} \dot{\vec{x}} \cdot \hat{M}(t, \vec{x}) \cdot \dot{\vec{x}} + \vec{K}(t, \vec{x}) \cdot \dot{\vec{x}} - U(t, \vec{x}). \quad (2.1.12)$$

By performing the Legendre transformation, it is possible for us to arrive at the Hamiltonian (assuming the matrix $\hat{M}$ is invertible). First, compute $\vec{p}$ from (1.7.28):

$$\vec{p} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \hat{M} \cdot \dot{\vec{x}} + \vec{K} \implies \dot{\vec{x}} = \hat{M}^{-1}(\vec{p} - \vec{K}). \quad (2.1.13)$$

Then, compute $\mathcal{H}$ from (1.7.29):

$$\mathcal{H} = \vec{p} \cdot \dot{\vec{x}} - \mathcal{L} \quad (2.1.14)$$

$$= \dot{\vec{x}} \cdot (\hat{M} \cdot \dot{\vec{x}} + \vec{K}) - \frac{1}{2} \dot{\vec{x}} \cdot \hat{M} \cdot \dot{\vec{x}} - \vec{K} \cdot \dot{\vec{x}} + U \quad (2.1.15)$$

$$= \frac{1}{2} \dot{\vec{x}} \cdot \hat{M} \cdot \dot{\vec{x}} + U \quad (2.1.16)$$

$$= \frac{1}{2} (\vec{p} - \vec{K}) \cdot \hat{M}^{-1} \cdot (\vec{p} - \vec{K}) + U. \quad (2.1.17)$$

Hence we have the Hamiltonian or Lagrangian for a Galilean symmetric particle in terms of three unknown functions, a real valued function $U(t, \vec{x})$, a vector valued function $\vec{K}(t, \vec{x})$, and a symmetric matrix valued function $\hat{M}(t, \vec{x})$. It is actually possible to be slightly more restrictive. Not only does space seem smooth, it also seems to be flat/unwarped, static, and without any holes. Thus, we also assume:

Assumption :: GCMIII - Space is static and Euclidean

The background space in which objects move is not itself dynamical and is instead fixed without any curvature or holes, extending infinitely in all directions.

By this we mean that we assume actual physical space is not only three dimensional, but also does not change with time and is flat/has no curvature or punctures. We assume it is just the Euclidean space $\mathbb{R}^3$. Any theory which assumes GCMII and GCMIII is called a Galilean theory or nonrelativistic theory. We can see the implications of the Euclidean assumption if we try to derive the Galilean Hamiltonian by looking at the Lie algebra of the boost. Let $\vec{G}(t, \vec{x}, \vec{p})$ be the generator of velocity boosts at the time the boost is applied. Then, by definition:

$$\frac{df}{d\vec{v}} = \{f, \vec{G}\}. \quad (2.1.18)$$

At the time the boost is applied $\vec{x}$ is unchanged (set $t = t_b$ in (2.1.4)). Therefore:

$$\frac{d\vec{x}}{d\vec{v}} = \{\vec{x}, \vec{G}\} = \frac{\partial \vec{G}}{\partial \vec{v}} = 0 \implies \vec{G} = \vec{G}(t, \vec{x}). \quad (2.1.19)$$

We can compute the bracket of the generator with the momentum by the method of (1.11.25). Consider the transformations $T(\vec{a})$ which translates the position by $\vec{a}$ and $B(\vec{v})$ which boosts the velocity by $\vec{v}$. Then:

$$B(-\vec{v})T(-\vec{a})B(\vec{v})T(\vec{a}) \begin{pmatrix} \vec{x} \\ \vec{p} \end{pmatrix} = B(-\vec{v})T(-\vec{a})B(\vec{v}) \begin{pmatrix} \vec{x} + \vec{a} \\ \vec{p} \end{pmatrix} \quad (2.1.20)$$

$$= B(-\vec{v})T(-\vec{a}) \begin{pmatrix} \vec{x} + \vec{a} + \vec{v}(t - t_b) \\ B(\vec{v})\vec{p} \end{pmatrix} \quad (2.1.21)$$

$$= B(-\vec{v}) \begin{pmatrix} \vec{x} + \vec{v}(t - t_b) \\ B(\vec{v})\vec{p} \end{pmatrix} \quad (2.1.22)$$

$$= \begin{pmatrix} \vec{x} \\ \vec{p} \end{pmatrix}. \quad (2.1.23)$$

Because these transformations commute on the entire phase space, by equation (1.11.25) the bracket of the generators of these two transformations must not be a function of either $\vec{x}$ or $\vec{p}$. Because the space is static, the boost operation has the same definition at all times and so the bracket cannot depend on t either:

$$\{\vec{p}, \vec{G}\} = \hat{M}' \quad (2.1.24)$$

for a constant matrix $\hat{M}'$. Now we have:

$$\{\vec{p}, \vec{G}\} = -\frac{\partial \vec{G}}{\partial \vec{x}} = \hat{M}' \implies \vec{G} = -\hat{M}' \cdot \vec{x} + \vec{f}(t). \quad (2.1.25)$$

$$\frac{d\vec{x}}{d\vec{v}} = \{\vec{x}, \vec{G}\} = \mathbb{1} \implies \{\dot{\vec{x}}, -\hat{M}' \cdot \vec{x} + \vec{f}\} = \mathbb{1} \quad (2.1.26)$$

$$\implies \hat{M}' \cdot \{\vec{x}, \dot{\vec{x}}\} = \mathbb{1} \implies \hat{M}' \frac{\partial \dot{\vec{x}}}{\partial \vec{p}} = \mathbb{1} \quad (2.1.27)$$

$$\implies \frac{\partial \vec{x}}{\partial \vec{p}} = \hat{M}'^{-1} \implies \dot{\vec{x}} = \hat{M}'^{-1}(\vec{p} - \vec{K}'(t, \vec{x})) \quad (2.1.28)$$

where $\vec{K}'(t, \vec{x})$ comes from integrating with respect to $\vec{p}$. By matching (2.1.13) to (2.1.28), we identify $\hat{M}' = \hat{M}$ and $\vec{K}' = \vec{K}$. Hence, $\hat{M}$ is actually a constant matrix. Now we will use that space is Euclidean. If we rotate both vectors $\vec{p}$ and $\vec{G}$ in $\{\vec{p}, \vec{G}\}$, because space is Euclidean and therefore rotationally invariant, we have essentially done nothing and must get the same result. So, $\hat{M}$ must be the same after this rotation. That is, for $\hat{R}$ a rotation matrix:

$$\{\hat{R}\vec{p}, \hat{R}\vec{G}\} = \{\vec{p}, \vec{G}\} = \hat{M}. \quad (2.1.29)$$

By explicitly calculating the left hand side in components:

$$\{\hat{R}\vec{p}, \hat{R}\vec{G}\}^{ab} = \{R^a{}_c p^c, R^b{}_d G^d\} = R^a{}_c \{p^c, G^d\} R^b{}_d = R^a{}_c M^{cd} R^b{}_d = R^a{}_c M^{cd} (R^T)_d{}^b \quad (2.1.30)$$

$$\implies \{\hat{R}\vec{p}, \hat{R}\vec{G}\} = \hat{R} \hat{M} \hat{R}^T. \quad (2.1.31)$$

Therefore, matching (2.1.29) and (2.1.31) we have:

$$\hat{R} \hat{M} \hat{R}^T = \hat{M}. \quad (2.1.32)$$

$\hat{M}$ is a real symmetric matrix and therefore diagonalizable with real eigenvalues m_1, m_2, m_3 and orthonormal eigenvectors $\vec{e}_1, \vec{e}_2, \vec{e}_3$ by standard linear algebra. Writing $\hat{M}$ in its eigenbasis:

$$\hat{M} = m_1 \vec{e}_1 \vec{e}_1^T + m_2 \vec{e}_2 \vec{e}_2^T + m_3 \vec{e}_3 \vec{e}_3^T. \quad (2.1.33)$$

Under the rotation then:

$$\hat{R} \hat{M} \hat{R}^T = \hat{R} (m_1 \vec{e}_1 \vec{e}_1^T + m_2 \vec{e}_2 \vec{e}_2^T + m_3 \vec{e}_3 \vec{e}_3^T) \hat{R}^T \quad (2.1.34)$$

$$= m_1 (\hat{R} \vec{e}_1) (\hat{R} \vec{e}_1)^T + m_2 (\hat{R} \vec{e}_2) (\hat{R} \vec{e}_2)^T + m_3 (\hat{R} \vec{e}_3) (\hat{R} \vec{e}_3)^T. \quad (2.1.35)$$

Hence, $\hat{R} \hat{M} \hat{R}^T$ simply rotates the eigenvectors of $\hat{M}$. By considering a rotation which rotates one eigenvector into another, the requirement that $\hat{M}$ must be unchanged under this rotation thus implies that the eigenvalues of the different eigenvectors are the same. Hence, $m_1 = m_2 = m_3 = m$. So, $\hat{M}$ is proportional to the identity matrix:

$$\hat{M} = m \mathbb{1} \quad (2.1.36)$$

for some constant m . Inserting this result into our Hamiltonian and Lagrangian from earlier, we have:

Theorem 2.1: Galilean Particle General Lagrangian

The most general Lagrangian for the dynamics of a particle with configuration $Q = \vec{x}$ which has Galilean boost symmetry in static Euclidean space is given by:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \vec{K}(t, \vec{x}) \cdot \dot{\vec{x}} - U(t, \vec{x}). \quad (2.1.37)$$

This Lagrangian has the associated Hamiltonian:

$$\mathcal{H} = \frac{|\vec{p} - \vec{K}(t, \vec{x})|^2}{2m} + U(t, \vec{x}). \quad (2.1.38)$$

U is called the potential energy and $\vec{K}$ is called the potential momentum.

It is a common mistake in some books to say that the Lagrangian is defined by “kinetic energy” minus “potential energy” where kinetic energy is the sum of terms in the energy which depend on velocity and potential energy is the sum of terms which don’t. It should be transparent from equation (2.1.37) and expressing (2.1.38) in terms of velocity (instead of $\vec{p}$) that no such thing is true for this Lagrangian when $\vec{K} \neq 0$. In fact no such statement is true in general and kinetic energy and potential energy are not useful or even consistently-defined concepts for most theories in physics. Saying the Lagrangian is the difference of kinetic and potential energy is a misguided appeal to history. It is valid for the physics which was known at the time the Lagrangian was discovered. It is not valid for the physics which is known now. It is now known that the Lagrangian is far more fundamental of a concept than kinetic or potential energy. One may retort that it is a useful shorthand for remembering some Lagrangians. However, given that one has to remember for which systems said incorrect rule happens to work out for in order to use it and still has to remember the

expressions for the kinetic and potential energies when it does work, it doesn't really save any effort. A much better method for remembering Lagrangians is outlined in Appendix C.

Exercises

Problem 2.1: The free particle. Consider the Lagrangian in (2.1.37) with $U = 0$ and $\vec{K} = 0$. This is called a “free particle” because it is the case of nothing external influencing the motion of the particle (this will be explained in the coming sections). Compute the Euler-Lagrange equations for this Lagrangian and solve them.

Problem 2.2: No $\vec{K}$ in 1 spatial dimension. Consider the Lagrangian in (2.1.37) but in 1 dimension.

- (a) Show that the term $K(t, x)\dot{x}$ in the Lagrangian can always be removed by changing the Lagrangian by a total time derivative (add a $\frac{df}{dt}$ and choose f so that it works out). This is special to 1 dimension.
- (b) Assuming you have “removed” K as done in part (a), now consider the special case of $U = \frac{1}{2}kx^2$ for constant $k > 0$. Find the Euler-Lagrange equations and solve them. This is called a simple harmonic oscillator.
- (c) Assuming you have “removed” K as done in part (a), now consider the special case of $U = mgx$ for constant $g > 0$. Find the Euler-Lagrange equations and solve them.

2.2 Time Translational Symmetry

Equation (2.1.37) gives us the general Lagrangian for a Galilean boost invariant point object. In it we see that there are two unknown functions, the scalar function $U(t, \vec{x})$ and the vector function $\vec{K}(t, \vec{x})$. For our case at the moment, we will consider a special case of the Lagrangian (2.1.37) when the object is **isolated**. An isolated system is a system in which the only dynamics are the system's dynamics. That is, there is no interaction between the system and any external variables. In terms of our point object, this would mean that the object is all alone in the universe with nothing else to interact with. Just as before when we observed boost symmetry and so required it of our Lagrangian, for isolated systems we observe more symmetries which we will also require.

Every day of your life the physics of everything around you has worked the same way as it did any other day. That is, as time passes the rules by which dynamics happen don't change. The logic used to design the first car's engine still works today because the rules are the same. And so, we believe:

Assumption :: PHSXIII - Time Translational Symmetry

Isolated systems have time translational symmetry.

This assumption is taken only to apply to isolated systems because an external effect may break the symmetry. While the rules governing my car do not change, the behavior of my car does change under the external effect of filling it with fuel or not. This assumption will turn out to apply to all of physics, not just GCM. Let us see what implications this has for a Lagrangian in general and then apply those restrictions to equation (2.1.37). Time translation is the canonical transformation in which the time variable has its definition shifted while the coordinates are unchanged:

$$t' = t + \varepsilon, \quad Q'^a = Q^a. \quad (2.2.1)$$

This is an extended point transformation and so by equations (1.9.107) and (1.9.108) we have that for some function $f(\varepsilon, t, Q)$ the Lagrangian must satisfy:

$$\mathcal{L}(t + \varepsilon, Q, \dot{Q}) = \mathcal{L}(t, Q, \dot{Q}) + \frac{df(\varepsilon, t, Q)}{dt}. \quad (2.2.2)$$

Differentiating with respect to ε at $\varepsilon = 0$ we have:

$$\frac{\partial \mathcal{L}}{\partial t} = \frac{d\mathcal{D}f}{dt}. \quad (2.2.3)$$

We know the Lagrangian is not uniquely defined. We can redefine the Lagrangian for our theory by considering an action gauge transformation. In particular, for a given Lagrangian satisfying the above, consider defining the new equivalent Lagrangian by using the gauge function $\chi(t, Q)$ defined as:

$$\chi(t, Q) = \chi_1(Q) - \int_{t_1}^t \mathcal{D}f(t', Q) dt' \quad (2.2.4)$$

where t_1 is some arbitrary constant value and $\chi_1(Q)$ is some well behaved function of Q . Then, after this gauge transformation:

$$\mathcal{L}'(t, Q, \dot{Q}) = \mathcal{L}(t, Q, \dot{Q}) + \frac{d\chi}{dt} = \mathcal{L}(t, Q, \dot{Q}) + \frac{\partial \chi_1}{\partial Q^a} \dot{Q}^a - \mathcal{D}f(t, Q) - \dot{Q}^a \int_{t_1}^t \frac{\partial \mathcal{D}f(t', Q)}{\partial Q^a} dt' \quad (2.2.5)$$

$$\implies \frac{\partial \mathcal{L}'}{\partial t} = \frac{\partial \mathcal{L}}{\partial t} - \frac{\partial \mathcal{D}f}{\partial t} - \dot{Q}^a \frac{\partial \mathcal{D}f}{\partial \dot{Q}^a} = \frac{\partial \mathcal{L}}{\partial t} - \frac{d\mathcal{D}f}{dt}. \quad (2.2.6)$$

Now using (2.2.3) we see that this gauge transformation Lagrangian satisfies:

$$\frac{\partial \mathcal{L}'}{\partial t} = 0. \quad (2.2.7)$$

Therefore, if a theory has time translational symmetry it is always possible to go to a gauge in which its Lagrangian has no explicit dependence on time. In that gauge, it immediately follows that the Hamiltonian has no explicit time dependence by (1.7.22):

$$\frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t} = 0. \quad (2.2.8)$$

In this gauge the surface term f added by the transformation is automatically 0. Then, the generator given

by Noether's theorem in this gauge is:

$$G = P_a 0 - \mathcal{H} 1 - 0 = -\mathcal{H}. \quad (2.2.9)$$

So, for a system with time translational symmetry, we can always transform into a gauge in which the Lagrangian does not depend explicitly on time. In that gauge, the generator of time translations of the system is $G = -\mathcal{H}$ and so $-\mathcal{H}$ (equivalently, $\mathcal{H}$) is conserved by the dynamics. In that gauge, the value of the Hamiltonian is called the **(total) Energy** of the system and it is conserved. So, $-\mathcal{H}$ is the generator of time translations. Recall that by definition $\mathcal{H}$ is the generator of time evolution. Time evolution is the canonical transformation in which Q, P change by evolving using the equations of motion. This is not the same thing as time translation in which the time parameter is changed and the system state is held fixed. Because time translation is the canonical transformation $\mathcal{D}Q = 0, \mathcal{D}P = 0$ and we made $\mathcal{D}f = 0$ by our choice of gauge, any function on phase space $g(Q', P')$ also has $\mathcal{D}g = 0$. Then, by the chain rule:

$$\mathcal{D}g = \mathcal{D}|_t g + \frac{dg}{dt} \mathcal{D}t = \{g, -\mathcal{H}\} + \{g, \mathcal{H}\} = 0. \quad (2.2.10)$$

Hence essentially the generator of time translations has to cancel the effect of time evolution to make $\mathcal{D}g = 0$ and so we can see that the two are inverse processes. This is why we found $G = -\mathcal{H}$. By explicit calculation, in any gauge:

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial t} + \frac{\partial\mathcal{H}}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial\mathcal{H}}{\partial P_a} \frac{dP_a}{dt} = \frac{\partial\mathcal{H}}{\partial t} - \dot{P}_a \dot{Q}^a + \dot{Q}^a \dot{P}_a = \frac{\partial\mathcal{H}}{\partial t} = -\frac{\partial\mathcal{L}}{\partial t}. \quad (2.2.11)$$

This confirms that the Hamiltonian is conserved whenever the Hamiltonian/Lagrangian does not explicitly depend on time. Thus, we have as a direct corollary of Noether's theorem:

Theorem 2.2: Energy Conservation

The Energy E of a system is negative the generator of time translations of that system. If the system has time translation symmetry (and all isolated systems do), there exists a gauge in which its Lagrangian and Hamiltonian have no explicit dependence on time. In that gauge, the value of the Hamiltonian is the energy E and it is conserved.

Now let us return to our specific theory. Consider a gauge transformation of our Lagrangian in equation (2.1.37):

$$\mathcal{L}'(t, \vec{x}, \dot{\vec{x}}) = \mathcal{L}(t, \vec{x}, \dot{\vec{x}}) + \frac{df}{dt} \quad (2.2.12)$$

$$= \frac{1}{2} m |\dot{\vec{x}}|^2 + \vec{K}(t, \vec{x}) \cdot \dot{\vec{x}} - U(t, \vec{x}) + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{x}} \cdot \dot{\vec{x}} \quad (2.2.13)$$

$$= \frac{1}{2} m |\dot{\vec{x}}|^2 + \left(\vec{K}(t, \vec{x}) + \frac{\partial f}{\partial \vec{x}} \right) \cdot \dot{\vec{x}} - \left(U(t, \vec{x}) - \frac{\partial f}{\partial t} \right). \quad (2.2.14)$$

Hence, we can see that a gauge transformation of the Lagrangian is equivalent to transforming U and $\vec{K}$ by:

$$U' = U - \frac{\partial f}{\partial t}, \quad \vec{K}' = \vec{K} + \frac{\partial f}{\partial \vec{x}}. \quad (2.2.15)$$

With this induced transformation on the potentials, the form of our Lagrangian in equation (2.1.37) is unchanged by gauge transformation. The gauge transformation of the potentials comes from the action gauge transformation of the Lagrangian but in language one will often refer to gauge transforming the potentials whether or not one is talking about a particular Lagrangian. So, the phrase “gauge transformation” takes on a life of its own in reference to the potentials even though it fundamentally comes from the Lagrangian. We can see that this use of the phrase gauge transformation is consistent with how we defined it at the end of section 1.8 because the potentials are only defined up to modifying them in a well defined way determined by this function $f(t, \vec{x})$.

Theorem 2.3: Gauge Transformation of the Potentials

The potentials $U(t, \vec{x})$ and $\vec{K}(t, \vec{x})$ are transformed under gauge transformation by $f(t, \vec{x})$ as:

$$U'(t, \vec{x}) = U - \frac{\partial f}{\partial t} \quad (2.2.16)$$

$$\vec{K}'(t, \vec{x}) = \vec{K} + \nabla f. \quad (2.2.17)$$

By Theorem 2.2, time translational symmetry of the Lagrangian implies there exists a gauge in which the Lagrangian has no explicit time dependence. Because the form of the Lagrangian (2.1.37) is unchanged by gauge transformation, we can use that form in any gauge. So, time translational symmetry implies there exists a gauge in which the Lagrangian of the isolated particle reduces to:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \vec{K}(\vec{x}) \cdot \dot{\vec{x}} - U(\vec{x}). \quad (2.2.18)$$

Exercises

Problem 2.3: A common Lagrangian. Consider the Lagrangian $\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = \frac{1}{2}m|\dot{\vec{x}}|^2 + t\nabla u \cdot \dot{\vec{x}}$ for some function $u(\vec{x})$.

- Verify that this Lagrangian is of the same form as (2.1.37).
- By using the equations of motion, verify that the quantity $E = \frac{1}{2}m|\dot{\vec{x}}|^2 + u(\vec{x})$ is conserved in this system.
- By using a gauge transformation, show that the given Lagrangian can be transformed to $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 - u(\vec{x})$ which now visibly has time-translation symmetry.
- By using the transformed Lagrangian, verify that the conserved quantity predicted by Noether's theorem is the one given in (b) and thus we identify this quantity with the Energy.
- Compute the Hamiltonians of the untransformed and transformed Lagrangian, show that only the transformed one is conserved, and show that the two are related by gauge transformation.

2.3 Translational Symmetry

Another symmetry we observe in our daily life is that physics works the same everywhere. That is, as you translate a whole system through space, the rules by which it evolves remain that same. The Earth is whirling around space all the time yet every day I can play guitar at my new point in space as if nothing had happened. The same mechanics apply. And so, similarly to time, we believe:

Assumption :: PHSXIV - Space Translational Symmetry

Isolated systems have space translational symmetry.

A space translation is mathematically the transformation $t' = t$, $\vec{x}' = \vec{x} + \vec{\varepsilon}$. By Noether's theorem, this symmetry will imply a corresponding conserved quantity. The quantity which generates translations in space is called the **(total) Linear Momentum**. Thus, we have:

Theorem 2.4: Linear Momentum Conservation

The Linear Momentum $\vec{P}$ is the generator of spatial translations of a system. If the system has space translational symmetry (and all isolated systems do), then its total Linear Momentum is conserved.

We should note that the linear momentum is not in general the same thing as the canonical momenta P_a . The linear momentum is the generator of translations of a whole system in space. The canonical momenta P_a are the generators of translations of coordinates Q^a in configuration space. Those coordinates may or may not correspond to spatial locations, depending on what one is describing.

Now, let us return to our isolated particle and see what space translation symmetry tells us about our Lagrangian. The transformation is an extended point transformation and so the symmetry condition from Noether's theorem is that there exists a function $\mathcal{D}f(t, \vec{x})$ so that:

$$\left. \frac{d}{d\varepsilon} \left(\frac{dt'}{dt} \mathcal{L}(t', Q', \dot{Q}') \right) \right|_{\varepsilon=0} = \frac{d\mathcal{D}f(t, Q)}{dt} \quad (2.3.1)$$

$$\Rightarrow \left. \frac{d}{d\vec{\varepsilon}} \left(\frac{dt}{dt} \mathcal{L}(t, \vec{x} + \vec{\varepsilon}, \dot{\vec{x}}) \right) \right|_{\varepsilon=0} = \frac{d\mathcal{D}f(t, \vec{x})}{dt} \quad (2.3.2)$$

$$\Rightarrow \frac{\partial \mathcal{L}}{\partial \vec{x}} = \frac{d\mathcal{D}f}{dt}. \quad (2.3.3)$$

Let $\vec{g}(t, \vec{x}) = \mathcal{D}f$. For now we will not actually use the form of the Lagrangian in (2.1.37) because it will save us effort later to be general right now. Instead, we will use what we learned last section, that due to time translational symmetry we can require the Lagrangian to not depend explicitly on time. So, for now we will just assume $\mathcal{L} = \mathcal{L}(\vec{x}, \dot{\vec{x}})$. Then, the translational symmetry requirement is:

$$\frac{\partial \mathcal{L}(\vec{x}, \dot{\vec{x}})}{\partial \vec{x}} = \frac{\partial \vec{g}(t, \vec{x})}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}(t, \vec{x}). \quad (2.3.4)$$

Taking the partial t derivative of both sides:

$$0 = \frac{\partial^2 g_a}{\partial t^2} + \dot{x}^b \frac{\partial g_a}{\partial x^b}. \quad (2.3.5)$$

Because this is true for all $\dot{\vec{x}}$, consider it at $\dot{\vec{x}} = 0$:

$$\frac{\partial^2 g_a}{\partial t^2} = 0 \Rightarrow g_a(t, \vec{x}) = h_a(\vec{x})t + i_a(\vec{x}) \quad (2.3.6)$$

for some functions $\vec{h}(\vec{x})$ and $\vec{i}(\vec{x})$. Then, returning this to the $\dot{\vec{x}}$ derivative of (2.3.5):

$$\frac{\partial^2 g_a}{\partial t \partial x^b} = 0 \Rightarrow \frac{\partial h_a}{\partial x^b} = 0 \Rightarrow g_a(t, \vec{x}) = tA_a + i_a(\vec{x}) \quad (2.3.7)$$

for a constant vector $\vec{A}$. Returning this to (2.3.4):

$$\frac{\partial \mathcal{L}(\vec{x}, \dot{\vec{x}})}{\partial x^a} = A_a + \dot{x}^b \frac{\partial i_a(\vec{x})}{\partial x^b}. \quad (2.3.8)$$

The $\dot{\vec{x}}$ derivative of this gives:

$$\frac{\partial^2 \mathcal{L}}{\partial x^a \partial \dot{x}^b} = \frac{\partial i_a}{\partial x^b}. \quad (2.3.9)$$

Then, the $\vec{x}$ derivative of this gives:

$$\frac{\partial^3 \mathcal{L}}{\partial x^a \partial \dot{x}^b \partial x^c} = \frac{\partial^2 i_a}{\partial x^b \partial x^c}. \quad (2.3.10)$$

The left hand side is automatically symmetric under interchanging the a and c indices because mixed partial derivatives commute. Therefore, the right hand side must also be symmetric under that interchange:

$$\frac{\partial^2 i_a}{\partial x^b \partial x^c} = \frac{\partial^2 i_c}{\partial x^b \partial x^c} \quad (2.3.11)$$

$$\implies \frac{\partial}{\partial x^b} \left(\frac{\partial i_a}{\partial x^c} - \frac{\partial i_c}{\partial x^a} \right) = 0. \quad (2.3.12)$$

$$\implies \frac{\partial i_b}{\partial x^a} - \frac{\partial i_a}{\partial x^b} = B_{ab} \quad (2.3.13)$$

for a constant matrix $\hat{B}$ with components B_{ab} . The left hand side is antisymmetric under interchanging a and b and so $B_{ab} = -B_{ba}$. Then, this can be rewritten as:

$$\frac{\partial}{\partial x^a} \left(i_b + \frac{1}{2} B_{bc} x^c \right) - \frac{\partial}{\partial x^b} \left(i_a + \frac{1}{2} B_{ac} x^c \right) = 0. \quad (2.3.14)$$

The curl of $\vec{i}(\vec{x})$ in components is defined by:

$$\vec{i}(\vec{x}) = \begin{pmatrix} \frac{\partial i_x}{\partial y} - \frac{\partial i_y}{\partial x} \\ \frac{\partial i_y}{\partial z} - \frac{\partial i_z}{\partial y} \\ \frac{\partial i_z}{\partial x} - \frac{\partial i_x}{\partial z} \end{pmatrix}. \quad (2.3.15)$$

These antisymmetric derivative combinations are precisely what occur in (2.3.14). So, we can express (2.3.14) as:

$$\nabla \times \left(\vec{i} + \frac{1}{2} \hat{B} \vec{x} \right) = 0. \quad (2.3.16)$$

The combination $\hat{B} \vec{x}$ can be written nicely in terms of the cross product. Because $\hat{B}$ is antisymmetric, we can write it down in terms of the most general antisymmetric matrix:

$$\hat{B} = \begin{pmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{pmatrix} \quad (2.3.17)$$

for some coefficients C_1, C_2, C_3 . Then, $\hat{B} \vec{x}$ is given by:

$$\hat{B} \vec{x} = \begin{pmatrix} C_2 z - C_3 y \\ C_3 x - C_1 z \\ C_1 y - C_2 x \end{pmatrix} = \vec{C} \times \vec{x} \quad (2.3.18)$$

where we have used the definition of the cross product and defined the vector $\vec{C} = (C_1, C_2, C_3)$. With this:

$$\nabla \times \left(\vec{i} + \frac{1}{2} \vec{C} \times \vec{x} \right) = 0. \quad (2.3.19)$$

Because this combination has vanishing curl, it can be written as a gradient by standard vector calculus:

$$\vec{i}(\vec{x}) = -\frac{1}{2} \vec{C} \times \vec{x} + \nabla j(\vec{x}) \quad (2.3.20)$$

for some scalar function $j(\vec{x})$.

Returning all of this to (2.3.8):

$$\frac{\partial \mathcal{L}(\vec{x}, \dot{\vec{x}})}{\partial x^a} = A_a - \frac{1}{2} (\vec{C} \times \dot{\vec{x}})_a + \dot{x}^b \frac{\partial^2 j(\vec{x})}{\partial x^a \partial x^b} \quad (2.3.21)$$

$$\implies \frac{\partial}{\partial x^a} \left(\mathcal{L}(\vec{x}, \dot{\vec{x}}) - \vec{A} \cdot \dot{\vec{x}} + \frac{1}{2} \dot{\vec{x}} \cdot (\vec{C} \times \dot{\vec{x}}) - \dot{x}^b \frac{\partial j}{\partial x^b} \right) = 0 \quad (2.3.22)$$

$$\implies \mathcal{L}(\vec{x}, \dot{\vec{x}}) - \vec{A} \cdot \vec{x} + \frac{1}{2} \vec{x} \cdot (\vec{C} \times \dot{\vec{x}}) - \dot{x}^b \frac{\partial j}{\partial x^b} = \ell(\dot{\vec{x}}) \quad (2.3.23)$$

where $\ell(\dot{\vec{x}})$ is an integration “constant” (with respect to $\vec{x}$) gotten from integrating this partial derivative with respect to x^a . Using the cyclicity and antisymmetry of the cross product:

$$\vec{x} \cdot (\vec{C} \times \dot{\vec{x}}) = \dot{\vec{x}} \cdot (\vec{x} \times \vec{C}) = -\dot{\vec{x}} \cdot (\vec{C} \times \vec{x}) \quad (2.3.24)$$

(this can be checked quickly using the component expression for the cross product) we can rewrite $\mathcal{L}$ as:

$$\mathcal{L}(\vec{x}, \dot{\vec{x}}) = \ell(\dot{\vec{x}}) + \vec{A} \cdot \vec{x} + \frac{1}{2} \dot{\vec{x}} \cdot (\vec{C} \times \vec{x}) + \frac{d}{dt} j(\vec{x}) \quad (2.3.25)$$

$$\simeq \ell(\dot{\vec{x}}) + \vec{A} \cdot \vec{x} + \frac{1}{2} \dot{\vec{x}} \cdot (\vec{C} \times \vec{x}) \quad (2.3.26)$$

for some unspecified function $\ell(\dot{\vec{x}})$ and constant vectors $\vec{A}$ and $\vec{C}$. (2.3.26) is therefore the most general Lagrangian for a point particle with dynamics that have time translational and space translational symmetry (up to the addition of total time derivatives).

Now let us actually put in the reduced form of the Lagrangian due to Galilean boost symmetry. By equation (2.2.18):

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \vec{K}(\vec{x}) \cdot \dot{\vec{x}} - U(\vec{x}). \quad (2.3.27)$$

This is only in the form of (2.3.26) with the identification:

$$\ell(\dot{\vec{x}}) = \frac{1}{2} m |\dot{\vec{x}}|^2, \quad \vec{K}(\vec{x}) = \frac{1}{2} \vec{C} \times \vec{x}, \quad U(\vec{x}) = -\vec{A} \cdot \vec{x}. \quad (2.3.28)$$

Therefore, when Galilean boost symmetry, time translational symmetry, and translational symmetry are applied the Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \vec{B} \times \vec{x} + \vec{E} \cdot \vec{x} \quad (2.3.29)$$

for constant vectors $\vec{B}$ and $\vec{E}$ (these are just renamings of $\vec{C}$ and $\vec{A}$ to some more common/suggestive names to those familiar with Lagrangians of this form).

Exercises

Problem 2.4: Translationally symmetric equations of motion. Consider our Lagrangian (2.3.29).

(a) From the Lagrangian compute the Euler-Lagrange equation of motion and show that it is:

$$m\ddot{\vec{x}} = \vec{E} + \dot{\vec{x}} \times \vec{B}.$$

(b) Show by direct calculation that this Lagrangian has time translational symmetry. Compute the Noether charge corresponding to that symmetry (the Energy) and show that it is given by:

$$E = \frac{1}{2} m |\dot{\vec{x}}|^2 - \vec{E} \cdot \vec{x}.$$

As well, explicitly verify that this energy is conserved by the equation of motion.

(c) Show by direct calculation that this Lagrangian has space translational symmetry. Compute the Noether charge corresponding to that symmetry (the linear momentum) and show that it is given by:

$$\vec{P} = m\dot{\vec{x}} + \vec{B} \times \vec{x} - \vec{E}t.$$

As well, explicitly verify that this linear momentum is conserved by the equation of motion.

2.4 Rotational Symmetry

Finally, we note that physics seems to work the same in all directions. As the Earth turns about its axis or I change the way I face, there is no apparent difference in how physics works. So, we have another key assumption which we believe in general:

Assumption :: PHSXV: Rotational Symmetry

Isolated systems have rotational symmetry.

While time translations and space translations are relatively easy to write down (just shift t or $\vec{x}$), rotations are slightly harder. Consider a vector $\vec{u}$ of length 1 in two spatial dimensions and write it in polar coordinates: $\vec{u} = (\cos \alpha, \sin \alpha)$ for some angle α . Now consider $\vec{v}$ to be $\vec{u}$ rotated by an angle θ . The angle between $\vec{v}$ and the x -axis is therefore $\theta + \alpha$ and so $\vec{v}$ can be written in coordinates as $\vec{v} = (\cos(\theta + \alpha), \sin(\theta + \alpha))$. By definition, $\vec{v} = \hat{R}(\theta)\vec{u}$ where $\hat{R}(\theta)$ is the rotation operator representing a rotation by an angle θ . Now using the angle addition trigonometry identities:

$$\vec{v} = \begin{pmatrix} \cos(\theta + \alpha) \\ \sin(\theta + \alpha) \end{pmatrix} = \begin{pmatrix} \cos \theta \cos \alpha - \sin \theta \sin \alpha \\ \sin \theta \cos \alpha + \cos \theta \sin \alpha \end{pmatrix} \quad (2.4.1)$$

$$= \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \cos \alpha \\ \sin \alpha \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \vec{u}. \quad (2.4.2)$$

Because $\vec{v} = \hat{R}(\theta)\vec{u}$, we then conclude that:

$$\hat{R}(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}. \quad (2.4.3)$$

So, we have an explicit matrix representation for rotations in 2 dimensions. In more than two dimensions, rotations act on a two dimensional subspace by taking an initial vector and after 90° rotating to an orthogonal final vector while leaving all vectors orthogonal to the plane made by the two unchanged. In two dimensions, the initial vector could be the x direction unit vector which goes to the y direction unit vector (the final vector) after 90° and there are no vectors orthogonal to both. In three dimensions, specifying which direction is unchanged defines the plane of rotation uniquely. This unchanged direction is called the axis of rotation. If we keep the z -axis unchanged, we simply have a rotation in the xy -plane which is the 2 dimensional result with the necessary entries to leave the z -axis unchanged:

$$\hat{R}_z(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2.4.4)$$

To get rotations about the x and y -axes all we have to do is “rotate” our definition of coordinate system by taking x to y , y to z , and z to x . Doing this to the components we get:

$$\hat{R}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}, \quad \hat{R}_y(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}. \quad (2.4.5)$$

We can get a rotation in any plane by simply specifying the initial vector $\vec{t}$ and orthogonal final vector $\vec{f}$ (the vector which $\vec{t}$ is taken to when the rotation angle is 90°). Then:

$$\hat{R}(\theta) = \cos \theta \vec{t}\vec{t}^T - \sin \theta \vec{t}\vec{f}^T + \sin \theta \vec{f}\vec{t}^T + \cos \theta \vec{f}\vec{f}^T + \mathbb{1} - \vec{t}\vec{t}^T - \vec{f}\vec{f}^T. \quad (2.4.6)$$

The first four terms are just the matrix representation in equation (2.4.3) translated into $\vec{t}$ and $\vec{f}$ and the final $\mathbb{1} - \vec{t}\vec{t}^T - \vec{f}\vec{f}^T$ is the identity matrix on the space orthogonal to both $\vec{t}$ and $\vec{f}$ but 0 on the space spanned by $\vec{t}$ and $\vec{f}$ and so ensures that components orthogonal to the rotation are unaffected.

Rotations satisfy an important geometric property: rotation by an angle θ_1 followed by rotation by an angle θ_2 about the same axis is equivalent to just a single rotation about that axis by angle $\theta_1 + \theta_2$. (One can verify this by explicitly calculating from (2.4.6).) Therefore:

$$\hat{R}(\theta_1 + \theta_2) = \hat{R}(\theta_2)\hat{R}(\theta_1). \quad (2.4.7)$$

By taking a derivative at 0, we get a convenient result:

$$\frac{d\hat{R}(\theta_1 + \theta_2)}{d\theta_2} = \frac{d\hat{R}(\theta_2)}{d\theta_2} \hat{R}(\theta_1) \quad (2.4.8)$$

$$\implies \frac{d\hat{R}(\theta_1 + \theta_2)}{d\theta_1} = \frac{d\hat{R}(\theta_2)}{d\theta_2} \hat{R}(\theta_1) \quad (2.4.9)$$

$$\implies \frac{d\hat{R}(\theta + 0)}{d\theta} = \frac{d\hat{R}(\theta_2)}{d\theta_2} \Big|_{\theta_2=0} \hat{R}(\theta) \quad (2.4.10)$$

$$\implies \frac{d\hat{R}(\theta)}{d\theta} = \hat{R}'(0) \hat{R}(\theta). \quad (2.4.11)$$

We get from equation (2.4.8) to (2.4.9) by identifying that a function of only $\theta_1 + \theta_2$ has the same derivative with respect to either and we get from equation (2.4.9) to (2.4.10) by considering $\theta_2 = 0$. Equation (2.4.11) is a first order linear homogeneous differential equation for the rotation matrix. This is just an explicit form of what we found in (1.11.8). Following the same steps as then to solve, we arrive at the equivalent of (1.11.10):

$$\frac{d\hat{R}(\theta)}{d\theta} = \hat{R}'(0) \hat{R}(\theta) \quad (2.4.12)$$

$$\implies \frac{d^n \hat{R}(\theta)}{d\theta^n} = (\hat{R}'(0))^n \hat{R}(\theta) \quad (2.4.13)$$

$$\implies \hat{R}(\theta) = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \frac{d^n \hat{R}(\theta')}{d\theta'^n} \Big|_{\theta'=0} \quad (2.4.14)$$

$$\implies \hat{R}(\theta) = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} (\hat{R}'(0))^n \hat{R}(0) \quad (2.4.15)$$

$$\implies \hat{R}(\theta) = e^{\hat{R}'(0)\theta}. \quad (2.4.16)$$

Functions of matrices such as $\sin \hat{A}$ and $e^{\hat{A}}$ are defined just as before in section 1.11 by putting the matrix into the Taylor series of the function. As such:

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}. \quad (2.4.17)$$

Because we already know what $\hat{R}(\theta)$ is supposed to be from equation (2.4.6), we can check that our solution in equation (2.4.16) actually works. Consider rotations in two dimensions. Then:

$$\hat{R}'(0) = \frac{d}{d\theta} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \Big|_{\theta=0} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \implies \hat{R}'(0)^2 = -\mathbb{1} \quad (2.4.18)$$

$$e^{\hat{R}'(0)\theta} = \sum_{n=0}^{\infty} \frac{(\theta \hat{R}'(0))^n}{n!} = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \hat{R}'(0)^n = \sum_{n=0}^{\infty} \frac{\theta^{2n}}{(2n)!} \hat{R}'(0)^{2n} + \sum_{n=0}^{\infty} \frac{\theta^{2n+1}}{(2n+1)!} \hat{R}'(0)^{2n+1} \quad (2.4.19)$$

$$= \sum_{n=0}^{\infty} \frac{\theta^{2n}}{(2n)!} (-\mathbb{1})^n + \sum_{n=0}^{\infty} \frac{\theta^{2n+1}}{(2n+1)!} (-\mathbb{1})^n \hat{R}'(0) \quad (2.4.20)$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n \theta^{2n}}{(2n)!} \mathbb{1} + \sum_{n=0}^{\infty} \frac{(-1)^n \theta^{2n+1}}{(2n+1)!} \hat{R}'(0) \quad (2.4.21)$$

$$= \cos \theta \mathbb{1} + \sin \theta \hat{R}'(0) = \cos \theta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin \theta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (2.4.22)$$

$$= \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} = \hat{R}(\theta). \quad (2.4.23)$$

And so our solution actually does produce the correct matrix. Doing this same thing for the x , y , and z axis rotations we found earlier:

$$\hat{R}_x(\theta) = e^{\theta \hat{J}_x}, \quad \hat{R}_y(\theta) = e^{\theta \hat{J}_y}, \quad \hat{R}_z(\theta) = e^{\theta \hat{J}_z}, \quad (2.4.24)$$

$$\hat{J}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \hat{J}_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.4.25)$$

For a general rotation as in equation (2.4.6), we find that:

$$\hat{J} = \hat{R}'(0) = -\vec{t}\vec{f}^T + \vec{f}\vec{t}^T \implies \hat{J}^T = -\vec{f}\vec{t}^T + \vec{t}\vec{f}^T = -\hat{J}. \quad (2.4.26)$$

Thus in general for a rotation, the matrix in the exponential is antisymmetric. A general antisymmetric 3x3 matrix can be written as:

$$\hat{J} = \begin{pmatrix} 0 & -\theta_z & \theta_y \\ \theta_z & 0 & -\theta_x \\ -\theta_y & \theta_x & 0 \end{pmatrix} = \theta_x \hat{J}_x + \theta_y \hat{J}_y + \theta_z \hat{J}_z \quad (2.4.27)$$

$$\implies \hat{R}(\theta) = e^{\theta \hat{J}} = e^{\theta_x \hat{J}_x + \theta_y \hat{J}_y + \theta_z \hat{J}_z}. \quad (2.4.28)$$

The group of matrices $\hat{R}(\theta)$ that correspond to rotations in 3 dimensions is called the special orthogonal group SO(3). The matrices are called special because they all have determinant 1 and orthogonal because they satisfy $\hat{R}\hat{R}^T = \mathbb{1}$ (these are both proven in the homework). The 3 is because they correspond to the group of rotations in 3 spatial dimensions. We see that a general element of SO(3) can be written as an exponential of a linear combination of $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$. Thus, these $\hat{J}$ matrices are the generators of the Lie algebra for this group. That Lie algebra is called so(3). Because rotations transform the position as $\vec{x}' = \hat{R}\vec{x}$, they are a linear point transformation. Therefore, these $\hat{J}_a$ matrices form a matrix representation of so(3) by theorem 1.11. Directly computing their commutators gives:

$$[\hat{J}_x, \hat{J}_y] = \hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = \hat{J}_x, \quad [\hat{J}_z, \hat{J}_x] = \hat{J}_y. \quad (2.4.29)$$

All other commutators of the $\hat{J}_a$ not written here are determined by antisymmetry of the commutator. These commutators define the structure constants of so(3), but we will find a nicer form for them in a moment after introducing some notation.

It is convenient to define $\vec{\theta} = (\theta_x, \theta_y, \theta_z)$ and $\hat{\vec{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$. The notation $\hat{\vec{J}}$ is a bit of silly notation meaning the list of three matrices $\hat{J}_x, \hat{J}_y, \hat{J}_z$ treated as the components of a vector for the purposes of computing dot products. Then, $\theta_x \hat{J}_x + \theta_y \hat{J}_y + \theta_z \hat{J}_z = \vec{\theta} \cdot \hat{\vec{J}}$. It is a useful observation to see how this is related to the cross product. The cross product of two vectors is defined as:

$$\vec{u} \times \vec{v} = \begin{pmatrix} u_y v_z - u_z v_y \\ u_z v_x - u_x v_z \\ u_x v_y - u_y v_x \end{pmatrix}. \quad (2.4.30)$$

Notice that for fixed $\vec{u}$, this can actually be viewed as a linear operator on $\vec{v}$ and as such has a matrix representation:

$$\vec{u} \times \vec{v} = \begin{pmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{pmatrix} \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = (\vec{u} \cdot \hat{\vec{J}}) \vec{v}. \quad (2.4.31)$$

Consequently it is convenient to define the operator $\vec{u} \times$ as:

$$\vec{u} \times = \vec{u} \cdot \hat{\vec{J}} = \begin{pmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{pmatrix}. \quad (2.4.32)$$

Then we can write an arbitrary rotation as:

$$\hat{R}(\vec{\theta}) = e^{\vec{\theta} \times}. \quad (2.4.33)$$

We can actually compute the exponential by hand as well. Let $\theta = |\vec{\theta}|$ be the angle of rotation and $\vec{n} = \frac{\vec{\theta}}{|\vec{\theta}|}$ be the axis of rotation. Then, using the double cross product identity (proven in the homework):

$$\vec{u} \times (\vec{v} \times \vec{w}) = \vec{v}(\vec{u} \cdot \vec{w}) - \vec{w}(\vec{u} \cdot \vec{v}) \quad (2.4.34)$$

we can compute:

$$(\vec{\theta} \times)^2 \vec{u} = \vec{\theta} \times (\vec{\theta} \times \vec{u}) = \vec{\theta}(\vec{\theta} \cdot \vec{u}) - \vec{u}(\vec{\theta} \cdot \vec{\theta}) \quad (2.4.35)$$

$$= \theta^2 \vec{n} \vec{n} \cdot \vec{u} - \theta^2 \vec{u} = -\theta^2 (\mathbb{1} - \vec{n} \vec{n}^T) \vec{u}. \quad (2.4.36)$$

Thus:

$$(\vec{\theta} \times)^2 = -\theta^2 (\mathbb{1} - \vec{n} \vec{n}^T). \quad (2.4.37)$$

This allows us to compute even powers of $\vec{\theta} \times$ quite nicely:

$$(\vec{\theta} \times)^{2k} = (-1)^k \theta^{2k} (\mathbb{1} - \vec{n} \vec{n}^T)^k. \quad (2.4.38)$$

The matrix $\mathbb{1} - \vec{n} \vec{n}^T$ very conveniently squares to itself and so it raised to the k power is also itself by induction:

$$(\mathbb{1} - \vec{n} \vec{n}^T)^2 = (\mathbb{1} - \vec{n} \vec{n}^T) \cdot (\mathbb{1} - \vec{n} \vec{n}^T) = \mathbb{1} - \vec{n} \vec{n}^T - \vec{n} \vec{n}^T + \vec{n}(\vec{n} \cdot \vec{n})\vec{n}^T = \mathbb{1} - \vec{n} \vec{n}^T \quad (2.4.39)$$

$$\implies (\mathbb{1} - \vec{n} \vec{n}^T)^k = \mathbb{1} - \vec{n} \vec{n}^T. \quad (2.4.40)$$

Thus:

$$(\vec{\theta} \times)^{2k} = (-1)^k \theta^{2k} (\mathbb{1} - \vec{n} \vec{n}^T). \quad (2.4.41)$$

Now computing the series formula for $\hat{R}(\vec{\theta})$:

$$\hat{R}(\vec{\theta}) = e^{\vec{\theta} \times} = \sum_{k=0}^{\infty} \frac{(\vec{\theta} \times)^k}{k!} = \mathbb{1} + \vec{\theta} \times + \sum_{k=2}^{\infty} \frac{(\vec{\theta} \times)^k}{k!} \quad (2.4.42)$$

$$= \mathbb{1} + \vec{\theta} \times + \sum_{k=1}^{\infty} \frac{(\vec{\theta} \times)^{2k}}{(2k)!} + \sum_{k=1}^{\infty} \frac{(\vec{\theta} \times)^{2k+1}}{(2k+1)!} \quad (2.4.43)$$

$$= \mathbb{1} + \vec{\theta} \times + \sum_{k=1}^{\infty} \frac{(-1)^k \theta^{2k}}{(2k)!} (\mathbb{1} - \vec{n} \vec{n}^T) + \sum_{k=1}^{\infty} \frac{(-1)^k \theta^{2k}}{(2k+1)!} (\mathbb{1} - \vec{n} \vec{n}^T) \vec{\theta} \times \quad (2.4.44)$$

$$= \mathbb{1} + \vec{\theta} \times + \left(\sum_{k=1}^{\infty} \frac{(-1)^k \theta^{2k}}{(2k)!} - 1 \right) (\mathbb{1} - \vec{n} \vec{n}^T) + \left(\sum_{k=1}^{\infty} \frac{(-1)^k \theta^{2k+1}}{(2k+1)!} - \theta \right) (\mathbb{1} - \vec{n} \vec{n}^T) \vec{n} \times \quad (2.4.45)$$

$$= \mathbb{1} + \vec{\theta} \times + (\cos \theta - 1) (\mathbb{1} - \vec{n} \vec{n}^T) + (\sin \theta - \theta) \vec{n} \times \quad (2.4.46)$$

$$= \cos \theta \mathbb{1} + (1 - \cos \theta) \vec{n} \vec{n}^T + \sin \theta \vec{n} \times. \quad (2.4.47)$$

So, for an axis of rotation $\vec{n}$ and angle of rotation θ , an arbitrary rotation matrix is given by:

$$\hat{R}(\vec{\theta}) = \cos \theta \mathbb{1} + (1 - \cos \theta) \vec{n} \vec{n}^T + \sin \theta \vec{n} \times. \quad (2.4.48)$$

One can check by hand that this matches (2.4.6).

All of these results so far are useful, but sometimes it is difficult to work with the matrices and objects with multiple components like $\hat{\vec{J}}$ directly and instead easier to work directly with their components. As such, we define ϵ_{abc} , called the **Levi-Civita symbol**, as the components of $\hat{\vec{J}}$. From equation (2.4.31) this means that component a of the cross product is given by:

$$\boxed{(\vec{u} \times \vec{v})_a = \epsilon_{abc} u^b v^c.} \quad (2.4.49)$$

It follows from the definition of the cross product then that $\epsilon_{123} = 1$ and $\epsilon_{abc} = -\epsilon_{bac} = -\epsilon_{cba}$. With this definition of the Levi-Civita symbol, it immediately follows that the commutators of the $\hat{J}_a$ can be written as:

$$[\hat{J}_a, \hat{J}_b] = \epsilon_{ab}{}^c \hat{J}_c. \quad (2.4.50)$$

Thus, the $\epsilon_{ab}{}^c$ coefficients are precisely the structure constants of $\mathfrak{so}(3)$. (Recall that the choice to write this c index as a superscript instead of a subscript is arbitrary in our current notation. It will be given a meaning in chapter 4.)

Under a rotation, position transforms as:

$$\vec{x}' = \hat{R}(\vec{\theta}) \vec{x} = e^{\vec{\theta} \times} \vec{x} = \left(\mathbb{1} + \vec{\theta} \times + \mathcal{O}(\theta^2) \right) \vec{x} = \vec{x} + \vec{\theta} \times \vec{x} + \text{H.O.T.} \quad (2.4.51)$$

$$\implies x'^a = x^a + \epsilon^a{}_{bc} \theta^b x^c + \text{H.O.T.} \implies \boxed{\mathcal{D}_b x^a = \left. \frac{dx'^a}{d\theta^b} \right|_{\theta=0} = \epsilon^a{}_{bc} x^c.} \quad (2.4.52)$$

A convenient formula will be how this transforms the dot product with a generic vector $\vec{v}$:

$$\left((\vec{\mathcal{D}} \vec{x}) \cdot \vec{v} \right)_a = v_b \mathcal{D}_a x^b = v_b \epsilon^b{}_{ac} x^c = \epsilon_{ac}{}^b x^c v_b = (\vec{x} \times \vec{v})_a \implies (\vec{\mathcal{D}} \vec{x}) \cdot \vec{v} = \vec{x} \times \vec{v}. \quad (2.4.53)$$

This formula only required the transformation property of $\vec{x}$ under a rotation to derive it. Because under a

rotation of space any vector in space rotates that same way, we have that under a rotation for vectors $\vec{u}$ and $\vec{v}$:

$$v_b \mathcal{D}_a u^b = \epsilon_{ac}{}^b u^c v_b. \quad (2.4.54)$$

Now that we finally know how to write down a rotation, the symmetry requirement gives us by Noether's theorem a conserved generator which we call the **(total) Angular Momentum** of the system.

Theorem 2.5: Angular Momentum Conservation

The Angular Momentum $\vec{J}$ is the generator of rotations of a system. If the system has rotational symmetry (and all isolated systems do), then its total angular momentum is conserved.

Because J_a is by definition the generator rotations about the axis with coordinate a , it satisfies:

$$\mathcal{D}_a f = \left. \frac{df}{d\theta^a} \right|_{\theta=0} = \{f, J_a\} \quad (2.4.55)$$

for a function f on phase space. For a vector $\vec{v}$ then using equation (2.4.54):

$$\mathcal{D}_b v^a = \epsilon^a{}_{bc} v^c \implies \boxed{\{v^a, J_b\} = \epsilon^a{}_{bc} v^c}. \quad (2.4.56)$$

However, rotations in how they act on the coordinates of a point particle with position $\vec{x}$ are just a simple linear point transformation. So, for such a particle we have from the linear point transformation theorem:

$$J_a = p_b (\hat{J}_a)^b{}_c x^c = (\vec{x} \times \vec{p})_a. \quad (2.4.57)$$

Then, from (2.4.50), it follows that the J_a must satisfy:

$$\boxed{\{J_a, J_b\} = \epsilon_{ab}{}^c J_c}. \quad (2.4.58)$$

In particular this means:

$$\mathcal{D}_b J^a = \{J^a, J_b\} = \epsilon^a{}_{bc} J^c. \quad (2.4.59)$$

Therefore, the components of $\vec{J}$ rotate exactly like any other vector under a rotation and so we call $\vec{J}$ the angular momentum vector³.

Let us now apply rotational symmetry to our Lagrangian and see what conditions it imposes. Under a rotation:

$$t' = t, \quad \vec{x}' = \hat{R} \vec{x} \implies \dot{\vec{x}}' = \hat{R} \dot{\vec{x}}. \quad (2.4.60)$$

We know from equation (2.3.26) that time translational and space translational symmetry ensure that the Lagrangian for a point particle has the form (up to the addition of total time derivatives):

$$\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = \ell(\dot{\vec{x}}) + \frac{1}{2} \dot{\vec{x}} \cdot (\vec{B} \times \vec{x}) + \vec{E} \cdot \vec{x} \quad (2.4.61)$$

for constant vectors $\vec{E}$ and $\vec{B}$ and unspecified function $\ell(\dot{\vec{x}})$. To have rotational symmetry, we know that under a rotation we must have for some function $f(\varepsilon, t, \vec{x})$:

$$\left. \frac{d}{d\varepsilon} \left(\frac{dt'}{dt} \mathcal{L}(t', \vec{x}', \dot{\vec{x}}') \right) \right|_{\varepsilon=0} = \frac{d\vec{\mathcal{D}}f}{dt} \quad (2.4.62)$$

$$\implies \mathcal{D}_a x^b \frac{\partial \mathcal{L}}{\partial x^b} + \mathcal{D}_a \dot{x}^b \frac{\partial \mathcal{L}}{\partial \dot{x}^b} = \frac{d\mathcal{D}_a f}{dt}. \quad (2.4.63)$$

Let $g_a(t, \vec{x}) = \mathcal{D}_a f(t, \vec{x})$ and use (2.4.53):

$$\vec{x} \times \frac{\partial \mathcal{L}}{\partial \vec{x}} + \dot{\vec{x}} \times \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{\partial \vec{g}(t, \vec{x})}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}(t, \vec{x}). \quad (2.4.64)$$

Now using the form from equation (2.3.26):

$$\frac{1}{2} \vec{x} \times (\dot{\vec{x}} \times \vec{B}) + \vec{x} \times \vec{E} + \dot{\vec{x}} \times \frac{\partial \ell(\dot{\vec{x}})}{\partial \dot{\vec{x}}} + \frac{1}{2} \dot{\vec{x}} \times (\vec{B} \times \vec{x}) = \frac{\partial \vec{g}(t, \vec{x})}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}(t, \vec{x}). \quad (2.4.65)$$

³Later we will see that under an inversion of space (sending every point to its negative), $\vec{J}$ behaves opposite to what a typical vector does and so it is typically called a pseudovector.

Using the double cross product identity (proven in the homework):

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B}) \quad (2.4.66)$$

we can simplify the above to:

$$\dot{\vec{x}} \times \frac{\partial \ell(\dot{\vec{x}})}{\partial \dot{\vec{x}}} + \frac{1}{2} \dot{\vec{x}}(\dot{\vec{x}} \cdot \vec{B}) - \frac{1}{2} \vec{x}(\dot{\vec{x}} \cdot \vec{B}) + \vec{x} \times \vec{E} = \frac{\partial \vec{g}(t, \vec{x})}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}(t, \vec{x}). \quad (2.4.67)$$

Evaluating this at $\dot{\vec{x}} = 0$:

$$\vec{x} \times \vec{E} = \frac{\partial \vec{g}(t, \vec{x})}{\partial t} \implies g(t, \vec{x}) = t \vec{x} \times \vec{E} + \vec{h}(\vec{x}) \quad (2.4.68)$$

for a vector field $\vec{h}(\vec{x})$. Then the $\dot{\vec{x}}$ derivative of (2.4.67) gives:

$$\frac{\partial}{\partial \dot{x}^b} \left(\left(\dot{\vec{x}} \times \frac{\partial \ell(\dot{\vec{x}})}{\partial \dot{\vec{x}}} \right)_a \right) + \frac{1}{2} \delta_{ab} (\dot{\vec{x}} \cdot \vec{B}) - \frac{1}{2} x_a B_b = t \frac{\partial}{\partial x^b} \left((\vec{x} \times \vec{E})_a \right) + \frac{\partial h_a}{\partial x^b}. \quad (2.4.69)$$

The partial t derivative of this gives:

$$\frac{\partial}{\partial x^b} (\vec{x} \times \vec{E}) = 0 \quad (2.4.70)$$

which is only true if $\vec{E} = 0$. Then, the partial $\vec{x}$ derivative of (2.4.69) gives:

$$\frac{1}{2} \delta_{ab} B_c - \frac{1}{2} \delta_{ac} B_b = \frac{\partial^2 h_a}{\partial x^b \partial x^c}. \quad (2.4.71)$$

The right hand side is symmetric under interchanging b and c while the left hand side is antisymmetric under interchanging b and c . The only matrix which is both antisymmetric and symmetric is the 0 matrix. Therefore the above must equal 0. Considering $a = b \neq c$ this implies:

$$B_c = 0 \implies \vec{B} = 0. \quad (2.4.72)$$

Further, we then have:

$$\frac{\partial h_a}{\partial x^b \partial x^c} = 0 \implies h_a(\vec{x}) = M_{ab} x^b + N_a \quad (2.4.73)$$

for a constant matrix $\hat{M}$ and constant vector $\vec{N}$. Returning all of this to (2.4.67) gives:

$$\dot{\vec{x}} \times \frac{\partial \ell(\dot{\vec{x}})}{\partial \dot{\vec{x}}} = \hat{M} \dot{\vec{x}}. \quad (2.4.74)$$

Taking the inner product of both sides with $\dot{\vec{x}}$ and using that $\vec{u} \times \vec{v}$ is orthogonal to $\vec{u}$ for all $\vec{v}$:

$$0 = \dot{\vec{x}} \cdot \left(\dot{\vec{x}} \times \frac{\partial \ell}{\partial \dot{\vec{x}}} \right) = M_{ab} \dot{x}^a \dot{x}^b. \quad (2.4.75)$$

This is true for all $\dot{x}^a$ and so differentiating twice with respect to $\dot{x}^a$ we find:

$$0 = M_{ab} + M_{ba}. \quad (2.4.76)$$

Therefore $\hat{M}$ must be antisymmetric. Consequently, for a constant vector $\vec{M}$ we can write it as:

$$\hat{M} = \begin{pmatrix} 0 & -M_3 & M_2 \\ M_3 & 0 & -M_1 \\ -M_2 & M_1 & 0 \end{pmatrix} = \vec{M} \times. \quad (2.4.77)$$

Then (2.4.74) becomes:

$$\dot{\vec{x}} \times \left(\frac{\partial \ell}{\partial \dot{\vec{x}}} + \vec{M} \right) = 0 \quad (2.4.78)$$

$$\implies \vec{\mathcal{D}} \left(\ell(\dot{\vec{x}}) + \vec{M} \cdot \dot{\vec{x}} \right) = 0. \quad (2.4.79)$$

So, the combination $\ell + \vec{M} \cdot \dot{\vec{x}}$ must be a function of $\dot{\vec{x}}$ only which is invariant under all rotations (because its derivative with respect to all rotations is 0). The vector $\dot{\vec{x}}$ can be written in terms of its magnitude $v = |\dot{\vec{x}}|$ and spherical coordinate angles θ, φ to parameterize the direction of $\dot{\vec{x}}$ in the usual way for a vector. Under rotations, the magnitude v is unchanged but the angles θ and φ are. Under rotations θ and φ can be made to take any values within their ranges on the sphere and so there are no rotational invariants that can be made

using θ or φ . Therefore, for a function of $\dot{\vec{x}}$ to be invariant under rotations it must purely be a function of $v = |\dot{\vec{x}}|$. That is, for some function $L(|\dot{\vec{x}}|)$:

$$\ell(\dot{\vec{x}}) + \vec{M} \cdot \dot{\vec{x}} = L(|\dot{\vec{x}}|). \quad (2.4.80)$$

Returning all of this to (2.4.61):

$$\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = L(|\dot{\vec{x}}|) - \vec{M} \cdot \dot{\vec{x}} = L(|\dot{\vec{x}}|) - \frac{d}{dt}(\vec{M} \cdot \vec{x}) \quad (2.4.81)$$

$$\simeq L(|\dot{\vec{x}}|). \quad (2.4.82)$$

Hence, **in order for our particle to have time translational, space translational, and rotational symmetry, its Lagrangian must be a function of the speed $|\dot{\vec{x}}|$ only** (up to adding total time derivatives).

Now let us finally include Galilean boost symmetry. By (2.3.29) the most general point particle Lagrangian with time translational symmetry, space translational symmetry, and Galilean boost symmetry is:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \frac{1}{2}\vec{B} \times \vec{x} + \vec{E} \cdot \vec{x}. \quad (2.4.83)$$

We just found that $\vec{E}$ and $\vec{B}$ must be 0 once we include rotational symmetry and that the remaining term $\frac{1}{2}m|\dot{\vec{x}}|^2$ is rotationally symmetric because it only depends on $|\dot{\vec{x}}|$. Thus, after including all symmetries:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2. \quad (2.4.84)$$

From Noether's theorem, the angular momentum of this theory is then:

$$\vec{L} = \vec{p} \cdot \vec{\mathcal{D}}\vec{x} - \mathcal{H}\vec{\mathcal{D}}t - \vec{\mathcal{D}}f = \vec{x} \times \vec{p}. \quad (2.4.85)$$

Here we use $\vec{L}$ for the angular momentum instead of $\vec{J}$. Soon we will learn that in general there are two kinds of angular momentum, orbital angular momentum for which we write $\vec{L}$ and spin angular momentum for which we write $\vec{S}$. There is a notion of the “center of motion” of a system (the center of motion is the point within a system that is conjugate to the total linear momentum of the system) which we will study later in this chapter and many times after. The spin angular momentum of a system is the generator of rotations of the system about its center. The total angular momentum is the generator of rotations of the system about the origin (and so depends on your choice of origin). The difference between the total and spin angular momentum is called the orbital angular momentum. When only one type of angular momentum is present (such as here where the only angular momentum is orbital angular momentum) we will use the appropriate symbol $\vec{L}$ or $\vec{S}$ for that one type. A single point particle carries no spin angular momentum because its center of motion is just its position and a rotation about that position leaves all the coordinates and momenta of that point particle unchanged, making the generator of that rotation (the spin) equal to 0.

So, after all symmetries are considered, we are left with:

Theorem 2.6: Galilean Particle Isolated Lagrangian

The most general Lagrangian for the dynamics of an isolated point particle with configuration $Q = \vec{x}$ which has Galilean boost symmetry in Euclidean space is given by:

$$\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = \frac{1}{2}m|\dot{\vec{x}}|^2 \quad (2.4.86)$$

for some constant m .

In the text of the above theorem we did not explicitly state that we require time translational, space translational, and rotational symmetry. However, those are all required by our general assumptions PHSXIII, PHSXIV, PHSXV, and so go into the definition of the word “isolated”. The group of transformations formed by compositions of time translations, space translations, rotations, and Galilean boosts is known as the connected Galilean group⁴. So, when we say Galilean system, we mean a system that has symmetry under the full connected Galilean group of transformations⁵.

⁴There is also the improper Galilean group which consists further of transformations that invert space $\vec{x}' = -\vec{x}$, called parity, and transformations that invert time $t' = -t$, called time reversal.

⁵Typically one even assumes further that it has symmetry under the improper Galilean group, but this distinction does not matter for us right now

Exercises

Problem 2.5: ★ Newton's First Law. Return to problem 2.1 and explain why the scenario described in that problem is called a “free particle”. Explain how the conditions necessary to derive that Lagrangian and the solutions to its equations of motion are what is meant by Newton's First Law: “An isolated object moves at constant velocity.”. It should be clear then that Newton's first law is not a basic postulate of the universe but instead a specific result about derived from symmetries applied to a specific Lagrangian which is only valid insofar as that system is a good model for reality.

Problem 2.6: ★ Cross Product Identities.

- (a) Show by direct calculation from (2.4.30) that for vectors $\vec{A}$ and $\vec{B}$: $\vec{A} \times \vec{B} = -\vec{B} \times \vec{A}$. This property is known as anti-symmetry.
- (b) Show by direct calculation from (2.4.30) that for vectors $\vec{A}$, $\vec{B}$, and $\vec{C}$: $\vec{A} \cdot (\vec{B} \times \vec{C}) = \vec{B} \cdot (\vec{C} \times \vec{A})$. This property is known as cyclicity.
- (c) Show for the basis $\vec{e}_a$ where $\vec{e}_1 = (1, 0, 0)$, $\vec{e}_2 = (0, 1, 0)$, and $\vec{e}_3 = (0, 0, 1)$ that:

$$\vec{e}_a \times \vec{e}_b = \epsilon_{ab}^c \vec{e}_c.$$

- (d) Show using the above properties and (2.4.49) that:

$$\epsilon_{abc} = \epsilon_{bca} = \epsilon_{cab} = -\epsilon_{bac} = -\epsilon_{acb} = -\epsilon_{cba}.$$

- (e) Use the definition of the cross product to show the double cross product identity:

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B}).$$

- (f) Show, either using the cross product or indices, that the Levi-Civita symbol satisfies the identity:

$$\epsilon^{abc} \epsilon_{ade} = \delta_d^b \delta_e^c - \delta_e^b \delta_d^c$$

where δ_b^a is the Kronecker delta symbol.

Problem 2.7: ★ Rotation Identities.

- (a) Show that for an orthonormal basis $\vec{e}_a$:

$$\vec{e}^a \vec{e}_a^T = \mathbb{1}.$$

- (b) Show using induction that for a unit vector $\vec{n}$ and natural number k :

$$(\mathbb{1} - \vec{n} \vec{n}^T)^k = \mathbb{1} - \vec{n} \vec{n}^T.$$

- (c) For vectors $\vec{u}$ and $\vec{v}$ and a rotation matrix $\hat{R}$, show using (2.4.48) by direct calculation that:

$$(\hat{R}\vec{u}) \times (\hat{R}\vec{v}) = \hat{R}(\vec{u} \times \vec{v}).$$

- (d) Let $\vec{n}$ be a unit vector, $\vec{t}$ be a unit vector orthogonal to $\vec{n}$, and $\vec{f} = \vec{n} \times \vec{t}$. Consider a rotation by $\hat{R}(\theta \vec{n})$. Show that the expression given by (2.4.48) matches that given by (2.4.6).
- (e) Show that if a vector $\vec{u}$ satisfies $\hat{R}\vec{u} = \vec{u}$ for all rotation matrices $\hat{R}$ then $\vec{u} = 0$. Thus there are no nonzero rotationally invariant vectors.
- (f) Show that if a matrix $\hat{M}$ satisfies $\hat{R}\hat{M}\hat{R}^T = \hat{M}$ for all rotation matrices $\hat{R}$ then $\hat{M}$ is proportional to the identity matrix. Thus (up to scalar multiplication) the identity matrix is the only rotationally invariant matrix. Hint: show first that for any antisymmetric matrix $\hat{J}$, $\hat{M}\hat{J} - \hat{J}\hat{M} = 0$.
- (g) Consider an object M^{abc} with three coordinate indices which satisfies $R^a_d R^b_e R^c_f M^{def} = M^{abc}$ for all rotation matrices $\hat{R}$. Such an object is called a rotationally invariant rank 3 tensor. Let $\hat{M}^a$ be the matrix with components M^{abc} (b for rows and c for columns). Show that for any antisymmetric matrix $\hat{J}$:

$$\hat{M}^a \hat{J} - \hat{J} \hat{M}^a = J^a_b \hat{M}^b.$$

Use this to show that M^{abc} is proportional to the Levi-Civita symbol ϵ^{abc} . Thus (up to scalar multiplication) the Levi-Civita symbol is the only rotationally invariant rank 3 tensor.

- (h) Consider an object M^{abcd} with four coordinate indices which satisfies $R^a_e R^b_f R^c_g R^d_h M^{efgh} = M^{abcd}$ for all rotation matrices $\hat{R}$. Such an object is called a rotationally invariant rank 4 tensor. Let $\hat{M}^{ab}$ be the matrix with components M^{abcd} . Show that for any antisymmetric matrix $\hat{J}$:

$$\hat{M}^{ab} \hat{J} - \hat{J} \hat{M}^{ab} = J^a_c \hat{M}^{cb} + J^b_c \hat{M}^{ac}.$$

Use this to show that M^{abcd} must be a linear combination of $\delta^{ab}\delta^{cd}$, $\delta^{ac}\delta^{bd}$, $\delta^{ad}\delta^{bc}$. Thus, these three combinations form a basis for all rotationally invariant rank 4 tensors.

Problem 2.8: Characterizing rotation matrices.

- Let $\hat{R}$ be a rotation matrix. Show that $\det(\hat{R}) = 1$ and that $\hat{R}^T = \hat{R}^{-1}$.
- Let $\hat{M}$ be a matrix so that $\hat{M}^T = \hat{M}^{-1}$. Show that $\det(\hat{M}) = \pm 1$.
- Assume the $\hat{M}$ above has $\det(\hat{M}) = 1$. Show that $\hat{M}$ is a rotation matrix. (Hint: consider the action of $\hat{M}$ on a right-handed orthonormal basis or its diagonalizability.) Hence, conclude that a matrix $\hat{M}$ is a rotation matrix if and only if $\hat{M}^T = \hat{M}^{-1}$ and $\det(\hat{M}) = 1$.
- Assume the $\hat{M}$ in (b) has $\det(\hat{M}) = -1$. Show that $-\hat{M}$ is a rotation matrix. Thus, conclude that any such matrix is a combination of a rotation and an inversion of space.
- Consider a matrix $\hat{M}$ so that it preserves the inner product between any two vectors: $(\hat{M}\vec{u}) \cdot (\hat{M}\vec{v}) = \vec{u} \cdot \vec{v}$. Show that this implies $\hat{M}^T = \hat{M}^{-1}$ and thus that only compositions of rotations and spatial inversions can have this property.

Problem 2.9: Dependence of Angular Momentum on the origin. Show how the angular momentum of a particle is changed when the origin of the coordinate system used to define $\vec{x}$ is changed.

Problem 2.10: Conservation of Angular Momentum by a central potential. Show that if a particle is not isolated but instead has a Lagrangian $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 - U(|\vec{x}|)$ then its linear momentum $\vec{p}$ is not conserved but its angular momentum $\vec{L}$ and energy E are. Explain how all three of those conclusions can be seen directly from the Lagrangian using Noether's theorem.

2.5 Interpreting the Galilean Lagrangian

Theorem 2.1 gives that the general Lagrangian for a particle in Galilean Classical Mechanics (GCM) is:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \vec{K}(t, \vec{x}) \cdot \dot{\vec{x}} - U(t, \vec{x}). \quad (2.5.1)$$

Further, Theorem 2.6 gives that the Lagrangian for a GCM particle when it is isolated is:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2. \quad (2.5.2)$$

We know that when all alone a particle acts like (2.5.2) and in general acts like (2.5.1) (unless something breaks Galilean symmetry). We can use this to start to interpret m , $\vec{K}$, and U . When the particle is isolated, we are left with only m . Because the particle is isolated, all that is left in the description must be properties of the particle. Hence, this parameter m whose meaning we have not yet identified must be a property of the particle. We shall call it **mass** and develop an interpretation for it soon. From Noether's theorem, one can see that in fact the total linear momentum of our free particle is its canonical momentum $\vec{p}$ and so often physicists will just call both the momentum. However, in general the two are of course distinct (such as when the particle is not free).

Now let us develop an interpretation for U and $\vec{K}$. They vanish when the particle is isolated and so must represent the effects of variables external to the particle. That is, the particle interacts with other things through U and $\vec{K}$. They are both inhomogeneities in space in the sense that they add explicit spatial dependence to the theory. Further, they may also add explicit time dependence. Our particle carries neither of these. We observed that because m remains when the particle is isolated, m must be a property of the particle. Hence, different particles may have different values of m . As well, it is possible that different particles may interact with external variables and inhomogeneities they induce differently but because the spatial and time dependence are external, the difference in interaction cannot be dependent on space and time. As such, there must be functions $\phi_s(t, \vec{x})$ and $\vec{A}_s(t, \vec{x})$ (with s an index) which represent the external variables and carry all the space and time dependence of the interaction. The only thing that can be different from particle to particle is how strongly each particle is affected by each ϕ_s and $\vec{A}_s$. The strength with which a particle is affected by ϕ_s and $\vec{A}_s$ is called its **charge** q_s . That is:

$$U(t, \vec{x}) = \sum_s q_s \phi_s(t, \vec{x}) \quad (2.5.3)$$

$$\vec{K}(t, \vec{x}) = \sum_s q_s \vec{A}_s(t, \vec{x}). \quad (2.5.4)$$

The sum over s will be over however many different kinds of charge there are. So, to clarify ϕ_s (called a **scalar potential**) and $\vec{A}_s$ (called a **vector potential**) represent some at the moment unknown variables external to the particle which the particle may interact with and q_s (called the interaction charge or just charge) is a property of the particle which gives how strongly it interacts with a given ϕ_s and $\vec{A}_s$. There may be multiple kinds of charge and correspondingly multiple scalar and vector potentials. We can insert these expressions into our Lagrangian and Hamiltonian to find:

Theorem 2.7: Galilean Particle in Euclidean space

The most general Lagrangian for the dynamics of a point-particle of mass m in Euclidean space with configuration $Q = \vec{x}$ which has Galilean boost symmetry is given by:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \sum_s q_s \left(\vec{A}_s(t, \vec{x}) \cdot \dot{\vec{x}} - \phi_s(t, \vec{x}) \right). \quad (2.5.5)$$

This theory has corresponding Hamiltonian:

$$\mathcal{H} = \frac{|\vec{p} - \sum_s q_s \vec{A}_s(t, \vec{x})|^2}{2m} + \sum_s q_s \phi_s(t, \vec{x}). \quad (2.5.6)$$

We saw in equation Theorem 2.3 that U and $\vec{K}$ are not uniquely defined because the following transformation turns out to just be a gauge transformation:

$$U' = U - \frac{\partial f}{\partial t} \quad \vec{K}' = \vec{K} + \nabla f. \quad (2.5.7)$$

By considering f in the same form as equations (2.5.3) and (2.5.4), we can see that this gauge transformation freedom extends down to the scalar and vector potentials:

$$\text{Let } f = \sum_s q_s f_s(t, \vec{x}) \quad (2.5.8)$$

$$U' = U - \frac{\partial f}{\partial t} = \sum_s q_s \phi_s(t, \vec{x}) - \frac{\partial}{\partial t} \sum_s q_s f_s(t, \vec{x}) = \sum_s q_s \left(\phi_s - \frac{\partial f_s}{\partial t} \right) \quad (2.5.9)$$

$$\vec{K}' = \vec{K} + \nabla f = \sum_s q_s \vec{A}_s(t, \vec{x}) + \nabla \sum_s q_s f_s(t, \vec{x}) = \sum_s q_s \left(\vec{A}_s + \nabla f_s \right) \quad (2.5.10)$$

$$\Rightarrow \phi'_s = \phi_s - \frac{\partial f_s}{\partial t} \quad \vec{A}'_s = \vec{A}_s + \nabla f_s. \quad (2.5.11)$$

And so $\phi_s, \vec{A}_s$ carry the same arbitrariness due to gauge freedom that is carried by $U, \vec{K}$. The last line of this calculation holds because since q_s is to represent properties of the particle, the transformation properties of ϕ_s and $\vec{A}_s$ should not depend on q_s as they are external to the particle, so we can require equality for all values of q_s .

Something very significant has happened, and noticing it is rather subtle. We have found that our general massive point particle in the Galilean theory interacts with the rest of the world through these potentials $\phi_s, \vec{A}_s$. At this point we have no idea what these potentials should be. We won't answer that question directly until next chapter but at this point it is still worth noting that we have discovered new variables (the potentials). And, now that we have these new variables we know what the correct thing to do is; we should treat them as new variables and thus should change our action from only depending on the position of our particle ($S[\vec{x}]$) to also depending on the values of the potentials ($S[\vec{x}, \phi, \vec{A}]$). We should find the appropriate action for this whole system from symmetries and use that action to find equations of motion for $\vec{x}, \phi$, and $\vec{A}$ all together. That is, while we have come upon the potentials by studying the dynamics of a particle, the self-consistent way to treat the potentials now that we know about them is to treat them as their own dynamical variables with a dynamical life of their own and with status as part of our Hamiltonian/Lagrangian/Action formalism equal to the status of the particle. Treating the potentials seriously as variables will lead us to discover the laws of gravity, electricity, and magnetism.

Let me comment further on a remark made in section 2.1. It is a very common mistake for physicists to say that the Lagrangian is defined as the kinetic energy minus the potential energy, often written as $\mathcal{L} = T - V$ where $T = \frac{1}{2}m|\dot{\vec{x}}|^2$ for a point mass m and V is usually assumed to be a function of position and time only, not of the velocity. We can see in equation (2.5.5) that the presence of any vector potential in the Lagrangian means that Lagrangian does not satisfy this wrong definition. One could generalize the definition to say that V may depend on time, position, and velocity, in which case one has $\mathcal{L}(t, \vec{x}, \dot{\vec{x}}) = \frac{1}{2}m|\dot{\vec{x}}|^2 - V(t, \vec{x}, \dot{\vec{x}})$ which is trivially true as for any particle system one could define $V(t, \vec{x}, \dot{\vec{x}}) = \frac{1}{2}m|\dot{\vec{x}}|^2 - \mathcal{L}(t, \vec{x}, \dot{\vec{x}})$ no matter what the Lagrangian is. Using equation (2.5.1) this would give $V = U - \vec{K} \cdot \dot{\vec{x}}$. However, the T and V are generally called the kinetic energy and potential energy by such physicists as they eventually intend the total energy of the system, given by the Hamiltonian, to be $\mathcal{H} = T + V$. And, if V depends on $\dot{\vec{x}}$, it will not be true that $\mathcal{L} = T - V$ and $\mathcal{H} = T + V$. The Hamiltonian we found in equation (2.5.6) reveals $\mathcal{H} = T + U$ and $\mathcal{L} = T + \vec{K} \cdot \dot{\vec{x}} - U$. Or, in terms of V , $\mathcal{H} = T + V + \vec{K} \cdot \dot{\vec{x}}$ and $\mathcal{L} = T - V$. Therefore, in general, for a Galilean particle there is no way to simultaneously make the Hamiltonian the sum of kinetic and potential energy, the Lagrangian the difference of kinetic and potential energy, and the kinetic energy correspond to the usual expression $\frac{1}{2}m|\dot{\vec{x}}|^2$. The wrong definition $\mathcal{L} = T - V$ is propagated because it is used to show the ability of the Lagrangian to describe the far less general and less powerful case of Newtonian mechanics, which people are usually already familiar with, and in the case of old fashioned Newtonian mechanics $\vec{K} = 0$ giving $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 - U(t, \vec{x})$ for a point mass m . Please do not continue the tradition of propagating this wrong definition.

In defensiveness, some physicists are likely to retort that $\mathcal{L} = T - V$ for everything they care about, which is almost certainly not true unless they live in 1790. Because $\mathcal{H} = T + U$ for a Galilean particle and they intend $\mathcal{H} = T + V$, they intend $U = V$. Then, $\mathcal{L} = T - V$ becomes $\mathcal{L} = T - U$ which by equation (2.5.1) is equivalent to the statement that $\vec{K}$ and consequently any form of vector potential is 0. We will see when we study electromagnetism, any time dependence in electromagnetism implies there are both electric and magnetic fields to worry about. As well, we will see that in this case it is impossible for the vector potential to be 0 and so the fact that magnets and time dependent electromagnetic phenomena exist means that $\vec{K} \neq 0$ and $\mathcal{L} \neq T - V$ for many very common and important physical systems. Essentially every piece of modern

technology rests on $\mathcal{L} = T - V$ being **WRONG**. The final retort you are likely to hear when telling someone $\mathcal{L} \neq T - V$ is that $T - V$ is a useful rule of thumb for remembering what the Lagrangian is, at least for some systems. I personally prefer my rules of thumb to give correct answers, and so if you are interested in replacing this wrong rule with a correct one, please read Appendix C.

Not only does the $T - V$ rule fail for equation (2.5.1), literally the very first theory we have come up with, but it does not become true later on nor successfully describe the majority of the theories we will discuss in the remaining chapters of this book. It is fundamentally not the right way to think about the Lagrangian. **The right way to think about the Lagrangian is that it is some function which gives the dynamics of your system by the Euler-Lagrange equation. You pick the function to have the symmetries you think your system should have.** Appendix C gives a dictionary of common terms in the Lagrangian. The point of the rest of this book to understand where that dictionary comes from.

Exercises

Problem 2.11: Gauge transformation practice. Show that the potentials $(\phi_1, \vec{A}_1) = (0, kt\vec{x})$ and $(\phi_2, \vec{A}_2) = (\frac{1}{2}k|\vec{x}|^2, 0)$ are related by gauge transformation and find the gauge function $f(t, \vec{x})$ which relates them.

2.6 Equations of Motion

Now that we have our Lagrangian and Hamiltonian, let us compute the equation of motion:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} = \sum_s q_s \left(\nabla \left(\vec{A}_s \cdot \dot{\vec{x}} \right) - \nabla \phi_s \right) \quad (2.6.1)$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = m \dot{\vec{x}} + \sum_s q_s \vec{A}_s(t, \vec{x}(t)) \quad (2.6.2)$$

$$\Rightarrow \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = m \ddot{\vec{x}} + \sum_s q_s \left(\frac{\partial \vec{A}_s}{\partial t} + \left(\dot{\vec{x}} \cdot \nabla \right) \vec{A}_s \right) \quad (2.6.3)$$

Putting these pieces into the Euler-Lagrange equation of motion:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{\partial \mathcal{L}}{\partial \vec{x}} \quad (2.6.4)$$

$$\Rightarrow m \ddot{\vec{x}} + \sum_s q_s \left(\frac{\partial \vec{A}_s}{\partial t} + \left(\dot{\vec{x}} \cdot \nabla \right) \vec{A}_s \right) = \sum_s q_s \left(\nabla \left(\vec{A}_s \cdot \dot{\vec{x}} \right) - \nabla \phi_s \right) \quad (2.6.5)$$

$$\Rightarrow m \ddot{\vec{x}} = \sum_s q_s \left(-\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s + \nabla \left(\vec{A}_s \cdot \dot{\vec{x}} \right) - \left(\dot{\vec{x}} \cdot \nabla \right) \vec{A}_s \right). \quad (2.6.6)$$

At this point it is very convenient to use the double cross product identity:

$$\dot{\vec{x}} \times (\nabla \times \vec{A}) = \nabla (\dot{\vec{x}} \cdot \vec{A}) - (\dot{\vec{x}} \cdot \nabla) \vec{A}. \quad (2.6.7)$$

Therefore:

$$m \ddot{\vec{x}} = \sum_s q_s \left(-\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s + \dot{\vec{x}} \times (\nabla \times \vec{A}_s) \right). \quad (2.6.8)$$

The equation of motion for the particle only depends on two specific combinations of derivatives of the potentials ϕ_s and $\vec{A}_s$. These combinations are called the **electric fields** $\vec{E}_s$ and **magnetic fields** $\vec{B}_s$:

$$\vec{E}_s \stackrel{\text{def}}{=} -\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s \quad \vec{B}_s \stackrel{\text{def}}{=} \nabla \times \vec{A}_s. \quad (2.6.9)$$

(In physics, the word **field** is used for any function of position. So, the scalar and vector potentials are also fields even though their most common names don't use the word explicitly. This is entirely distinct from the use of the word field in math, such as the field of real numbers.) We know that the potentials (ϕ_s and $\vec{A}_s$) have a gauge transformation (2.5.11) under which the physical predictions (the equation of motion of the particle) are necessarily unchanged. Let us see how the electric and magnetic fields transform under this gauge transformation:

$$\vec{E}'_s = -\frac{\partial \vec{A}'_s}{\partial t} - \nabla \phi'_s = -\frac{\partial}{\partial t} (\vec{A}_s + \nabla f_s) - \nabla \left(\phi_s - \frac{\partial f}{\partial t} \right) = -\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s = \vec{E}_s \quad (2.6.10)$$

$$\vec{B}'_s = \nabla \times \vec{A}'_s = \nabla \times (\vec{A}_s + \nabla f_s) = \nabla \times \vec{A}_s = \vec{B}_s. \quad (2.6.11)$$

Thus, we see that the $\vec{E}_s$ and $\vec{B}_s$ are **gauge invariant**. That is, they are unchanged by gauge transformation. In terms of the fields, we get the general Galilean symmetric dynamics:

Theorem 2.8: Galilean Particle Equations of Motion in Euclidean Space

The equation of motion for a GCM point-particle is:

$$m \ddot{\vec{x}} = \sum_s q_s \left(\vec{E}_s + \dot{\vec{x}} \times \vec{B}_s \right). \quad (2.6.12)$$

The $\vec{E}_s$ and $\vec{B}_s$ fields are defined by:

$$\vec{E}_s = -\nabla \phi_s - \frac{\partial \vec{A}_s}{\partial t} \quad \vec{B}_s = \nabla \times \vec{A}_s. \quad (2.6.13)$$

And so, specifying the $\vec{E}_s$ and $\vec{B}_s$ fields determines the motion of our particle. However, it should be pointed out that $\vec{E}_s$ and $\vec{B}_s$ cannot be given arbitrarily. For example, consider the divergence of the $\vec{B}_s$ field:

$$\nabla \cdot \vec{B}_s = \nabla \cdot \nabla \times \vec{A}_s = 0. \quad (2.6.14)$$

The divergence of any curl is automatically 0 by a short calculation and so the divergence of $\vec{B}_s$ is always 0. Equation (2.6.14) is sometimes called the **Solenoid Law**. Further, by the commutativity of partial derivatives and that the curl of any gradient is 0:

$$\nabla \times \vec{E}_s = \nabla \times \left(-\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s \right) = -\frac{\partial}{\partial t} \nabla \times \vec{A}_s - \nabla \times \nabla \phi_s = -\frac{\partial \vec{B}_s}{\partial t} - 0 = -\frac{\partial \vec{B}_s}{\partial t} \quad (2.6.15)$$

$$\implies \nabla \times \vec{E}_s = \frac{\partial \vec{B}_s}{\partial t}. \quad (2.6.16)$$

Hence, some of the derivatives of $\vec{E}_s$ and $\vec{B}_s$ are related to each other. (2.6.16) is called **Faraday's Law**.

As long as we keep our assumption of space not having any holes, the Solenoid law and Faraday's law are "invertible" in the sense that they imply the existence of potentials ϕ_s and $\vec{A}_s$. First, use the fact that any divergenceless vector field can be written as the curl of another vector field:

$$\nabla \cdot \vec{B}_s = 0 \implies \exists \vec{A}_s : \nabla \times \vec{A}_s = \vec{B}_s. \quad (2.6.17)$$

This implication only holds because $\nabla \cdot \vec{B}_s = 0$ everywhere on space and we have assumed space is contractible. (In short, mathematically a space is contractible if you can make a transformation that continuously shrinks the space down to a single point. This isn't possible if the space has any "missing points" i.e. holes. For example, a ball is contractible but a donut is not. We assumed in GCMIII that space is topologically like the volume of ball with the radius taken to infinity and not like a donut or something more complicated.) Then, use the fact that a curl-free vector field can be written as the gradient of a scalar field:

$$\nabla \times \vec{E}_s = -\frac{\partial \vec{B}_s}{\partial t} = -\frac{\partial}{\partial t} \nabla \times \vec{A}_s = -\nabla \times \left(\frac{\partial \vec{A}_s}{\partial t} \right) \quad (2.6.18)$$

$$\implies \nabla \times \left(\vec{E}_s + \frac{\partial \vec{A}_s}{\partial t} \right) = 0 \implies \exists \phi_s : \vec{E}_s + \frac{\partial \vec{A}_s}{\partial t} = -\nabla \phi_s \implies \vec{E}_s = -\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s. \quad (2.6.19)$$

This implication also depends on the contractibility of space. For one final note on the relationship between the $\vec{E}_s$ and $\vec{B}_s$ fields and their potentials, we have already seen that if two potentials are related by a gauge transformation then they produce the same fields. The converse of this is also true (if space is contractible); that is, if two potentials produce the same fields, they are related by a gauge transformation. We can see this by considering two sets of potentials $\phi'_s, \vec{A}'_s$ and $\phi_s, \vec{A}_s$ which produce the same fields everywhere:

$$\vec{B}_s = \nabla \times \vec{A}_s = \nabla \times \vec{A}'_s \implies \nabla \times (\vec{A}'_s - \vec{A}_s) = 0 \implies \exists f_{s0}(t, \vec{x}) : \vec{A}'_s = \vec{A}_s + \nabla f_{s0}. \quad (2.6.20)$$

$$\vec{E}_s = -\frac{\partial \vec{A}_s}{\partial t} - \nabla \phi_s = -\frac{\partial \vec{A}'_s}{\partial t} - \nabla \phi'_s \implies \nabla \phi'_s = \nabla \phi_s - \frac{\partial}{\partial t} (\vec{A}'_s - \vec{A}_s) = \nabla \phi_s - \frac{\partial}{\partial t} \nabla f_{s0} \quad (2.6.21)$$

$$\implies \nabla (\phi'_s - \phi_s + \frac{\partial f_{s0}}{\partial t}) = 0 \implies \exists f_{s1}(t) : \phi'_s = \phi_s - \frac{\partial f_{s0}}{\partial t} + f_{s1}(t). \quad (2.6.22)$$

If we now define $f_s(t, \vec{x})$ by:

$$f_s(t, \vec{x}) = f_{s0}(t, \vec{x}) - \int_{t_0}^t f_{s1}(t') dt' \quad (2.6.23)$$

for an arbitrary constant time t_1 , we have:

$$\vec{A}'_s = \vec{A}_s + \nabla f_s, \quad \phi'_s = \phi_s - \frac{\partial f_s}{\partial t}. \quad (2.6.24)$$

Hence, the potentials are related by a gauge transformation.

We will often assume we are only dealing with one type of charge at a time for simplicity and so we will often not put an index on ϕ_s or $\vec{A}_s$ as there will only be one value for that index under such circumstances. Experimentally, there are only two types of charges found in the Galilean theory anyway (electric charge and gravitational charge) which we will explicitly discuss in the next chapter. Going forward we will just write as if we are considering one charge at a time and if one would like to consider a second type of charge we see here how to do so.

We have found that not only are $\vec{E}$ and $\vec{B}$ gauge invariant, but on a contractible space they are the complete set of independent gauge invariants as they can be used to reconstruct the potentials up to a gauge. This gives us:

Theorem 2.9: Gauge Transformations of the potentials

The potentials ϕ and $\vec{A}$ are only defined up to gauge transformation by the function f as:

$$\phi' = \phi - \frac{\partial f}{\partial t}, \quad \vec{A}' = \vec{A} + \nabla f. \quad (2.6.25)$$

This f necessarily drops out of any physical predictions of the theory. The $\vec{E}$ and $\vec{B}$ fields defined in terms of the potentials by:

$$\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t}, \quad \vec{B} = \nabla \times \vec{A} \quad (2.6.26)$$

are gauge invariant and satisfy:

$$\nabla \times \vec{E} = -\frac{\partial\vec{B}}{\partial t}, \quad \nabla \cdot \vec{B} = 0 \quad (2.6.27)$$

from their definition in terms of the potentials.

In a contractible region of space, $\vec{E}$ and $\vec{B}$ form a complete set of gauge invariants of the potentials. On such a domain, equation (2.6.27) in isolation is sufficient to imply the existence of potentials so that $\vec{E}$ and $\vec{B}$ can be written in terms of them in the form of (2.6.26). Two different pairs of potentials $(\phi, \vec{A})$ and $(\phi', \vec{A}')$ produce the same $\vec{E}$ and $\vec{B}$ on a contractible domain if and only if they are related by a gauge transformation.

It is often said (incorrectly) that the potentials $(\phi, \vec{A})$ are “unphysical” while the fields $\vec{E}$ and $\vec{B}$ are “physical”. (It is common to just call $\vec{E}$ and $\vec{B}$ “the fields” for short.) The more careful statement is that $(\phi, \vec{A})$ are not uniquely defined (because of the gauge transformation) while the $\vec{E}$ and $\vec{B}$ fields are (because of gauge invariance). However, because $\vec{E}$ and $\vec{B}$ can always be computed from the potentials, all of the “physics” of $\vec{E}$ and $\vec{B}$ is necessarily contained in $(\phi, \vec{A})$. Therefore, $(\phi, \vec{A})$ are at least as “physical” as $\vec{E}$ and $\vec{B}$. It is the gauge transformation function f which is “unphysical” because it always drops out of the equations of motion (by Theorem 1.6). Further, on a non-contractible domain it turns out to not be possible to infer the potentials up to gauge transformation from the $\vec{E}$ and $\vec{B}$ fields and so on a non-contractible domain **the potentials carry more physical information than the fields**. We will see in later chapters that this affects the outcomes of some real experiments! (An experimentally relevant example of a non-contractible domain is if you are studying the physics of a cylinder of material with a hole through the center down the cylinder axis. Particles that are trapped in that holey cylindrical body/long donut live in a non-contractible space.) **The potentials are the true physical variables.** The fields-only perspective is historically motivated and empirically outdated. One should view the non-uniqueness of the definition of the potentials as an ability to make a “choice of coordinates”. The coordinates of a point $\vec{x}$ are not uniquely defined (because we can apply a translation or rotation and our laws give the same description) but certainly the location of a point is “physical” as it is how we identify the motions of objects. Once you define your coordinate axes the coordinates of a point are well-defined. Similarly so, once you define your gauge the potentials are well-defined. Later in chapter 3 when we treat the potentials as variables to be varied, the gauge transformation will literally be a symmetry that they carry in the same way that translations and rotations are symmetries carried by the point particle. There is nothing “unphysical” about the situation, you just have to finish defining your variables to use them.

Exercises

Problem 2.12: The interpretation of mass. The goal of this question is to understand why it is reasonable to think about mass as “how difficult” an object is to move and charge as “how strongly” an object is affected by the potentials.

- (a) Taking (2.6.12), show that two objects with all the same charges and initial conditions experiencing $\vec{E}$ and $\vec{B}$ fields will have accelerations which are related inversely proportionally to their masses (1 line

to solve). Explain how this means that the mass m measures the difficulty of moving the object (its “inertia”).

- (b) More completely, consider an object experiencing only 1 $\vec{E}$ and for which that $\vec{E}$ field does not depend explicitly on time: $\vec{E}(t, \vec{x}) = \vec{E}(\vec{x})$ and no $\vec{B}$ fields: $\vec{B} = 0$. Show that the solution to the equation of motion (2.6.12) is:

$$\vec{x}(t) = \vec{x}_1 \left(\sqrt{\frac{q}{m}} t \right)$$

where $\vec{x}_1(t)$ is the solution to the differential equation:

$$\ddot{\vec{x}}_1 = \vec{E}(\vec{x}_1).$$

- (c) Explain how the relationship between $\vec{x}$ and $\vec{x}_1$ further justifies the interpretation of m as a property of an object which makes that object more difficult to move and how it also motivates interpretation q as how strongly an object is effected by $\vec{E}$.

Problem 2.13: Particle in a uniform $\vec{E}$ field. Consider a particle experiencing a constant and uniform $\vec{E}$ field and no $\vec{B}$ field. (Constant meaning $\vec{E}(t, \vec{x}) = \vec{E}(\vec{x})$ does not change with time and uniform field meaning $\vec{E}(\vec{x}) = \vec{E}$ is the same at all spatial locations.)

- Show that one choice of corresponding potentials is: $\phi = -\vec{E} \cdot \vec{x}$ and $\vec{A} = 0$.
- With this choice, show that the Lagrangian for this particle is $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + q\vec{E} \cdot \vec{x}$.
- Show that the particle moves with equation of motion $m\ddot{\vec{x}} = q\vec{E}$.
- Solve the equation of motion above.
- What geometric shape does the path followed by the particle in space make? (Hint: define the y direction as the direction of the $\vec{E}$ field, define the origin as the initial position of the particle, and define the xy plane as the plane spanned by $\vec{E}$ and the initial velocity of the particle.)

Problem 2.14: Particle in a uniform $\vec{B}$ field. Consider a particle experiencing a constant and uniform $\vec{B}$ field and no $\vec{E}$ field.

- Show that one choice of corresponding potentials is: $\phi = 0$ and $\vec{A} = \frac{1}{2}\vec{B} \times \vec{x}$.
- With this choice, show that the Lagrangian for this particle is $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \frac{q}{2}\vec{B} \cdot (\vec{x} \times \dot{\vec{x}})$.
- Show that the particle moves with equation of motion $m\ddot{\vec{x}} = q\dot{\vec{x}} \times \vec{B}$.
- Define the z direction as the direction in which $\vec{B}$ is pointing. Write the equations of motion above in components and solve them.
- What geometric shape does the path followed by the particle in space make?

Problem 2.15: Particle in both a uniform $\vec{E}$ and $\vec{B}$ field. Consider a particle experiencing a constant and uniform $\vec{E}$ field and a constant and uniform $\vec{B}$ field.

- Show that one choice of corresponding potentials is: $\phi = -\vec{x} \cdot \vec{E}$ and $\vec{A} = \frac{1}{2}\vec{B} \times \vec{x}$.
- With this choice, show that the Lagrangian for this particle is $\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \frac{q}{2}\vec{B} \cdot (\vec{x} \times \dot{\vec{x}}) + q\vec{E} \cdot \vec{x}$.
- Show that the particle moves with equation of motion $m\ddot{\vec{x}} = q(\vec{E} + \dot{\vec{x}} \times \vec{B})$.
- Define the z direction as the direction in which $\vec{B}$ is pointing and the yz plane to be the plane spanned by $\vec{E}$ and $\vec{B}$. Write the equations of motion above in components and solve them.
- What geometric shape does the path followed by the particle in space make?

Problem 2.16: ★ Aristotle’s Force. This question is credited to John P. Ralston. Let us go back to section 1.3, when we had coordinates only and before we had doubled to the phase space. For our configuration $Q = \vec{x}$ for a point-mass we would by equation (1.1.6) write that for some velocity field $\vec{v}(t, \vec{x})$:

$$\frac{d\vec{x}}{dt} = \vec{v}(t, \vec{x}).$$

- Argue based on time translational and space translational symmetry considerations that when isolated the function $\vec{v}(t, \vec{x})$ must be constant.
- Argue that different particles may respond to spatial/temporal inhomogeneities differently so that the

equation of motion can be rewritten:

$$\frac{d\vec{x}}{dt} = \frac{\vec{V}(t, \vec{x})}{m}$$

for some constant m which indicates the strength with which the particle is affected by the inhomogeneities and $\vec{V}(t, \vec{x})$ is some vector-field external to the particle.

- (c) Explain that any vector-field $\vec{V}(t, \vec{x})$ can be decomposed as:

$$\vec{V}(t, \vec{x}) = \nabla S(t, \vec{x}) - \vec{K}(t, \vec{x})$$

for some vector field $\vec{K}$ and scalar field S . As well, show that S and $\vec{K}$ are only defined up to modifying them by a function $f(t, \vec{x})$:

$$\vec{K}' = \vec{K} + \nabla f, \quad S' = S + f.$$

- (d) Differentiate the first order equation of motion for $\vec{x}$ to receive a second order equation of motion. Verify that by defining the function U as:

$$U(t, \vec{x}) = -\frac{\partial S}{\partial t} - \frac{|\vec{V}|^2}{2m}$$

the equation of motion becomes:

$$m \frac{d^2 \vec{x}}{dt^2} = -\frac{\partial \vec{K}}{\partial t} - \nabla U + \frac{d\vec{x}}{dt} \times (\nabla \times \vec{K}).$$

Compare this equation of motion with (2.6.8) (and so identify that (2.6.8) is trivially true for some potentials once we assume our configuration is given by a point).

- (e) Show that under the modification by f from earlier that U changes as:

$$U' = U - \frac{\partial f}{\partial t}.$$

As well, explain how the definition of U given above could have been predicted from the Hamilton-Jacobi equation and what we have learned in this chapter about a Galilean particle.

- (f) Show that the function S can be determined as:

$$S(t, \vec{x}) = S_0 + \int_0^t \left(\frac{1}{2} m |\dot{\vec{x}}|^2 + \vec{K}(t, \vec{x}) \cdot \dot{\vec{x}} - U(t, \vec{x}) \right) dt$$

(for some constant S_0) and that its variation, viewed as a functional of $\vec{x}(t)$, is 0 under the equation of motion. Thus conclude (as we had already established) that there is ultimately no content to the use of a stationary action to find equations of motion for this system beyond the assumption that equations of motion exist and that your set of variables is complete.

Problem 2.17: Poincare Gauge. Consider the Poincare gauge potentials defined by the following:

$$\phi(t, \vec{x}) = -\vec{x} \cdot \int_0^1 \vec{E}(t, \lambda \vec{x}) d\lambda, \quad \vec{A}(t, \vec{x}) = -\vec{x} \times \int_0^1 \vec{B}(t, \lambda \vec{x}) \lambda d\lambda.$$

Show by direct calculation that if the functions $\vec{E}(t, \vec{x})$ and $\vec{B}(t, \vec{x})$ satisfy the Solenoid law and Faraday's law (equation (2.6.27)) in all of space, then the potentials ϕ and $\vec{A}$ above reproduce $\vec{E}$ and $\vec{B}$ as their derivatives in the way demanded by definition (equation (2.6.26)). This explicitly shows that $\vec{E}(t, \vec{x})$ and $\vec{B}(t, \vec{x})$ determine the potentials up to a gauge transformation in a contractible region as in this Poincare gauge we are able to construct potentials from the electric and magnetic fields directly. Those potentials, as always, can be modified by a gauge transformation to give equivalent predictions for the motions of any charges. Explain how contractibility is assumed in the above integral formulas.

2.7 Effective Theories, Top Down and Bottom Up

So far we have considered particle motion to always have Galilean Boost Symmetry. This is true for a particle experiencing potentials (provided the potentials are transformed correctly with the particle, a point we will cover carefully next chapter) and even systems of particles experiencing potentials when we consider the motion of all of them. In this chapter so far, we have seen how the potentials affect the particle. In the next chapter, we will see how the particles affect the potentials. We will find that particles can affect each other indirectly through the potentials. That is, one particle affects the potential which another particle experiences and thus the two particles indirectly affect each other. Historically, before the potentials or even the fields were understood it was thought that the particles affected each other directly. We know now this is incorrect as we will see in chapter 4 (having point-particles interact directly we will learn is incompatible with the ideas of locality, that what happens at a point in the universe only depends on data around that point, and causality, that causes must happen before their effects). While the whole system of interacting particles and potentials has Galilean Boost Symmetry, it may not be the case (and usually isn't) that any particular subsystem will have Galilean Boost Symmetry (recall in section 1.2 the example of a mass on a spring, the wall, and translational symmetry). This is somewhat problematic when we consider that realistically describing the motion of objects means only describing a few variables and not all of the objects in the universe. Therefore, we do need to know how to consider subsystems to do the physics of anything practical. As well, we also at the moment have developed a theory for a single particle interacting with potentials. What happens when we would like to consider multiple particles? Do we have to start over? We need to also know how to compose subsystems together to form a larger system. Learning how to compose systems will give us hints on how to decompose them into subsystems as well, so let's go that way first.

The easiest case is when the subsystems that we would like to consider as one total system do not affect each other. Suppose Q_1 is the configuration of system 1 and that its equations of motion are given by the action $S_1[Q_1]$ and that Q_2 is the configuration of system 2 with its equations of motion given by the action $S_2[Q_2]$. By “do not affect each other” or “non-interacting” we mean that the equations of motion for Q_1 do not depend on Q_2 and the equations of motion for Q_2 do not depend on Q_1 . Then, because we would like to consider these both as part of one system we would have our total configuration $Q = (Q_1, Q_2)$ and we seek an action $S[Q]$ which produces both sets of equations of motion. Thus, we need the combined action to produce the same equation of motion functions as each subsystem action:

$$\frac{\delta S}{\delta Q_1^a} = \frac{\delta S_1}{\delta Q_1^a}, \quad \frac{\delta S}{\delta Q_2^a} = \frac{\delta S_2}{\delta Q_2^a}. \quad (2.7.1)$$

By the action recovery theorem (Theorem 1.7) then we can write:

$$S[Q_1, Q_2] \simeq \int_{t_0}^{t_f} Q^a \int_0^1 \frac{\delta S}{\delta Q^a} [\lambda Q] d\lambda dt \quad (2.7.2)$$

$$= \int_{t_0}^{t_f} Q_1^a \int_0^1 \frac{\delta S}{\delta Q_1^a} [\lambda Q] d\lambda dt + \int_{t_0}^{t_f} Q_2^a \int_0^1 \frac{\delta S}{\delta Q_2^a} [\lambda Q] d\lambda dt \quad (2.7.3)$$

$$= \int_{t_0}^{t_f} Q_1^a \int_0^1 \frac{\delta S_1}{\delta Q_1^a} [\lambda Q_1] d\lambda dt + \int_{t_0}^{t_f} Q_2^a \int_0^1 \frac{\delta S_2}{\delta Q_2^a} [\lambda Q_2] d\lambda dt \quad (2.7.4)$$

$$\simeq S_1[Q_1] + S_2[Q_2]. \quad (2.7.5)$$

Hence the action of a system composed of non-interacting subsystems is the sum of the actions of the individual subsystems. By the linearity of differentiation, this sum law carries down to the Lagrangian and the Hamiltonian:

$$\mathcal{L} = \frac{dS}{dt}[Q_1, Q_2] = \frac{dS_1}{dt}[Q_1] + \frac{dS_2}{dt}[Q_2] = \mathcal{L}_1(t, Q_1, \dot{Q}_1) + \mathcal{L}_2(t, Q_2, \dot{Q}_2) \quad (2.7.6)$$

$$\implies P'_1 = \frac{\partial \mathcal{L}}{\partial \dot{Q}_1} = \frac{\partial \mathcal{L}_1}{\partial \dot{Q}_1} = P_1, \quad P'_2 = \frac{\partial \mathcal{L}}{\partial \dot{Q}_2} = \frac{\partial \mathcal{L}_2}{\partial \dot{Q}_2} = P_2 \quad (2.7.7)$$

$$\implies \mathcal{H} = P'_1 \dot{Q}_1 + P'_2 \dot{Q}_2 - \mathcal{L} = P_1 \dot{Q}_1 - \mathcal{L}_1 + P_2 \dot{Q}_2 - \mathcal{L}_2 = \mathcal{H}_1(t, Q_1, P_1) + \mathcal{H}_2(t, Q_2, P_2). \quad (2.7.8)$$

Thus:

Theorem 2.10: Composition of non-interacting systems

If system 1 is described by the action $S_1[Q_1]$, Lagrangian $\mathcal{L}_1$, or Hamiltonian $\mathcal{H}_1$ and system 2 is described by the action $S_2[Q_2]$, Lagrangian $\mathcal{L}_2$, or Hamiltonian $\mathcal{H}_2$, then the composite system of both in which they do not interact is described by the action $S[Q_1, Q_2]$, Lagrangian $\mathcal{L}$, or Hamiltonian $\mathcal{H}$ defined by:

$$S[Q_1, Q_2] = S_1[Q_1] + S_2[Q_2] \quad (2.7.9)$$

$$\mathcal{L}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) = \mathcal{L}_1(t, Q_1, \dot{Q}_1) + \mathcal{L}_2(t, Q_2, \dot{Q}_2) \quad (2.7.10)$$

$$\mathcal{H}(t, Q_1, Q_2, P_1, P_2) = \mathcal{H}_1(t, Q_1, P_1) + \mathcal{H}_2(t, Q_2, P_2). \quad (2.7.11)$$

When the Q_1 and Q_2 do interact, they will then have some joint action $S[Q_1, Q_2]$ which is not simply the sum of their free actions $S_1[Q_1]$ and $S_2[Q_2]$. As such, the “interaction” term is defined as the difference between the joint action and the free actions:

$$S_{\text{int}}[Q_1, Q_2] \stackrel{\text{def}}{=} S[Q_1, Q_2] - S_1[Q_1] - S_2[Q_2] \quad (2.7.12)$$

$$\implies S[Q_1, Q_2] = S_1[Q_1] + S_2[Q_2] + S_{\text{int}}[Q_1, Q_2]. \quad (2.7.13)$$

This way, when there is no interaction the interaction term vanishes automatically. If we were only interested in the dynamics of the Q_1 , we would only need to consider the terms which depend on the Q_1 . Therefore, the action for “ Q_1 given Q_2 ” $S_{1|2}[Q_1|Q_2]$ which produces the correct dynamics for Q_1 at fixed Q_2 is defined as:

$$S_{1|2}[Q_1|Q_2] \stackrel{\text{def}}{=} S_1[Q_1] + S_{\text{int}}[Q_1, Q_2] \quad (2.7.14)$$

$$\implies S[Q_1, Q_2] = S_{1|2}[Q_1|Q_2] + S_2[Q_2]. \quad (2.7.15)$$

One can equivalently define the action of 2 given 1 by swapping all 1’s with 2’s and 2’s with 1’s in the previous two equations. By taking time derivatives, we can find that our decomposition extends down to the Lagrangian as well:

$$\mathcal{L}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) = \frac{dS[Q]}{dt} = \frac{dS_1[Q_1]}{dt} + \frac{dS_2[Q_2]}{dt} + \frac{dS_{\text{int}}[Q_1, Q_2]}{dt} \quad (2.7.16)$$

$$= \mathcal{L}_1(t, Q_1, \dot{Q}_1) + \mathcal{L}_2(t, Q_2, \dot{Q}_2) + \mathcal{L}_{\text{int}}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) \quad (2.7.17)$$

$$\mathcal{L}_{1|2}(t, Q_1, \dot{Q}_1|Q_2, \dot{Q}_2) = \frac{dS_{1|2}[Q_1|Q_2]}{dt} = \frac{dS_1[Q_1]}{dt} + \frac{dS_{\text{int}}[Q_1, Q_2]}{dt} \quad (2.7.18)$$

$$= \mathcal{L}_1(t, Q_1, \dot{Q}_1) + \mathcal{L}_{\text{int}}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) \quad (2.7.19)$$

Unfortunately, because any $\dot{Q}$ dependence in $\mathcal{L}_{\text{int}}$ affects the relationship between the conjugate momenta and the coordinates in the Legendre transformation, the pieces of the Lagrangian are not related to specific pieces of the Hamiltonian in a simple way. However, we can identify pieces of the Hamiltonian with the understanding that the only way to relate them to the Lagrangian is through the Legendre transformation between the total Lagrangian and the total Hamiltonian. Just as with the action, the interaction term of the Hamiltonian is simply defined as the difference between the total Hamiltonian and the sum of the free Hamiltonians:

$$\mathcal{H}_{\text{int}}(t, Q_1, Q_2, P_1, P_2) \stackrel{\text{def}}{=} \mathcal{H}(t, Q_1, Q_2, P_1, P_2) - \mathcal{H}_1(t, Q_1, P_1) - \mathcal{H}_2(t, Q_2, P_2). \quad (2.7.20)$$

Thus:

Theorem 2.11: Composition of Interacting Systems

If $S_{1|2}$ (or $\mathcal{L}_{1|2}$) is the Action (or Lagrangian) for the configuration Q_1 in the presence of a fixed Q_2 , then the Action (or Lagrangian) for the combined system (Q_1, Q_2) is:

$$S[Q_1, Q_2] = S_{1|2}[Q_1, Q_2] + S_2[Q_2] \quad (2.7.21)$$

$$\mathcal{L} = \mathcal{L}_{1|2} + \mathcal{L}_2 \quad (2.7.22)$$

where S_2 is the action of Q_2 when unaffected by Q_1 and $\mathcal{L}_2$ is the corresponding Lagrangian to that

action. Equivalently, the total action/Lagrangian/Hamiltonian are given by:

$$S[Q_1, Q_2] = S_1[Q_1] + S_2[Q_2] + S_{\text{int}}[Q_1, Q_2] \quad (2.7.23)$$

$$\mathcal{L}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) = \mathcal{L}_1(t, Q_1, \dot{Q}_1) + \mathcal{L}_2(t, Q_2, \dot{Q}_2) + \mathcal{L}_{\text{int}}(t, Q_1, Q_2, \dot{Q}_1, \dot{Q}_2) \quad (2.7.24)$$

$$\mathcal{H}(t, Q_1, Q_2, P_1, P_2) = \mathcal{H}_1(t, Q_1, P_1) + \mathcal{H}_2(t, Q_2, P_2) + \mathcal{H}_{\text{int}}(t, Q_1, Q_2, P_1, P_2) \quad (2.7.25)$$

where the “int” terms determine the interaction between Q_1 and Q_2 .

Now that we know how to put systems together, let's try to take them apart. That is, we want to develop how to find the **effective theory** for some of our valuables Q_1 without working directly with the rest of our variables Q_2 . In an effective theory, instead of seeking to describe a system fully and under all circumstances, we only seek to describe it to a sufficiently good approximation under special circumstances of interest. Those circumstances of interest are called the domain of validity of the effective theory. This is in contrast to a fundamental theory which is precisely a theory that intends to describe a system exactly and always. Naturally a theory can be “more” fundamental than another by being more broadly applicable and carrying fewer restrictions or vice versa. In a sense, all science not directly taking into account all known variables that could exist in a system is effective science. Because no one has ever successfully written down the fundamental theory of the universe, all science is effective science and all theories are effective theories. But, some science is more effective than others. So far we have been building up our theory of particles as if it is fundamental. Certainly we would like to find a fundamental description of the world. But, from a practical perspective, one cannot be sure they have included literally every variable in existence, only those variables which are known so far. We will find that our theory of point particles certainly cannot be fundamental and will have to be replaced by a more fundamental theory in Part II. Thus, our theory of point particles is absolutely an effective theory. An effective theory is generically simpler (as it cuts out what is not needed) and the action S_{eff} corresponding to the effective theory is called the **effective action**.

Consider a system with configuration $Q = (Q_1, Q_2)$ just as before with combined action $S[Q]$. The Q_1 will be the variables we are interested in and want to study (the Q_1 will be our system) while the Q_2 will be the variables we want to remove (the Q_2 are called “external variables” to Q_1). For example, Q_1 could be the position of an object on a table and Q_2 could be all of the variables of the positions of the masses making up the table. In principle, when the object rolls on the table it and all the masses within the table interact by *some* action. Because the Q_1 are not isolated (due to the interaction with the Q_2) rather than being an isolated system, it is called a **open system**. From the total action, the equation of motions for the Q_2 would be:

$$\frac{\delta S}{\delta Q_2}[Q_1, Q_2] = 0. \quad (2.7.26)$$

We know this gives second order differential equations by Euler-Lagrange. These equations of motion though will depend in some way on Q_1 since the two are allowed to interact. Suppose that we could solve these equations of motion and get $Q_2(t)$ for an arbitrary Q_1 . Because this is a differential equation and so is solved by integration, $Q_2(t)$ could depend on all of the values of $Q_1(t')$ for $t' \leq t$. Thus the solution for Q_2 is actually a functional of Q_1 , $Q_2[Q_1]$. In principle, we could take the equations of motion for Q_1 :

$$\frac{\delta S}{\delta Q_1}[Q_1, Q_2] = 0 \quad (2.7.27)$$

and insert our solution for Q_2 as a functional of Q_1 to get a integro-differential equation for Q_1 only. That is, a differential equation which depends not only on Q_1 and its derivatives but also potentially on integrals of Q_1 over its past values. When the reduced equation of motion for Q_1 depends on the whole history of Q_1 , the Q_1 are said to exhibit **hysteresis**. Hysteresis is the general case when precisely removing external variables and usually makes the resulting differential equations quite difficult to solve. However, often it is possible to approximately remove external variables so that there approximate description has no hysteresis. We can also get the effective integro-differential equation for Q_1 from an action. Consider inserting the solution $Q_2[Q_1]$ into the original action:

$$S_{\text{eff}}[Q_1] \stackrel{\text{def}}{=} S[Q_1, Q_2[Q_1]]. \quad (2.7.28)$$

Then, by the chain rule:

$$\frac{\delta S_{\text{eff}}}{\delta Q_1(t)}[Q_1, Q_2[Q_1]] = \left. \frac{\delta S}{\delta Q_1(t)} \right|_{Q_2[Q_1]} + \int_0^t \frac{\delta S}{\delta Q_2(t')} \frac{\delta Q_2[Q_1](t')}{\delta Q_1(t)} dt'. \quad (2.7.29)$$

Because the solution $Q_2[Q_1]$ is defined by solving (2.7.26), the functional derivative of the action with respect to Q_2 along it necessarily vanishes at each point in time. Thus, the integrand above is 0 and so we are left with:

$$\frac{\delta S_{\text{eff}}}{\delta Q_1(t)}[Q_1, Q_2[Q_1]] = \left. \frac{\delta S}{\delta Q_1(t)} \right|_{Q_2[Q_1]}. \quad (2.7.30)$$

Equating the right hand side above to 0 is exactly what is done in (2.7.27) to get the equation of motion for Q_1 . Therefore, we can use $S_{\text{eff}}[Q_1]$ for Q_1 to get the equations of motion for the Q_1 only. However, one should be careful. The solution $Q_2[Q_1]$ is found by varying the original action while keeping the end-points of the path (Q_1, Q_2) fixed (as defined in section 1.5). Therefore, when inserted back into the action, we have to express the solution in terms of the path Q_1 and the initial and final coordinates of Q_2 , not the initial coordinate and velocity of Q_2 . (If you use the initial velocity instead, you have to account for the fact that it is changed in the variation of Q_1 so that the final condition remains fixed. If you do not, you will not get the correct result.)

Solution-insertion can be useful when solving problems where some variables can be solved along the way as it allows one to systematically manage reduce the number of variables remaining. When variables are solved for and reinserted into the action those variables are said to be “integrated out”. Going from our underlying description (of both Q_1 and Q_2) down to an effective description of just Q_1 is called doing **top-down effective theory**. The presence of hysteresis makes the effective action defined above often very difficult to use. When an action has hysteresis it is certainly not of the form of (1.5.41) and so we cannot formulate a typical Lagrangian in terms of the coordinates and derivatives or similarly a Hamiltonian with coordinates and momenta for the system. This is because when there is hysteresis in the action, the time derivative (the Lagrangian) will depend on the whole past history of the system, not just coordinates and derivatives at the current time. So, while the theory has an action it is often not directly useful. There are a few special cases that allow us to simplify things however.

A convenient special case to solution-insertion is when the Lagrangian does not depend on $\dot{Q}_2$. That is, we have:

$$S[Q_1, Q_2] = \int_0^t \mathcal{L}(t, Q_1, \dot{Q}_1, Q_2) dt. \quad (2.7.31)$$

Then, the equation of motion for Q_2 becomes:

$$\frac{\delta S}{\delta Q_2^a} = \frac{\partial \mathcal{L}}{\partial Q_2^a} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{Q}_2^a} \right) = \frac{\partial \mathcal{L}}{\partial Q_2^a} - 0 \stackrel{!}{=} 0. \quad (2.7.32)$$

This implicitly defines Q_2 in terms of t, Q_1 , and $\dot{Q}_1$ but it does so without referencing the initial or final conditions for Q_2 and so there is no challenge directly substituting it into the Lagrangian. Evaluating the Lagrangian along the solution, we have:

$$\mathcal{L}_{\text{eff}} = \mathcal{L}(t, Q_1, \dot{Q}_1, Q_2(t, Q_1, \dot{Q}_1)). \quad (2.7.33)$$

Then, the Euler-Lagrange equation applied to $\mathcal{L}_{\text{eff}}$ becomes:

$$\frac{\partial \mathcal{L}_{\text{eff}}}{\partial Q_1^a} - \frac{d}{dt} \frac{\partial \mathcal{L}_{\text{eff}}}{\partial \dot{Q}_1^a} = \frac{\partial}{\partial Q_1^a} \left(\mathcal{L}(t, Q_1, \dot{Q}_1, Q_2(t, Q_1, \dot{Q}_1)) \right) - \frac{d}{dt} \frac{\partial}{\partial \dot{Q}_1^a} \left(\mathcal{L}(t, Q_1, \dot{Q}_1, Q_2(t, Q_1, \dot{Q}_1)) \right) \quad (2.7.34)$$

$$= \left. \frac{\partial \mathcal{L}}{\partial Q_1^a} \right|_{Q_2[Q_1]} + \left. \frac{\partial \mathcal{L}}{\partial Q_2^b} \right|_{Q_2[Q_1]} \frac{\partial Q_2^b}{\partial Q_1^a} - \frac{d}{dt} \left(\left. \frac{\partial \mathcal{L}}{\partial \dot{Q}_1^a} \right|_{Q_2[Q_1]} + \left. \frac{\partial \mathcal{L}}{\partial \dot{Q}_2^b} \right|_{Q_2[Q_1]} \frac{\partial Q_2^b}{\partial \dot{Q}_1^a} \right) \quad (2.7.35)$$

$$= \left. \frac{\partial \mathcal{L}}{\partial Q_1^a} \right|_{Q_2[Q_1]} + 0 - \frac{d}{dt} \left(\left. \frac{\partial \mathcal{L}}{\partial \dot{Q}_1^a} \right|_{Q_2[Q_1]} + 0 \right) \quad (2.7.36)$$

$$= 0. \quad (2.7.37)$$

Hence, directly inserting the solution for Q_2 just gives us back our Euler-Lagrange equation for Q_1 . So, when the Lagrangian is of the form of (2.7.33), solution-insertion is easy. In this case Q_2 is called an **insertable coordinate**.

Another convenient special case to solution-insertion is when the Hamiltonian does not depend on Q_2 . That is, we have:

$$\mathcal{H} = \mathcal{H}(t, Q_1, P_1, P_2). \quad (2.7.38)$$

Then, Hamilton's equations for Q_2 become:

$$\frac{dP_{2a}}{dt} = -\frac{\partial \mathcal{H}}{\partial Q_2^a} = 0 \implies P_2 = P_2(0). \quad (2.7.39)$$

Inserting the solved constant value of P_2 into the Hamiltonian does not affect the equations of motion for Q_1 or P_1 at all (as P_2 is held fixed under partial derivatives with respect to them anyway). Therefore, this allows us to define the effective Hamiltonian:

$$\mathcal{H}_{\text{eff}}(t, Q_1, P_1) = \mathcal{H}(t, Q_1, P_1, P_2(0)). \quad (2.7.40)$$

One can then perform the Legendre transform to get the corresponding effective Lagrangian. In this case, Q_2 is called an **ignorable coordinate** because it doesn't appear at all in the equations of motion. Together, we then have:

Theorem 2.12: Solution Insertion Theorem

If $S[Q_1, Q_2]$ is the action for variables Q_1 and Q_2 and the equations of motion for Q_2 are solved for arbitrary Q_1 to define a functional $Q_2[Q_1]$ in terms of the path Q_1 and the initial and final values of Q_2 , then the equations of motion for Q_1 are equivalently given by the effective action:

$$S_{\text{eff}}[Q_1] = S[Q_1, Q_2[Q_1]]. \quad (2.7.41)$$

If the Lagrangian for Q_1 and Q_2 does not depend on $\dot{Q}_2$, $\mathcal{L} = \mathcal{L}(t, Q_1, \dot{Q}_1, Q_2)$, then the Euler-Lagrange solution for Q_2 is insertable directly into $\mathcal{L}$ to get the effective Lagrangian for Q_1 only:

$$\frac{\partial \mathcal{L}}{\partial Q_2} = 0 \implies Q_2 = Q_2(t, Q_1, \dot{Q}_1) \quad (2.7.42)$$

$$\mathcal{L}_{\text{eff}}(t, Q_1, \dot{Q}_1) = \mathcal{L}(t, Q_1, \dot{Q}_1, Q_2(t, Q_1, \dot{Q}_1)). \quad (2.7.43)$$

If the Hamiltonian for Q_1, Q_2, P_1 , and P_2 does not depend on Q_2 , $\mathcal{H} = \mathcal{H}(t, Q_1, P_1, P_2)$, then Q_2 is ignorable, P_2 is constant, and the Hamiltonian evaluated at P_2 's constant value is the effective Hamiltonian for Q_1 and P_1 :

$$\mathcal{H}_{\text{eff}}(t, Q_1, P_1) = \mathcal{H}(t, Q_1, P_1, P_2(0)). \quad (2.7.44)$$

In general, solution-insertion is not so easy because of hysteresis and because one has to know how to express solutions in terms of initial and final coordinates rather than initial coordinates and velocities. One way to mitigate the challenge of hysteresis is to use Taylor's theorem for analytic functions:

$$Q(t') = Q(t + t' - t) = \sum_{n=0}^{\infty} \frac{(t' - t)^n}{n!} \cdot {}^n Q(t). \quad (2.7.45)$$

This allows us to write $Q(t')$ at a time in the past $t' < t$ as a series in the derivatives of $Q(t)$ in the present. By truncating the series at a finite number of terms, one can approximate the hysteresis terms in the action and still have something expressed only in terms of the current variables, thus allowing one to formulate a higher-derivative Lagrangian and corresponding Hamiltonian.

The above is all good when the full underlying action $S[Q_1, Q_2]$ is known, so that the effective action may be calculated. Unfortunately, one often does not know S in detail. In fact, one often doesn't even know what all of the Q_2 's are. (For a ball experiencing friction on a table, there are countless little interactions with the surface causing the net effect of friction. One certainly doesn't go and solve the equations of motion for the full microscopic details of the ball's surface and the table's surface just to get the resulting friction on the ball.) Fortunately, we are not completely lost. We know from Theorem 2.11 that the full action of the interacting system is given by:

$$S[Q] = S_1[Q_1] + S_2[Q_2] + S_{\text{int}}[Q_1, Q_2]. \quad (2.7.46)$$

Then, the equation of motion of Q_1 in the full system is:

$$\frac{\delta S}{\delta Q_1} = \frac{\delta S_1[Q_1]}{\delta Q_1} + \frac{\delta S_{\text{int}}[Q_1, Q_2]}{\delta Q_1} = 0. \quad (2.7.47)$$

Now evaluating this at the solution $Q_2[Q_1]$ of the equation of motion for Q_2 in terms of the Q_1 :

$$\frac{\delta S_1[Q_1]}{\delta Q_1} = - \left. \frac{\delta S_{\text{int}}}{\delta Q_1} \right|_{Q_2[Q_1]}. \quad (2.7.48)$$

Somewhat trivially, when Q_1 is free its motion is given by the stationary variation of S_1 ; therefore, when Q_1 is interacting its motion is given by setting the variation of its free action S_1 to something other than 0. The extent to which the variation of the free action of a variable fails to be stationary is called the **external force** on that variable:

$$F_{\text{ext}} \stackrel{\text{def}}{=} - \frac{\delta S_1[Q_1]}{\delta Q_1} \implies F_{\text{ext}}[Q_1] = \left. \frac{\delta S_{\text{int}}}{\delta Q_1} \right|_{Q_2[Q_1]}. \quad (2.7.49)$$

If we know the underlying theory, we have the right side of (2.7.49) as an exact expression for the external force. If we don't know the underlying theory, then we can simply say that there will be some unknown external force and write F_{ext} as a generic Taylor series expansion in Q_1 and its derivatives with unknown coefficients to be determined by experiment (because the underlying theory is not known, there is no other way to get the values of the coefficients). In this way, the external force is just a name for however we model whatever "other stuff" is affecting our variables Q_1 ⁶. When one builds up an effective theory from a free theory without knowing the underlying nature of the interaction, it is called doing **bottom-up effective theory**.

Occasionally, by using the action recovery Theorem 1.7, it may be possible to define an effective action, $S_{\text{eff}}[Q_1]$, without hysteresis for an effective theory so that the left side of (2.7.49) is actually the equation of motion given by that action in terms of Q_1 only. But, there is no guarantee that such an action in terms of only the reduced variables exists. Unfortunately, we are cursed with the fact that **subsystems of Hamiltonian systems may not be Hamiltonian**. (When an action has hysteresis, it is said to be non-Hamiltonian, as it prevents the typical formulation of a Hamiltonian or Lagrangian in terms of only the remaining variables evaluated at the present moment in time. Or, if adding extra degrees of freedom to get a variational principle it is also said to be non-Hamiltonian.) In the case that a hysteresis-free effective action in terms of only the reduced variables does exist, the external force is called "conservative". In the case there does not, it is called "non-conservative" or "dissipative". It is often said that there is no way to formulate dissipative systems in terms of an action, which is incorrect. The authors of [32] and [33] explicitly demonstrate how to do so. However, it does involve a doubled set of degrees of freedom (as one would expect given that the stationary action theorem involves such a doubling in general). We will cover this approach briefly shortly. Some external forces such as friction and viscosity are unfortunately typically non-conservative (usually this is the case when entire variables, like those in the table, are thrown out as integrating them out generically produces hysteresis). One can often find decent approximate models without hysteresis for non-conservative forces just by fitting coefficients to data in the general Taylor expansion for the external force. This is ultimately because many of these non-conservative forces result from our system experiencing interactions from a large number of basically identical smaller systems (an object moving through the air colliding with air molecules) and so the net effect on the object is often well approximated by the effect of each interaction multiplied by the rate of interactions per time. What happens in each interaction can often be calculated approximately in terms of the variables Q_1 (as well as its derivatives and some parameters about the small system). Then, assuming each interaction happens only over a short period of time, one gets an expression which only depends on Q_1 and derivatives at that time. This is not exact, but often good enough for applications and we will explore it in more detail as a general concept in chapter 5. Bottom-up effective theories are by their nature not exact, but good enough for an intended purpose so this is fine.

Non-conservative forces are commonly found when considering a subsystem which breaks some symmetries of the full system. In the case of the mass on the table, the interaction between the mass and the table breaks Galilean symmetry because when only the mass is boosted the dynamics are not equivalent to the mass unboosted due to relative motion against the table. Galilean boost symmetry would be retained if both the mass and the table were boosted, but not when only one is. The presence of external forces generally breaks the conservation laws of the system on which they act (due to the broken symmetries and Noether's insightful relationship between symmetries and conservation laws). In particular let us look at the energy. Considering the external force F_{ext} on a system Q with free action S_0 , free Lagrangian $\mathcal{L}_0$, free Hamiltonian

⁶Ernst Mach (1838-1916) was thoroughly critical of Newton and specifically described Newton's concept of force as tautological and unnecessary [63]. Here we can see that force is not so much an "essential physical concept" as it is just a name we give to how we model the terms in an equation of motion added in the presence of an interaction. At the end of the day, it is the equations of motion which predict what happens. If something isn't in the equations of motion, it isn't part of the theory.

$\mathcal{H}_0$, and free momentum P_0 :

$$F_{\text{ext}} = -\frac{\delta S_0}{\delta Q} = -\frac{\partial \mathcal{L}_0}{\partial Q} + \frac{d}{dt} \left(\frac{\partial \mathcal{L}_0}{\partial \dot{Q}} \right) = \frac{\partial \mathcal{H}_0}{\partial Q} + \frac{dP_0}{dt}. \quad (2.7.50)$$

Thus, the modified Hamilton's equations in the presence of an external force become:

$$\frac{dQ}{dt} = \frac{\partial \mathcal{H}_0}{\partial P_0}, \quad \frac{dP_0}{dt} = -\frac{\partial \mathcal{H}_0}{\partial Q} + F_{\text{ext}}. \quad (2.7.51)$$

In this case, the time derivative of the Hamiltonian becomes:

$$\frac{d\mathcal{H}_0}{dt} = \frac{\partial \mathcal{H}_0}{\partial t} + \frac{\partial \mathcal{H}_0}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial \mathcal{H}_0}{\partial P_{0a}} \frac{dP_{0a}}{dt} \quad (2.7.52)$$

$$= \frac{\partial \mathcal{H}_0}{\partial t} + \left(F_a^{\text{ext}} - \frac{dP_{0a}}{dt} \right) \frac{dQ^a}{dt} + \frac{dQ^a}{dt} \frac{\partial P_{0a}}{dt} \quad (2.7.53)$$

$$= \frac{\partial \mathcal{H}_0}{\partial t} + F_a^{\text{ext}} \frac{dQ^a}{dt}. \quad (2.7.54)$$

In the case that the free Hamiltonian has time translation symmetry, we can ensure we are in a gauge so that its partial time derivative is 0. Then, the free Hamiltonian is the energy of the system and we have that the rate of change of the energy of the system of Q 's is:

$$\frac{dE}{dt} = \frac{d\mathcal{H}_0}{dt} = F_a^{\text{ext}} \frac{dQ^a}{dt}. \quad (2.7.55)$$

Thus, the total change in the system's energy between an initial and final time is:

$$\Delta E = \int_{t_0}^{t_f} \frac{dE}{dt} dt = \int_{t_0}^{t_f} F_a^{\text{ext}} \frac{dQ^a}{dt} dt \quad (2.7.56)$$

$$\implies \Delta E = \int_{Q(t)} F_a^{\text{ext}} dQ^a \quad (2.7.57)$$

where here the integral bound is to indicate that the integral must be taken over the path $Q(t)$ followed by the system. The integral on the right hand side defines "the Work done on the system by external forces" W :

$$W \stackrel{\text{def}}{=} \int_{Q(t)} F_a^{\text{ext}} dQ^a. \quad (2.7.58)$$

Sometimes this is written in differential form as:

$$dW = F_a^{\text{ext}} dQ^a \quad (2.7.59)$$

where the bar is put through the differential on dW to indicate that it is typically an inexact differential as the result of the integral generically depends on the path of integration.

Theorem 2.13: Work-Energy Theorem

If S and $\mathcal{H}$ are the action and Hamiltonian of a system with configuration Q when that system experiences no external forces then that system has equations of motion:

$$-\frac{\delta S}{\delta Q^a} = F_a^{\text{ext}} \quad (2.7.60)$$

in the presence of external forces where the F_a^{ext} functions must be supplied. In this case the modified Hamilton's equations become:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a} + F_a^{\text{ext}}. \quad (2.7.61)$$

When the system's free Hamiltonian is time-independent the change in the system's energy between an initial and final state is given by the work done by the external forces:

$$\Delta E = W \stackrel{\text{def}}{=} \int_{Q(t)} F_a^{\text{ext}} dQ^a. \quad (2.7.62)$$

Now let us see how to derive non-conservative forces from a variational principle. Suppose you have identified by some modeling a set of external force F_a^{ext} experienced by your coordinates and that you have written these external forces as a functional of your coordinates (typically just an ordinary function of your

coordinates and one or two orders of differentiation at the present time). How can you tell if there is an effective term you could add to the action for the coordinates that would produce this external force from the variational principle? That is, what is the test for whether this force is conservative? One direct route is to simply appreciate that by the action recovery theorem 1.7 if it can be produced by an action in terms of only the coordinates you simply need to feed it into (1.8.28) to find the action term and then vary that term to verify it reproduces F_a^{ext} . There is a simple mathematical reason why this will reproduce some external forces but not reproduce others. Suppose you have a conservative external force F_a^{con} , meaning an external force for which there does exist an action $S_F[Q]$ so that:

$$F_a^{\text{con}} = \frac{\delta S_F[Q]}{\delta Q^a(t)}. \quad (2.7.63)$$

Then, simply take a second functional derivative of this equation:

$$\frac{\delta F_a^{\text{con}}(t)}{\delta Q^b(t')} = \frac{\delta^2 S_F[Q]}{\delta Q^a(t) \delta Q^b(t')} = \frac{\delta F_b^{\text{con}}(t')}{\delta Q^a(t)} \quad (2.7.64)$$

by using the interchangeability of partial derivatives. Therefore, a conservative external force has vanishing “functional curl”:

$$\frac{\delta F_a^{\text{con}}(t)}{\delta Q^b(t')} - \frac{\delta F_b^{\text{con}}(t')}{\delta Q^a(t)} = 0 \quad (2.7.65)$$

in the exact same way that a vector field which can be written as the gradient of a scalar field has vanishing vector curl (in fact these are exactly the same if you treat functional derivatives as the limit of ordinary partial derivatives). The converse is also true, just as in vector calculus: if an external force has vanishing functional curl then it can be written as the functional derivative of an action. This can be seen by feeding a generic F_a into the action recovery theorem and enforcing that varying should actually give you F_a back (this is shown in the homework).

Assuming you have used the action recovery method to incorporate whatever conservative forces into your action you can, you now only have remaining F^{ext} pieces which are non-conservative. These can still be implemented into your action at the cost of doubling the number of degrees of freedom. This approach is often called the “in-in formalism”. Let $\mathcal{L}$ be the Lagrangian for our coordinates of interest including all conservative forces and let F^{ext} be the remaining non-conservative forces. We introduce a second set of degrees of freedom $q^a(t)$, one for each of our original coordinates $Q^a(t)$, and seek an action $S_2[Q, q]$ of the doubled set so that the equations of motion for Q^a are precisely as desired. We also define the extra degrees of freedom so that their true physical values when the equations of motion are satisfied are to simply remain 0 (as we have just conjured them for convenience anyway). Define the dissipation potential $K[Q, q]$ from our non-conservative external forces by:

$$K[Q, q](t) = F_a^{\text{ext}}[Q](t)q^a(t) + \mathcal{O}(q^2). \quad (2.7.66)$$

I have marked that corrections of order q^2 in the ancillary degrees of freedom are allowed because they can be chosen arbitrarily without affecting any of the results of later calculations. Sometimes it may be convenient for the purposes of making formulas more aesthetic to introduce q^2 and higher pieces, however they contribute no true effect. Now consider the action:

$$S_2[Q, q] = \int_{t_0}^{t_f} \left(\mathcal{L}(t, Q + q/2, \dot{Q} + \dot{q}/2) - \mathcal{L}(t, Q - q/2, \dot{Q} - \dot{q}/2) + K[Q, q](t) \right) dt. \quad (2.7.67)$$

Because the contribution of the dissipation potential to the action is through adding it to the Lagrangian, the dissipation potential is only truly defined up at modifying it by total time derivatives. With this form of S_2 , it immediately follows that by varying with respect to q and then setting $q \rightarrow 0$ we have:

$$\left. \frac{\delta S_2}{\delta q^a} \right|_{q=0} = \frac{\partial \mathcal{L}}{\partial Q^a}(t, Q, \dot{Q}) - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^a}(t, Q, \dot{Q}) + F_a^{\text{ext}} \stackrel{!}{=} 0 \quad (2.7.68)$$

thus giving the proper equation of motion for our coordinates Q^a with the non-conservative forces included.

We should of course verify that it is consistent with the variational principle to just assert that $q^a = 0$. As a shorthand, define the equation of motion function of the conservative pieces:

$$E_a(t, Q, \dot{Q}, \ddot{Q}) = \frac{\partial \mathcal{L}}{\partial Q^a} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^a}. \quad (2.7.69)$$

Then, varying the action with respect to Q^a yields:

$$\frac{\delta S_2}{\delta Q^a} = E_a(t, Q + q/2, \dot{Q} + \dot{q}/2, \ddot{Q} + \ddot{q}/2) - E_a(t, Q - q/2, \dot{Q} - \dot{q}/2, \ddot{Q} - \ddot{q}/2) + \int_{t_0}^{t_f} q^b(t') \frac{\delta F_b^{\text{ext}}(t')}{\delta Q^a(t)} dt' \stackrel{!}{=} 0 \quad (2.7.70)$$

We choose the initial and final conditions on $q^a(t)$ to be 0 by definition of our variational principle. You will notice that setting $q(t)$ to 0 at all times identically solves the above equation of motion and so in fact the variational principle for S_2 fully determines $q^a(t)$ to be constantly 0 and $Q^a(t)$ to follow the dissipative equations of motion once the stationary of the action is applied. Anyone who says you can't get dissipative equations of motion from an action is wrong.

Exercises

Problem 2.18: ★ Newton's Second Law. Consider our Galilean symmetric particle to be experiencing some external forces $\vec{F}$. Show using (2.5.2) (the Lagrangian for a free Galilean particle) and Theorem 2.13 Newton's second law: "The equation of motion for a mass m is $\vec{F} = m\ddot{\vec{x}}$ where $\vec{F}$ is the external force on that mass". It should now be clear then that Newton's second law⁷ is not a fundamental basic postulate of the universe but instead a specific result about a specific Lagrangian (which until you know what to put for the external forces isn't even capable of determining the motion) which is only valid insofar as that system is a good model of reality. Fallaciously, some sources misunderstand the whole picture and believe analytical mechanics to be a "reformulation" of Newton's laws (or worse, a special case). Given that analytical mechanics will be the foundation of all chapters in both volumes of this text but Newton's laws will break down before even chapter 4 it should be clear to the reader that such a picture is fundamentally wrong and exactly flipped around.

Problem 2.19: ★ Lorentz Force Law. Consider our Galilean symmetric particle to be experiencing some potentials (only consider one kind of charge) so that the particle (as we have derived) has the Lagrangian (2.5.5) and equation of motion given by (2.6.12). Treating S_0 as the action corresponding to the free Galilean Lagrangian (2.5.2), derive that the external force produced by the potentials $(\phi, \vec{A})$ is:

$$\vec{F} = q(\vec{E} + \dot{\vec{x}} \times \vec{B}).$$

This result is known as the Lorentz Force Law.

Problem 2.20: ★ Newton's Third Law. Suppose we have two objects with positions $\vec{x}_1$ and $\vec{x}_2$ interacting and that their combined action is invariant under a translation. (Note: invariant means that not only is the action symmetric under the transformation but the surface term is 0 as well.)

- Show using Noether's theorem and Theorem 2.11 that the generator of translations of the whole system is $\vec{p}_1 + \vec{p}_2$ (called the total linear momentum of the system) where $\vec{p}_1$ and $\vec{p}_2$ are the conjugate momenta of $\vec{x}_1$ and $\vec{x}_2$ respectively.
- Due to the interaction, each object will experience an external force "due to the other object" (thus it is said to be "exerted" by the other object "onto" this object). Call the external force experienced by object 1 due to object 2 $\vec{F}_{2 \rightarrow 1}$ and the external force experienced by object 2 due to object 1 $\vec{F}_{1 \rightarrow 2}$. Show that the equations of motion for the two objects would be:

$$\frac{d\vec{p}_{10}}{dt} = \vec{F}_{2 \rightarrow 1}, \quad \frac{d\vec{p}_{20}}{dt} = \vec{F}_{1 \rightarrow 2}.$$

where $\vec{p}_{10}$ and $\vec{p}_{20}$ are the momenta of objects 1 and 2 as derived from their respective free Lagrangians.

- Assuming the whole system has translational symmetry and that the interacting Lagrangian produces the same total momentum as the free Lagrangians, show by Noether's theorem that:

$$\vec{F}_{1 \rightarrow 2} = -\vec{F}_{2 \rightarrow 1}.$$

Hence, under these conditions the force one object exerts on another is equal in magnitude and opposite in direction of the force the second object exerts on the first. This is often said informally as Newton's third law: "for every action there is an equal and opposite reaction". This result is only valid under the additional assumptions we have made that the particles have the same expression for their total momentum in the interacting theory as they do in the free theory, which is not true in general. As well, the statement by its nature assumes that particles only interact pairwise (how would one define the

⁷It is called Newton's second law although Newton himself never actually wrote $\vec{F} = m\ddot{\vec{x}}$ [107].

“force of 1 on 2” if there was a three way interaction? Such interactions do happen in physics, as we will see). It should now be clear then that Newton’s third law is not a fundamental basic postulate of the universe but instead a specific result about a specific Lagrangian (which assumes restricted possibilities for interactions) which is only valid insofar as that system is a good model of reality. Fallaciously, some sources misunderstand Newton’s third law to be necessary for momentum conservation by having no idea how Noether’s theorem works or what the definition of momentum is. In summary, all three of Newton’s laws have long since been superseded by much more general and much more powerful physics but they have a domain of applicability for sufficiently simple systems.

Problem 2.21: Falling due to gravity. Galileo apocryphally dropped objects of different masses from the leaning tower of Pisa and famously found that the different masses hit the ground at the same time. As well, he found that in order to multiply the time taken to fall to the ground by a factor, the height from which the object is dropped must be multiplied by the square of that factor. We will derive these facts from more fundamental considerations in the next chapter but for now simply take them as given. (There is a subtlety here caused by air resistance against the objects when the experiment is done for real. Here we neglect air resistance for simplicity, which is a better approximation the denser the object is and the smaller the cross sectional area of the object.)

- Show that the given relationship between the drop time and drop height implies the position of the dropped mass in the direction of falling is given by $y(t) = y(0) - \frac{1}{2}gt^2$ where g is constant to be determined by experiment. Show that g corresponds to the acceleration due to the force causing the falling (called gravity) and that the fact that the fall time is the same for different bodies implies they experience the same g .
- Show that the force of gravity on the falling object is given by $\vec{F} = (0, -mg, 0)$. Using that g is observed to be the same for different objects, infer that m is the “interaction charge” for the force of gravity.
- Using the equation of motion (2.6.12), find potentials $(\phi, \vec{A})$ which would produce the found force.
- Write the Lagrangian for this system with the potentials found in the previous part. Find the equations of motion of this system and show that when the initial conditions are as setup by Galileo ($\vec{x}(0) = (0, h, 0)$ where h is the height of the tower and $\dot{\vec{x}}(0) = 0$), the described results are reproduced.
- Find the energy corresponding to this Lagrangian and show that it is conserved by the dynamics.
- Explain how by dropping the mass from a variety of heights (which can be measured with our meter stick) and measuring the time necessary to fall (which can be measured by counting cycles of a periodic process), one can measure the value of g . It’s experimental value on Earth is $g = (9.81 \pm 0.02) \frac{\text{m}}{\text{s}^2}$.⁸ Because precision time-keeping devices were unavailable, Galileo famously counted his own pulse, sang bars of his favorite songs, or counted swings of a homemade pendulum to keep time in his experiments [24].

Problem 2.22: Projectile Motion. For this and many of the following questions the results of the previous question will be necessary. Consider an object of mass m launched from the ground at some angle θ above horizontal with speed v . Find the geometric shape of the path traced through the air, how far away from the launching point the object lands on the ground, and what angle will maximize that distance. Assume the ground is flat in your calculations.

Problem 2.23: Archery. Consider an arrow of mass m which is launched from a bow at a speed v making an angle θ above horizontal from a height h_0 above the ground. Ignoring any air resistance, if the archer would like to hit a target a horizontal distance ℓ away at an elevation of h , how high δh above the target must the archer aim? Assume the archer would prefer the more direct shot due to it being less sensitive to errors. In addition to the full solution, Taylor expand your solution for high speed arrows (v large, $1/v$ small) to get a simple lowest order expression for δh . What angular adjustment $\delta\theta$ (to lowest order) should the archer aim above the direct line from themselves to the target in order to have a successful hit?

Problem 2.24: A water feature. Consider a fountain which sprays water in all directions from a height h off of the ground. All the water leaves with the same speed v . Let the z axis be pointing out of the ground. Find the shape of the plume of the fountain. That is, find the surface $z(x, y)$ which together with the surface

⁸ g has been measured to many digits of precision, but its value varies over the Earth due to the Earth not being a perfectly homogeneous ball. At the poles, it reaches up to $g_{\text{poles}} = 9.83218493(78) \frac{\text{m}}{\text{s}^2}$ and at the equator its value is as low as $g_{\text{e}} = 9.78032(7) \frac{\text{m}}{\text{s}^2}$ [38]. The “standard” value taken is by definition $g = 9.80665 \frac{\text{m}}{\text{s}^2}$, which is chosen to approximate the value at a latitude of 45° above the equator [78].

of the ground at $z = 0$ bounds the region in which there is water throughout. As well, find the volume of the region which gets wet. (Assume each bit of matter in the water does not interact with any other bits.)

Problem 2.25: ★ Hooke's Law and the Harmonic Oscillator. Consider an object with position given by $x(t)$ moving in 1 dimension and experiencing an external force of the form $F(x)$. Let x_{eq} be a stable equilibrium of this system (equilibrium means that if x starts at rest at $x = x_{\text{eq}}$ then it remains there for all time, stable means that if x starts in a neighborhood of x_{eq} then it accelerates toward x_{eq} instead of away from it).

- Show that $F(x_{\text{eq}}) = 0$.
- Show that the lowest order Taylor expansion of $F(x)$ around x_{eq} is $F(x) \approx -k(x - x_{\text{eq}})$ for some positive constant k (assume $F'(x_{\text{eq}}) \neq 0$). This result is called Hooke's law: the given expression for force is valid in the neighborhood of a stable equilibrium⁹ for any mechanical system experiencing a coordinate dependent force. A common example is a spring, which applies a force based on the amount the spring is compressed (therefore position dependent). As such, the k appearing above is often called "the spring constant" of the spring.
- Show that the equation of motion implied by the force in the previous part can be derived from an effective Lagrangian of the form of (2.1.37) with the appropriate choice of potentials and find those potentials. Thus, show this system has an effective action.
- Show that the energy implied by the Lagrangian in the previous part is conserved by the equation of motion.
- Show that the general solution to the equation of motion of this system is:

$$x(t) = x_{\text{eq}} + A \cos(\omega t) + B \sin(\omega t)$$

where A and B are constants determined by initial conditions and $\omega = \sqrt{k/m}$, the angular frequency of oscillation. Because the system oscillates with a single frequency which is independent of the amplitude, this system is called a **simple harmonic oscillator**.

Problem 2.26: Measurements with a Mass on a Spring. Consider a mass m hanging vertically from a spring of unstretched length l and of spring constant k experiencing acceleration due to gravity g .

- Suppose that the length l is known (it has been measured by a meter stick), the mass m is defined as our reference unit of mass, and g and k are unknown. Explain how defining the period of oscillation of this system as a unit of time gives one a way to measure time by counting bounces of the mass. Thus, this device is the last tool needed to measure g in Galileo's experiment. Assume the value of g is known from Galileo's experiment for the rest of the question.
- Explain how by setting the system in equilibrium we can determine k in terms of our reference units.
- Suppose we have such a reference spring system with our reference mass attached and whose period gives our reference time. Explain how if we have another mass M whose value is unknown we can determine that mass in two different ways by replacing the reference mass on our original spring with it. Thus, this gives us a way to measure masses.
- Suppose we have our reference mass-spring system again and that we have another spring of unknown spring constant K . Explain how we can measure that spring constant by attaching our reference mass to it.

Problem 2.27: ★ Fundamental Fourier Integral. There is an integral we need many times for later results, and now is as good of a time as any to evaluate it.

- Let $\varepsilon > 0$ and k be real. Show the following:

$$\int_0^\infty e^{-(\varepsilon - ik)x} dx = \frac{1}{\varepsilon - ik}.$$

⁹Technically we haven't only assumed stability but linear stability. By this I mean that the term which causes acceleration back toward equilibrium is required to appear at linear order. In principle, the first derivative could be 0 as well as the second and the stabilizing term could be at cubic order or higher for generic stability. Or, $F(x)$ could be poorly behaved enough to not even be differentiable but still produce stable dynamics. However, we are generally safe in physics to assume the functions we are working with are differentiable. As well, because for any value of the first derivative other than 0 the equilibrium is either entirely stable or unstable we exclude consideration of the exact value of 0 except in the case that a symmetry would force the first derivative to vanish. That is, Hooke's Law is applicable to any stable equilibrium in physics for which there is not an additional symmetry that forces the stability to occur at a higher order instead.

- (b) Use part (a) to show that:

$$\int_{-\infty}^{\infty} e^{-\varepsilon|x|+ikx} dx = \frac{2\varepsilon}{\varepsilon^2 + k^2}.$$

- (c) Consider a function $f(k)$ which is continuous at $k = 0$ and otherwise sufficiently nice for you to commute limits in this question. Show that:

$$\lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\varepsilon|x|+ikx} f(k) dx dk = 2\pi f(0).$$

To do so, you will want to use the u -substitution $u = \frac{1}{\varepsilon}k$.

- (d) From the previous part, conclude using the definition of the Dirac delta that:

$$\lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} e^{-\varepsilon|x|+ikx} dx = 2\pi\delta(k).$$

When integrating against functions $f(k)$ which decay sufficiently quickly for large $|k|$, the $\varepsilon \rightarrow 0^+$ limit and integration with respect to k commute. Thus, when integrating this against sufficiently quickly decaying $f(k)$, one is safe writing:

$$\int_{-\infty}^{\infty} e^{ikx} dx = 2\pi\delta(k).$$

This integral is called the fundamental Fourier integral. Very often we integrate this fact against functions $f(k)$ for which the integral of $|f(k)|^2$ over all k converges. Such f are called “square-integrable”.

Problem 2.28: ★ Fourier Transform Primer. Consider a function $x(t)$ which is square-integrable. Define the **Fourier Transform** of $x(t)$ by:

$$\tilde{x}(\omega) = \mathcal{F}[x](\omega) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{2\pi}} x(t) dt.$$

In different applications, $x(t)$ may be a real valued or complex valued function. So, for generality, allow $x(t)$ to be complex valued for this question.

- (a) Show using the fundamental Fourier integral that the inverse Fourier transform is given by:

$$x(t) = \mathcal{F}^{-1}[\tilde{x}](t) = \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\sqrt{2\pi}} \tilde{x}(\omega) d\omega.$$

Explain how conceptually this formula expresses any (square-integrable) function as a linear combination of sines and cosines (remember Euler’s formula) of different frequencies. Then, explain how the original Fourier transform allows one to compute the coefficients of linear combination in the preceding expression.

- (b) Show that both the Fourier transform and inverse Fourier transform are linear functionals of their arguments. That is, they satisfy for functions $x(t)$ and $y(t)$ and constants a and b :

$$\begin{aligned} \mathcal{F}[ax(t) + by(t)] &= a\mathcal{F}[x] + b\mathcal{F}[y] \\ \mathcal{F}^{-1}[a\tilde{x} + b\tilde{y}] &= a\mathcal{F}^{-1}[\tilde{x}] + b\mathcal{F}^{-1}[\tilde{y}]. \end{aligned}$$

- (c) Show using integration by parts and that $|x(t)| \rightarrow 0$ as $|t| \rightarrow \infty$ that:

$$\mathcal{F}\left[\frac{dx}{dt}\right] = -i\omega\tilde{x}(\omega).$$

Iterate your argument to show further that:

$$\mathcal{F}\left[\frac{d^n x}{dt^n}\right] = (-i\omega)^n \tilde{x}(\omega).$$

- (d) Directly compute the Fourier transforms of the following functions: $x(t) = e^{-rt}\vartheta(t)$, $x(t) = e^{-r|t|}$, $x(t) = \vartheta(t+r)\vartheta(r-t)$, $x(t) = \sin(\omega_0 t)$, $x(t) = \cos(\omega_0 t)$, $x(t) = e^{-i\omega_0 t}$. Here $r > 0$ and $\vartheta(t)$ is the Heaviside step function which is defined as 1 for argument greater than 0, 0 for argument less than 0, and 1/2 for argument equal to 0. The last three of these functions are not square-integrable and so if you are being careful, you would add the exponential factor from the previous question to help with convergence. However, being slightly casual about that issue here will not end up hurting you (don’t get too used to being so lucky).
- (e) Show by direct computation and the fundamental Fourier integral that for square-integrable functions

$x(t)$ and $y(t)$:

$$\int_{-\infty}^{\infty} \tilde{x}^*(\omega) \tilde{y}(\omega) d\omega = \int_{-\infty}^{\infty} x^*(t) y(t) dt.$$

This result is known as Parseval's theorem.

(f) Show by direct computation that:

$$\mathcal{F}^{-1}[\tilde{x}(\omega) \tilde{y}(\omega)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x(\tau) y(t - \tau) d\tau.$$

This result is known as the convolution theorem and the integral containing x and y on the right hand side is called the convolution of $x(t)$ and $y(t)$.

- (g) Compute the Fourier transform of $x(t - \tau)$ in terms of $\tilde{x}(\omega)$, the Fourier transform of $x(t)$. (Here τ is a real number.)
- (h) Assume $x(t)$ is a real valued function. Show then that $\tilde{x}(-\omega) = \tilde{x}^*(\omega)$ and thus the Fourier transform of x is specified completely by its behavior for positive frequencies.

Problem 2.29: ★ Driven Harmonic Oscillator. Consider again the harmonic oscillator. However, now allow the oscillator to experience an external force $F(t)$ provided in addition to the effect of the spring (of spring constant $k = m\omega_0^2$) so that the equation of motion of the position of the mass is:

$$\ddot{x} + \omega_0^2 x = \frac{F(t)}{m}.$$

(a) Define the functions $a(t)$ and $b(t)$ by:

$$a(t) = x(t) \cos \omega_0 t - \frac{\dot{x}(t)}{\omega_0} \sin \omega_0 t$$

$$b(t) = x(t) \sin \omega_0 t + \frac{\dot{x}(t)}{\omega_0} \cos \omega_0 t.$$

Show then that $a(t)$ and $b(t)$ satisfy:

$$x(t) = a(t) \cos \omega_0 t + b(t) \sin \omega_0 t, \quad \frac{da}{dt} = -\frac{F(t)}{\omega_0 m} \sin \omega_0 t, \quad \frac{db}{dt} = \frac{F(t)}{\omega_0 m} \cos \omega_0 t.$$

(b) Solve the differential equations for $a(t)$ and $b(t)$ and use them to show that:

$$x(t) = a(t_0) \cos(\omega_0(t - t_0)) + b(t_0) \sin(\omega_0(t - t_0)) + \int_{t_0}^t \frac{F(t')}{\omega_0 m} \sin(\omega_0(t - t')) dt'.$$

As well, assuming that the solution $x(t)$ goes to 0 as t_0 goes to $-\infty$ (long enough in the past, there was no swinging), show that:

$$x(t) = \int_{-\infty}^t \frac{F(t')}{\omega_0 m} \sin(\omega_0(t - t')) dt'.$$

- (c) Because we started with a linear differential equation, the solution is always linearly related to the initial conditions and driving function. Because $x(t)$ is linearly related to $F(t')$ but may depend on $F(t')$ for all $t' < t$, that linear relationship is generically an integral of $F(t')$ against some function $G(t, t')$ called the Green's function of that differential equation. Whenever that system has time translational symmetry the Green's function only depends on the combination $t - t'$ and so can be written by abuse of notation as $G(t, t') = G(t - t')$. Find the Green's function for the harmonic oscillator. That is, find the function $G(t)$ so that:

$$x(t) = \int_{-\infty}^{\infty} F(t') G(t - t') dt'.$$

To do so you will need to use the initial condition that $x(t)$ goes to 0 as $t \rightarrow -\infty$ (different initial/final conditions lead to different but related Green's functions; the Green's function with this boundary condition is called the delayed Green's function). It will be useful to use the Heaviside step function $\vartheta(t)$ which is defined as 1 for argument greater than 0, 0 for argument less than 0, and 1/2 for argument equal to 0.

- (d) It is also fruitful to analyze this problem in the Fourier domain. Show from our original equation of

motion that the Fourier transforms $\tilde{x}(\omega)$ and $\tilde{F}(\omega)$ are related by:

$$\tilde{x}(\omega) = \frac{\tilde{F}(\omega)}{m(\omega_0^2 - \omega^2)}.$$

- (e) Whenever we start with a linear differential equation with time translational symmetry the Fourier transforms of the solution and the driving function are always proportional. The ratio of the Fourier solution ($\tilde{x}$) to the Fourier driving function ($\tilde{F}$) is called the propagator or transfer function of the system $\tilde{G}(\omega)$. That is: $\tilde{G}(\omega) \stackrel{\text{def}}{=} \frac{\tilde{x}}{\tilde{F}}$. Show that $\tilde{G}(\omega)$ is related to the Green's function $G(t)$ by:

$$G(t) = \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{2\pi} \tilde{G}(\omega) d\omega, \quad \tilde{G}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} G(t) dt.$$

- (f) The propagator $\tilde{G}(\omega)$ by definition gives the component of the solution which has angular frequency ω per input component of angular frequency ω . Thus, the magnitude $A(\omega) = |\tilde{G}(\omega)|$ gives how much the input at a given frequency is amplified in the output (so it is called the amplification). Determine $\tilde{G}(\omega)$ and $A(\omega)$ for our oscillator and plot A .
- (g) A local maximum of the amplification is called a resonance. The frequency at which that resonance occurs is called the resonant frequency. Find the resonant frequency of our oscillator. Conceptually, such a frequency corresponds to a frequency at which the system responds most strongly. So, it is said to “resonate”. Consider the system $x(t)$ to be in equilibrium at $t = 0$ and for an external force $F(t) = F_0 \sin(\omega t)$ to then be turned on for all $t > 0$. Find $x(t)$ for all $t > 0$ and explain how the solution is qualitatively different when $F(t)$ has the resonant frequency.

Problem 2.30: Collision Kinematics. Consider two masses m_1 and m_2 , each moving freely for a while which then crash into each other and then again move freely afterward.

- (a) Argue based on symmetry considerations that the total energy of the system and total momentum of the system are conserved by the dynamics, including the collision.
- (b) Given that the total momentum of the two masses is conserved, write the momentum of particle 1 after the collision ($\vec{p}_{1f}$) in terms of its momentum before the collision ($\vec{p}_{10}$) as: $\vec{p}_{1f} = \vec{p}_{10} - \Delta p \hat{n}$ where Δp is the magnitude of momentum transferred from particle 1 to particle 2 and $\hat{n}$ is the unit vector pointing in the direction of the momentum transfer. Use this form to show that the momentum of particle 2 after the collision is related to its momentum before the collision as: $\vec{p}_{2f} = \vec{p}_{20} + \Delta p \hat{n}$.
- (c) Given that the total energy of the two masses is conserved, show using the above expressions that if $\Delta p \neq 0$ (meaning a collision actually happens), then:

$$\Delta p = 2 \frac{m_1 m_2}{m_1 + m_2} \hat{n} \cdot (\vec{v}_{10} - \vec{v}_{20})$$

where $\vec{v}_{10}$ and $\vec{v}_{20}$ are the velocities of the masses before the collision. Hence, the particle's momenta/velocities after the collision can be determined using only conservation laws without needing to refer to the specifics of what happened in the collision process. When something can be derived from conserved quantities only it is called “kinematic”.

- (d) The above is true when the total energy and momentum of the masses are conserved in the collision. Such a collision is called “elastic”. However, when objects collide they might deform each other (by making a dent for example) or interact with the air (to make the sound of a BANG!). Because of this, while total energy is conserved, some of that energy might go into other forms than simply the energy of the masses. Consequently, the energy of just the sum of their free Hamiltonians may not be conserved in the collision. Typically though these alternate possibilities for the energy are spherically symmetric and so momenta goes in all directions, for a net momentum of loss to the other variables of 0 (as the momentum loses in different directions average out to having no preferential direction). So, even in “inelastic” collisions, collisions in which free particle energy of the masses is not conserved, momentum is still typically assumed to be conserved. (In reality, this too can fail to be the case and one can study the case in which there is a net momentum transfer to these other neglected variables.) Assuming that the total energy of the two masses after the collision is less than or equal to the energy before but that the momentum is still conserved, show that the momentum transfer now satisfies:

$$\Delta p \leq 2 \frac{m_1 m_2}{m_1 + m_2} \hat{n} \cdot (\vec{v}_{10} - \vec{v}_{20}).$$

- (e) Let $u = \hat{n} \cdot (\vec{v}_1 - \vec{v}_2)$ be the relative velocity of the masses in the direction of the momentum transfer.

Show that u after the collision, u_f , is related to u before the collision, u_0 , by:

$$u_f = u_0 - \frac{m_1 + m_2}{m_1 m_2} \Delta p.$$

- (f) A useful quantity for studying inelastic collisions is the coefficient of restitution ε defined by $\varepsilon = -u_f/u_0$. Show that in order for the masses to not pass through each other in the collision, the sign of their relative velocities in the direction of momentum transfer before and after the collision must be different. Using that fact and the previous two parts, show that:

$$0 \leq \varepsilon \leq 1.$$

- (g) Show that the momentum transfer is given in terms of the coefficient of restitution by:

$$\Delta p = (1 + \varepsilon) \frac{m_1 m_2}{m_1 + m_2} \hat{n} \cdot (\vec{v}_{10} - \vec{v}_{20})$$

and that the energy lost by the masses in the collision is given by:

$$E_{\text{lost}} = E_0 - E_f = \frac{1 - \varepsilon^2}{2} \frac{m_1 m_2}{m_1 + m_2} u_0^2.$$

Problem 2.31: The Momentum Reservoir. When you jump, where does your momentum come from? Consider the Earth to be a very a large mass M and you to be a small mass m . Suppose you are at rest relative to the Earth initially and then “jump” off the ground with some speed v .

- Show that the Earth’s velocity is changed by $-\frac{m}{M}v$ in the direction perpendicular to the surface.
- Show that the Energy you must put into jumping (assume you don’t waste any energy into anything else, like moving air; this is a lower bound) is $E = \frac{1}{2}m(1 + \frac{m}{M})v^2$.
- Imagine that the Earth was taken to be infinitely large. Show that in that limit, at finite energy input you leave the ground with speed $v = \sqrt{\frac{2E}{m}}$, momentum $p = mv$, and that the Earth does not move at all. Thus, an infinite mass acts like a “Momentum Reservoir”, allowing one to seemingly produce momentum for free. It seems as if this violates Noether’s theorem, which guarantees momentum conservation from translational symmetry. Explain how the limit $M \rightarrow \infty$ breaks translational symmetry and thus causes the breakdown of momentum conservation.

Problem 2.32: The Momentum Bomb. This question is credited to John P. Ralston. An alien civilization a large distance l away from Earth has found out about us, and they are not peaceful. However, their post-apocalyptic civilization has overwhelmed itself in garbage and has very little expendable energy. So, while they have essentially unlimited mass to throw at us, they have very little energy. Their plan is to send a very large mass toward Earth to disrupt our orbit about the Sun. Why do we have no reason to be worried? Think about scaling properties.

Problem 2.33: The Rocket Equation. Consider a rocket which propels itself forward by ejecting mass behind it. Because mass is simply emitted by the rocket, the total mass of the rocket and the fuel together is constant. Energy is supplied by some source within the rocket (a chemical reaction), causing the emission of fuel so that the relative velocity of the rocket to the fuel immediately after the fuel is emitted is $\vec{u}$. Let $m(t)$ be the mass of the rocket and its contents at time t .

- (a) Using conservation of momentum, show that the velocity $\vec{v}(t)$ of the rocket satisfies the rocket equation:

$$m \frac{d\vec{v}}{dt} = - \frac{dm}{dt} \vec{u}.$$

- (b) Solve the rocket equation to show that the velocity of the rocket is given by:

$$\vec{v}(t) = \vec{v}(0) + \vec{u} \ln \left(\frac{m(0)}{m(t)} \right).$$

- (c) Show that the necessary **power** ($\mathcal{P}$, rate at which energy is supplied) from the chemical reaction to make the rocket eject fuel as described is:

$$\mathcal{P} \stackrel{\text{def}}{=} \frac{dE}{dt} = \frac{1}{2} \left(- \frac{dm}{dt} \right) |\vec{u}|^2.$$

Problem 2.34: Equivalent or inequivalent? Revisited. Return to problem 1.25. Now that we know precisely what is meant by an external force, show that if a system is experiencing an external force $J(t)$ which is a given function of time then its Lagrangian can be modified to incorporate this external force by

simply adding a term $+J(t)Q$. Further, explain how this shows that the entire free Lagrangian (up to gauge transformation) can be probed by providing different $J(t)$ to a system (thus the Lagrangians appearing in problem 1.25 are genuinely inequivalent even though their free equations of motion are the same).

Problem 2.35: Conservation law of Galilean Boost Symmetry. By Noether's theorem, the generator of any continuous symmetry of our theory is conserved. We have already found the conservation laws corresponding to time translation (Energy), space translation (Linear Momentum), and rotation (Angular Momentum) but there is one more continuous symmetry we have: Galilean Boost Symmetry. In this problem we will explore its conservation law. Consider a theory of N particles interacting via a Galilean invariant interaction:

$$\mathcal{L} = \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + \mathcal{L}_{\text{int}}$$

so that the total theory has Galilean boost symmetry.

- (a) Show by direct calculation that under a Galilean boost applied at time t_b the surface term f added to the action under the transformation satisfies:

$$\vec{\mathcal{D}}f = \frac{d}{d\vec{v}} \int_{t_b}^t \mathcal{L}(t, \vec{x}', \dot{\vec{x}}') dt \Big|_{\vec{v}=0} = \sum_{n=1}^N (m_n \vec{x}_n(t) - m_n \vec{x}_n(t_b)).$$

- (b) Show using Noether's theorem that the generator of the symmetry is then given by:

$$\vec{G} = \sum_{n=1}^N (\vec{p}_n(t - t_b) - m_n(\vec{x}_n - \vec{x}_n(t_b))).$$

- (c) Assuming additionally time-translational symmetry and space-translational symmetry, show that the generator is equivalently:

$$\vec{G} = \sum_{n=1}^N (\vec{p}_n t - m_n \vec{x}_n).$$

This $\vec{G}$ is called the “dynamic mass moment” of the system.

- (d) Using the conservation laws established, show that the center of mass velocity:

$$\vec{v}_{\text{COM}} \stackrel{\text{def}}{=} \frac{\sum_{n=1}^N m_n \dot{\vec{x}}_n}{\sum_{n=1}^N m_n}$$

is conserved. Thus, Galilean Boost Symmetry ultimately implies (together with our other conservation laws) that the center of mass of the system will move at constant velocity.

Problem 2.36: Functional Poincare Lemma. Consider some external forces $F_a[Q](t)$ which depend on our degrees of freedom $Q^a(t)$. By the action recovery theorem, if those external forces can be derived from a variational principle involving $Q^a(t)$ only then (up to a surface term) the appropriate action that does so is:

$$S[Q] = \int_{t_0}^{t_f} \int_0^1 Q^a F_a[\lambda Q](t) d\lambda dt.$$

Previously we showed that if $F_a[Q](t)$ is able to be written as the functional derivative of an action then the functional curl of $F_a[Q](t)$, defined by:

$$\Omega_{ab}[Q](t, t') = \frac{\delta F_b[Q](t')}{\delta Q^a(t)} - \frac{\delta F_a[Q](t)}{\delta Q^b(t')}$$

- (a) Take the variational of S as defined above. Show that it becomes:

$$\begin{aligned} \delta S &= \int_{t_0}^{t_f} \int_0^1 \delta Q^a(t) F_a[\lambda Q](t) d\lambda dt + \int_{t_0}^{t_f} \int_0^1 \int_{t_0}^{t_f} \lambda Q^a(t) \delta Q^b(t') \frac{\delta F_a}{\delta Q^b(t')} [\lambda Q](t) dt' d\lambda dt \\ &= \int_{t_0}^{t_f} \int_0^1 \delta Q^a(t) F_a[\lambda Q](t) d\lambda dt + \int_{t_0}^{t_f} \int_0^1 \int_{t_0}^{t_f} \lambda Q^b(t') \delta Q^a(t) \Omega_{ab}[\lambda Q](t, t') dt' d\lambda dt \\ &\quad + \int_{t_0}^{t_f} \int_0^1 \int_{t_0}^{t_f} \lambda Q^b(t') \delta Q^a(t) \frac{\delta F_a}{\delta Q^b(t')} [\lambda Q](t) dt' d\lambda dt \end{aligned}$$

where in the above the functional derivatives of F_a are understood as being taken before evaluating it at λQ .

(b) Show that:

$$\frac{d}{d\lambda}(F_a[\lambda Q](t)) = \int Q^b(t') \frac{\delta F_a}{\delta Q^b(t')}[\lambda Q](t) dt'. \quad (2.7.71)$$

(c) Combine the results of the previous parts and do some integration by parts to show that in general:

$$\frac{\delta S}{\delta Q^a} = F_a[Q](t) + \int_0^1 \int_{t_0}^{t_f} \lambda Q^b(t') \Omega_{ab}[\lambda Q](t, t') dt' d\lambda. \quad (2.7.72)$$

Thus conclude that if the functional curl of F_a vanishes then indeed S can be used as an action to produce it, completing the converse.

2.8 Incorporating Constraints

Often instead of being able to move freely an object's motion may be restricted by its environment. Such a restriction is called a constraint. That is, there could be external forces on an object or between objects which restrict variables from being able to access all different values independently. As an example, consider a ball which is attached to a rod of fixed length and where the end of the rod is fixed in place. Then, the rod provides external forces to the ball to keep it satisfying the constraint of being the rod's length away from the pivot of the rod. Essentially, constraints are a special case of external forces in which those external forces are taken to be whatever they have to be to make the constraint satisfied. A completely rigid rod would allow the ball to move freely in directions which wouldn't change the ball's distance from the pivot but would act to prevent any motion which would. Any real rod would stretch and bend a bit due to the ball. But, in the limit that the rod is unbending and unstretching the constraint becomes exact. Constrained motion is taken as the limit that the restrictions are applied completely rigidly so that permitted motions are unscathed and nonpermitted motions are completely forbidden. Thus, constrained motion is a bottom-up effective theory. (It is bottom-up because it doesn't reference what the underlying cause of the constraint is; the constraint is just taken as given.)

Constrained motion is most easily formulated in terms of the action. For an unconstrained system, the equations of motion are found by setting the variation of the action to 0 (or matching the variation against the external force when such forces are present) for arbitrary variations δQ^a of the coordinates. For a constrained system, not all variations of the coordinates are possible because only some such variations will satisfy the constraints. Because the constraint forces will act to allow any motion consistent with the constraints as normal but prevent any motion which is inconsistent, variations of the coordinates which violate the constraints are forbidden (by the constraints) and the action's variation will vanish with respect to only variations of the coordinates which are consistent with the constraints (as they are permitted as normally). This is called **d'Alembert's principle: constrained motion is given by requiring the action to be stationary with respect to all variations which are consistent with the constraints**. All this model for constrained motion actually says is that the constraint forces act to prevent any path which violates the constraints but do nothing to paths which satisfy the constraints.

A more realistic model of the rod example would be to consider it like a spring which pulls toward being straight and the correct length. Then, the exactly rigid case would be gotten by taking the limit that the spring constant goes to infinity at the end. This same idea can be generalized to other constraints by modeling the constraint force by Hooke's law to push the system toward satisfying the constraint. An exactly rigid constraint would then be the limit that the spring constant is taken to infinity. Suppose our system has coordinate Q and should have constrained value Q_* . In the large spring constant limit, because Hooke's law's external force of $-k(Q - Q_*)$ diverges for any value of Q which doesn't satisfy the constraint permitted value of Q_* , the system is forced to rigidly satisfy the constraint. So, it prevents any motion which violates the constraint. As well, for configurations satisfying the constraint we see that there would be no external force due to Hooke's law. As such, in the limit we are right back to allowing constraint satisfying variations freely and completely forbidding constraint violating variations. So, d'Alembert's principle is equivalent to the limit in which approximate constraints become completely stiff.

Now that we have a model for how constraints work, let us study a few different important classes of them. First, we distinguish between equality constraints and inequality constraints. An equality constraint is any restriction on our variables which can be expressed in an equation. That is, there will be some functions $C^1(t, \phi), C^2(t, \phi), \dots$ of time t and variables ϕ (which variables are allowed to appear in the list ϕ define the different kinds of equality constraints) so that the allowed motions are those and only those values of ϕ which make all of the constraint functions 0: $C^\alpha(t, \phi) = 0$. We will use α as an index to list all of our constraint functions. For example, for the ball on a rod, the constraint would be $|\vec{x}| = l$ where $\vec{x}$ is the position of the ball relative to the pivot of the rod and l is the length of the rod. So, the constraint function is $C(t, \vec{x}) = |\vec{x}| - l$. (In the rod example there is only one constraint function.)

As a general technical point, to do much with the constraints we will need to make sure we define our constraint functions so that all of the variations of the different constraint functions are linearly independent for arbitrary variations $\delta\phi$ near values of ϕ which satisfy the constraints. If some initial set of constraint functions does not satisfy this it is typically not much effort to define new equivalent constraints so that the new ones do. For example, if we had a constraint that two coordinates x and y should both be 0, one bad way to write this constraint is: $C(x, y) = x^2 + y^2$. Certainly this vanishes if and only if $x = y = 0$ but the variation of this function is $\delta C = 2x\delta x + 2y\delta y$ which for values of x and y which satisfy the constraint is 0

and thus not linearly independent. We can instead take the system to have the two constraint functions as $C^1 = x$ and $C^2 = y$ which then have $\delta C^1 = \delta x$ and $C^2 = \delta y$ which are now not able to be written as linear combinations of each other when considering general δx and δy . We will also assume that our constraint functions are sufficiently smooth functions (as many derivatives exist as we need) in a neighborhood of the application of the constraint.

Equality constraints can be divided into 3 important basic classes. The first class we will discuss are called coordinate constraints or holonomic constraints. These are constraints with constraint functions $C^\alpha(t, Q)$ that only depend on time and the coordinates Q^a of the configuration space. So, holonomic constraints restrict our coordinates. For our example of a ball on a rod we found our constraint function to be $C(t, \vec{x}) = |\vec{x}| - l$ which is holonomic. Because holonomic constraints don't depend on the velocities $\dot{Q}$ or the momenta P (by definition), they are the easiest to work with. As well, they are the most common type of constraint and so it is important to learn about them now. All other equality constraints are called nonholonomic. All of our coverage of nonholonomic constraints can be skipped now if you like and returned to when they are referenced later. Holonomic constraints we will use often; nonholonomic constraints we will use occasionally as needed. The second class of equality constraints we will discuss are called velocity constraints¹⁰. They are constraints where the constraint functions $C^\alpha(t, Q, \dot{Q})$ may depend on both the coordinates and their velocities. These types of constraints occur often when the motion of different parts of a system are connected to each other, like in a bicycle or car. These are less common than holonomic and more difficult to work with but still show up occasionally and are manageable. The third class of equality constraints we will discuss are called phase space constraints which are constraints of the form $C^\alpha(t, Q, P) = 0$ for some functions C^α on the extended phase space. These we will not use this chapter but they become essential in understanding electromagnetism and the other interactions in our universe later on. Phase space constraints arise in systems which have redundancies in their phase space. It should be noted that the methods for all the different constraints can be applied together without conflicting. That is, within a single situation one may have several simultaneous holonomic and nonholonomic constraints on the variables of the system.

An inequality constraint is any restriction on our variables which can only be expressed in an inequality. For example, if our object were in a box which is fixed in place and the box is completely impenetrable then we would have constraints that the position of our object must be within the box. If say the left end of the box is at $x = 0$ and the right end is at $x = l$ we would then have that the x coordinate of our object must satisfy $0 \leq x(t) \leq l$. We will not have much to say on inequality constraints but they are worth mentioning.

2.8.1 Holonomic Constraints

Holonomic constraints are the most important class of constraints and analytical mechanics handles them very efficiently. These are constraints which can be put in the form $C^\alpha(t, Q) = 0$ for some functions $C^\alpha(t, Q)$. By d'Alembert's principle the action for a holonomically constrained system is only allowed to be varied by a variation δQ^a if both Q^a and $Q^a + \delta Q^a$ satisfy the constraints. Hence, if δQ^a is an allowed variation, the C^α must not change under it. The fact that $C^\alpha(t, Q + \varepsilon \delta Q)$ must remain 0 for allowed δQ^a implies that the ε derivative of C^α vanishes at $\varepsilon = 0$:

$$\delta C^\alpha = \lim_{\varepsilon \rightarrow 0} \frac{C^\alpha(t, Q + \varepsilon \delta Q) - C^\alpha(t, Q)}{\varepsilon} = \frac{\partial C^\alpha}{\partial Q^a} \delta Q^a = 0. \quad (2.8.1)$$

The set of all variations δQ^a forms a vector space of dimension equal to the number of Q 's. The $\frac{\partial C^\alpha}{\partial Q^a}$ taken as components of a matrix define a matrix with its number of rows equal to the number of constraints and number of columns equal to the number of Q 's. By equation (2.8.1) when that matrix is multiplied onto a vector δQ of allowed variations the result is the 0 vector (the summation over the index a in the product is matrix multiplication). Thus, not all of the components of the δQ can be chosen independently because allowed variations must be in the null space of the given matrix. Equation (2.8.1) gives a number of vanishing linear combinations of the δQ^a equal to the number of constraint functions C^α and so reduces the dimension of the space of linearly independent allowed variations by that number (because we have made our constraints have linearly independent variations by definition, it will reduce the dimension of the linearly independent allowed variations by exactly that number). Equivalently, for each α we can define a vector V^α with components given by $\frac{\partial C^\alpha}{\partial Q^a}$ and equation (2.8.1) gives that a variation δQ^a is allowed if and only if it is orthogonal to all of the V^α vectors. When we take the variation of the action $S_0[Q]$ of the unconstrained

¹⁰It is also possible to have higher derivative constraints handled in a very similar way. See [28], [29].

theory we have:

$$\delta S_0 = \int_{t_0}^{t_f} \frac{\delta S_0}{\delta Q^a} \delta Q^a dt. \quad (2.8.2)$$

When we did unconstrained variation, the δQ^a could be chosen independently and so the variation of the action was guaranteed to vanish only when the coefficients $\frac{\delta S_0}{\delta Q^a}$ vanished. However, now that the δQ^a are not all independent, it is possible for the action's variation to vanish without all of the coefficients vanishing. Requiring equation (2.8.2) to vanish implies that at each time the integrand is 0 (the variations are independent of each other at different times because the constraints all only depend on the present time, they don't for example depend on both $Q(t)$ and $Q(t')$). Requiring the integrand in equation (2.8.2) to be 0 under all allowed variations looks like it gives a new linear combination of the δQ^a which must be 0. Consequently, it looks like it defines a new vector V' with components $\frac{\delta S_0}{\delta Q^a}$ that all of the allowed variations must be orthogonal to. However, we know that equation (2.8.1) gives the full set of linear redundancies because any variation satisfying equation (2.8.1) maintains the constraints and once the constraints are satisfied all remaining variations are allowed. Therefore, requiring the integrand in equation (2.8.2) to be 0 cannot provide a V' which is linearly independent of the V^α meaning V' must be a linear combination of the V^α . This is true separately for each time and so the coefficients of linear combination typically depend on time. In components the statement that V' must be a linear combination of the V^α is simply that for some $\lambda_\alpha(t)$:

$$\frac{\delta S_0}{\delta Q^a} = -\lambda_\alpha(t) \frac{\partial C^\alpha}{\partial Q^a}. \quad (2.8.3)$$

Equation (2.8.3) is the equation of motion for holonomic constraints. The coefficients λ_α have to be determined by algebraic manipulation of equation (2.8.3) and $C^\alpha(t, Q) = 0$. With the definition of external force in (2.7.49), equation (2.8.3) implies that the external force necessary to enforce the constraint (called the constraint force) is:

$$F_a^{\text{ext}} = \lambda_\alpha \frac{\partial C^\alpha}{\partial Q^a}. \quad (2.8.4)$$

By rearranging equation (2.8.3) we can also find that it can be derived directly from a modified action without assuming a constraint:

$$\frac{\delta S_0}{\delta Q^a} + \lambda_\alpha \frac{\partial C^\alpha}{\partial Q^a} = 0 \quad (2.8.5)$$

$$\Rightarrow \frac{\delta}{\delta Q^a} \left(S_0 + \int_{t_0}^{t_f} \lambda_\alpha C^\alpha dt \right) = 0 \quad (2.8.6)$$

where here the δQ^a are treated as independent of each other and of λ_α . Hence, if we define the action $S_\lambda[Q, \lambda]$ by:

$$S_\lambda[Q, \lambda] = S_0[Q] + \int_{t_0}^{t_f} \lambda_\alpha(t) C^\alpha(t, Q) dt \quad (2.8.7)$$

then the stationary variation of S_λ with respect to Q^a simply gives equation (2.8.5) and the stationary variation of S_λ with respect to λ_α gives:

$$\frac{\delta S_\lambda}{\delta \lambda_\alpha} = C^\alpha(t, Q) = 0 \quad (2.8.8)$$

which are simply our original constraints. Thus, the constrained variation of S_0 under the holonomic constraints $C^\alpha(t, Q)$ is equivalent to the unconstrained variation of $S_\lambda[Q, \lambda]$. This realization is actually just the Lagrange multiplier theorem of ordinary vector calculus but generalized to apply to functionals (where the $\lambda_\alpha(t)$ are the multipliers). For values of Q which satisfy the constraints, $S_\lambda[Q, \lambda] = S_0[Q]$ because the additional term is 0.

Holonomic constraints can also be formulated in a way which reduces the total number of variables in the problem and thus viewed as implying a redundancy on the configuration space. This is often the most useful approach. The set of configurations Q for which the constraint functions vanish defines some region in the configuration space called the constraint manifold. (Manifold is just an expensive word for surface smooth enough to do calculus on; we will use them in many different contexts and treat them more precisely later.) Because we will be restricted to being on this subset of the whole configuration space, it is a good idea to find coordinates that parameterize this region. That is, we find variables q^μ so that any

configuration Q which satisfies the constraints can be written in terms of these variables: $Q^a = f^a(t, q)$ for some functions f . Therefore, these functions must satisfy $C^\alpha(t, f(t, q)) = 0$ and the requirement $Q^a = f^a(t, q)$ is equivalent to our original constraints $C^\alpha(t, Q) = 0$. Because each independent constraint function can in principle be used to solve for one of the Q 's in terms of the others (using the inverse function theorem), the number of q 's (reduced coordinates) will be the number of Q 's minus the number of constraint functions. In our example of a ball on the end of a rod, the constraint is $C(\vec{x}) = |\vec{x}| - l = 0$. This means the constraint manifold is a sphere of radius l around the origin in the configuration space. We can parameterize a sphere by two angles in spherical coordinates as $\vec{x} = (l \cos \varphi \sin \theta, l \sin \varphi \sin \theta, l \cos \theta)$. Hence, for this example our q would be $q = (\theta, \varphi)$. There are two q 's because we had three Q 's: (x, y, z) minus one constraint. If we write equation (2.8.5) in terms of our reduced coordinates and contract it with $\frac{\partial f^a}{\partial q^\mu}$, we have:

$$\left. \frac{\delta S_0}{\delta Q^a} \right|_{Q=f(t,q)} + \lambda_\alpha \left. \frac{\partial C^\alpha}{\partial Q^a} \right|_{Q=f(t,q)} = 0 \quad (2.8.9)$$

$$\Rightarrow \left. \frac{\delta S_0}{\delta Q^a} \right|_{Q=f(t,q)} \frac{\partial f^a}{\partial q^\mu} + \lambda_\alpha \left. \frac{\partial C^\alpha}{\partial Q^a} \right|_{Q=f(t,q)} \frac{\partial f^a}{\partial q^\mu} = 0. \quad (2.8.10)$$

This first term can be rewritten using the functional derivative chain rule (1.6.8) as:

$$\left. \frac{\delta S_0}{\delta Q^a} \right|_{Q=f(t,q)} \frac{\partial f^a}{\partial q^\mu} = \frac{\delta}{\delta q^\mu} S_0[f(t, q)]. \quad (2.8.11)$$

This second term can be rewritten using the chain rule of ordinary vector calculus as:

$$\left. \frac{\partial C^\alpha}{\partial Q^a} \right|_{Q=f(t,q)} \frac{\partial f^a}{\partial q^\mu} = \frac{\partial C^\alpha(t, f(t, q))}{\partial q^\mu}. \quad (2.8.12)$$

Because $C^\alpha(t, f(t, q)) = 0$ for all values of q^μ , all of the partial derivatives in equation (2.8.12) vanish:

$$\left. \frac{\partial C^\alpha}{\partial Q^a} \right|_{Q=f(t,q)} \frac{\partial f^a}{\partial q^\mu} = \frac{\partial C^\alpha(t, f(t, q))}{\partial q^\mu} = 0. \quad (2.8.13)$$

Hence, equation (2.8.10) can be rewritten as:

$$\frac{\delta}{\delta q^\mu} S_0[f(t, q)] = 0. \quad (2.8.14)$$

Thus, for holonomic constraints, if one finds coordinates q^μ which parameterize the region in configuration space which satisfies the constraints then the constrained motion is simply given by the stationary variation of the action in which the $Q^a = f^a(t, q)$ are directly inserted into the unconstrained action:

$$S_{\text{con}}[q] = S_0[f(t, q)]. \quad (2.8.15)$$

The direct substitution of the constraints into the action is especially convenient as to do this method one never has to compute the multipliers λ_α .

I promised earlier that d'Alembert's principle is equivalent to the limit of an arbitrarily strong restoring force. Let us see how that works here. Consider a system which is not fully constrained but instead has the equation of motion of a restoring force toward the constraint:

$$\frac{\delta S_0}{\delta Q^a} = -F_a^{\text{ext}} = k(Q^a - f^a(t, q)). \quad (2.8.16)$$

This way, if the constraint is not satisfied (meaning $Q^a \neq f^a$), there is a term in the equation of motion which will accelerate the Q^a back in the direction of satisfying the constraint. By the action recovery theorem, we can actually integrate equation (2.8.16) to get an action which produces this equation of motion:

$$S_k[Q, q] = S_0[Q] - \frac{k}{2} \int_{t_0}^{t_f} (Q^a - f^a(t, q))(Q^a - f^a(t, q)) dt. \quad (2.8.17)$$

By direction calculation, this action does reproduce equation (2.8.16) as its equation of motion for Q^a . As well, varying with respect to q^μ gives:

$$\frac{\delta S_k}{\delta q^\mu} = -k \frac{\partial f^a}{\partial q^\mu}(t, q) (Q^a - f^a(t, q)) \stackrel{!}{=} 0. \quad (2.8.18)$$

By inserting equation (2.8.16) into equation (2.8.18), we get:

$$\frac{\partial f^a}{\partial q^\mu}(t, q) \frac{\delta S_0}{\delta Q^a}[Q] = 0. \quad (2.8.19)$$

By taking the $k \rightarrow \infty$ limit of equation (2.8.17) we get:

$$\frac{1}{k} \frac{\delta S_0}{\delta Q^a} = Q^a - f^a(t, q) \quad (2.8.20)$$

$$\implies \lim_{k \rightarrow \infty} (Q^a - f^a(t, q)) = \lim_{k \rightarrow \infty} \frac{1}{k} \frac{\delta S_0}{\delta Q^a} = 0. \quad (2.8.21)$$

Hence as promised, the constraint $Q^a = f^a(t, q)$ is satisfied in the $k \rightarrow \infty$ limit. In that limit then, we can replace Q in equation (2.8.19) by $f(t, q)$:

$$\frac{\partial f^a}{\partial q^\mu}(t, q) \frac{\delta S_0}{\delta Q^a} [f(t, q)] = 0. \quad (2.8.22)$$

This is exactly the same as equation (2.8.11) and so we see that the limit of strong restoring force does indeed reproduce our previous equations of motion. All of this together gives us:

Theorem 2.14: Holonomic Constraint Theorem

If a system with configuration Q whose unconstrained dynamics are given by the stationary variation of the action $S_0[Q]$ is constrained by the holonomic constraints $C^\alpha(t, Q) = 0$, then the constrained system has dynamics given by requiring that action be stationary under variations consistent with those constraints. That is equivalent to the unconstrained stationary variation of the action:

$$S_\lambda[Q, \lambda] = S_0[Q] + \int_{t_0}^{t_f} \lambda_\alpha(t) C^\alpha(t, Q) dt. \quad (2.8.23)$$

If the constraint manifold of points on the configuration space so that the constraints are satisfied is parameterized by coordinates q so that $Q^a = f^a(t, q)$, then the constrained equations of motion are equivalently given by the stationary variation of the action:

$$S_{\text{con}}[q] = S_0[Q]|_{Q=f(t, q)}. \quad (2.8.24)$$

All of this is equivalent to the limit of a restoring force of arbitrary strength which pulls the coordinates Q onto the constraint manifold.

2.8.2 Velocity Constraints

Velocity constraints are when we require functions $C^\alpha(t, Q, \dot{Q})$ to vanish. One has to be slightly more careful here to make sure they include only variations which satisfy the constraints. Now that our constraint functions depend on velocity, at a given value of t and Q , they restrict possible velocities $\dot{Q}$. Consider two paths $Q(t)$ and $Q'(t)$ which both satisfy the constraint and at a time t_* pass through the same value of the configuration Q_* . That is, $Q(t_*) = Q'(t_*) = Q_*$. Then, to both satisfy the constraint they must have:

$$C^\alpha(t_*, Q_*, \dot{Q}(t_*)) = C^\alpha(t_*, Q_*, \dot{Q}'(t_*)) = 0. \quad (2.8.25)$$

Then, in a time δt , the path difference which develops between $Q(t)$ and $Q'(t)$ is:

$$\delta Q^a = \lim_{\varepsilon \rightarrow 0} \frac{Q'^a(t_* + \varepsilon \delta t) - Q^a(t_* + \varepsilon \delta t)}{\varepsilon} \quad (2.8.26)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{Q'^a(t_* + \varepsilon \delta t) - Q_*^a + Q_*^a - Q^a(t_* + \varepsilon \delta t)}{\varepsilon} \quad (2.8.27)$$

$$= \dot{Q}'^a \delta t - \dot{Q}^a \delta t = (\dot{Q}'^a - \dot{Q}^a) \delta t. \quad (2.8.28)$$

Rearranging, we have:

$$\dot{Q}'^a(t_*) = \dot{Q}^a(t_*) + \frac{\delta Q^a}{\delta t}. \quad (2.8.29)$$

Because again the variation of the constraint necessarily vanishes we have:

$$0 = \delta C^\alpha = \lim_{\varepsilon \rightarrow 0} \frac{C^\alpha(t_*, Q_*, \dot{Q}(t_*) + \varepsilon \frac{\delta \dot{Q}}{\delta t}) - C^\alpha(t_*, Q_*, \dot{Q}(t_*))}{\varepsilon} = \frac{\partial C^\alpha}{\partial \dot{Q}^a} \frac{\delta \dot{Q}^a}{\delta t} \quad (2.8.30)$$

$$\implies \frac{\partial C^\alpha}{\partial \dot{Q}^a} \delta \dot{Q}^a = 0. \quad (2.8.31)$$

Hence, equation (2.8.31) gives the equivalent linear interdependencies of the variations for velocity

constraints that equation (2.8.1) gave for the coordinate constraints. Thus, by the same logic as before, in order for the action to be stationary under all variations satisfying equation (2.8.31), there must be coefficients λ_α (which may depend on time) so that:

$$\frac{\delta S_0}{\delta Q^a} = -\lambda_\alpha \frac{\partial C^\alpha}{\partial \dot{Q}^a}. \quad (2.8.32)$$

This follows immediately by our previous reasoning for holonomic constraints where instead of $\frac{\partial C^\alpha}{\partial Q^a}$ providing a matrix so that δQ^a must be in its null space, now $\frac{\partial C^\alpha}{\partial \dot{Q}^a}$ provides that matrix. Beyond that point the reasoning is identical.

Importantly, unlike in the holonomic case, this result is **not** the same as just naively adding Lagrange multipliers to the original action. To arrive at equation (2.8.32) we had to carefully only consider path variations which were consistent at each moment in time with our constraints. When we do Lagrange multipliers we actually take all variations, even ones which do not satisfy the constraints, and then the constraints are enforced at the end by the equations of motion given by the varying the action with respect to the multipliers. In the holonomic case, the operations of varying and then applying the constraints or applying the constraint and then varying are the same. They happen to commute. In the nonholonomic case, they do not. Thus it is **incorrect** to apply the Lagrange multiplier method for velocity constraints (because doing so includes paths in the variation which are inconsistent with those constraints even after constraints are imposed at the end). Let us see explicitly that these two methods are different. If we took the unconstrained action and added Lagrange multipliers for our constraints we would have:

$$\text{(Incorrect)} \quad S_\xi[Q, \xi] = S_0[Q] + \int_{t_0}^{t_f} \xi_\alpha C^\alpha(t, Q, \dot{Q}) dt \quad (2.8.33)$$

$$\text{(Incorrect)} \quad \Rightarrow \frac{\delta S_\xi}{\delta \xi_\alpha} = C^\alpha(t, Q, \dot{Q}) = 0 \quad (2.8.34)$$

$$\text{(Incorrect)} \quad \Rightarrow \frac{\delta S_\xi}{\delta Q^a} = \frac{\delta S_0}{\delta Q^a} + \xi_\alpha \frac{\partial C^\alpha}{\partial Q^a} - \frac{d}{dt} \left(\xi_\alpha \frac{\partial C^\alpha}{\partial \dot{Q}^a} \right) \stackrel{!}{=} 0 \quad (2.8.35)$$

This equation of motion is completely different than (2.8.32). The two do not match. Because the nonholonomic constraint is nonintegrable (cannot be rewritten as a reduction of the number of coordinates), naive variation of the Lagrange multiplier action includes paths in the variation which do not satisfy the constraints and so it produces the wrong result. Some sources [37] incorrectly state without justification that the Lagrange multiplier method applies to nonholonomic constraints but other sources [34], [28], [29] further explore why doing so is incorrect. (The error in [37] has since been acknowledged and corrected with an errata from the authors. They are far from the only authors to have ever made this mistake. This mistake has a history of rediscovery and redaction.)

Further, the nonintegrability of the constraints prevents a direct substitution rule like (2.8.24) from existing (which can also be used to show the multiplier method will fail). However, there is a weak sort of analog. The constraints (2.8.25) make the $\dot{Q}^a$'s not all independent. Using the constraints, it is possible to solve for some of the $\dot{Q}^a$ in terms of some of the other ones. So, let us partition the Q into two sets: $Q = (q, \tilde{q})$ where we will use the constraints to write the $\tilde{q}^\alpha$ in terms of the $\dot{q}^\mu$. Thus, there are the same number of $\tilde{q}^\alpha$ as there are constraints (assuming all of the constraints are linearly independent; if they are not you can reduce the number of constraints so that they are anyway). After solving for the $\tilde{q}^\alpha$, we will have that our constraints are reexpressed as:

$$\frac{d\tilde{q}^\alpha}{dt} = f^\alpha(t, q, \tilde{q}, \dot{q}) \quad (2.8.36)$$

for some functions f^α which are determined from the previous C^α . This reexpression of the constraints is done just by algebraically solving for some of the velocities. This reexpression is still in the same form as our original C^α if we identify new constraint functions C'^α as:

$$C'^\alpha(t, Q, \dot{Q}) = \dot{\tilde{q}}^\alpha - f^\alpha(t, q, \tilde{q}, \dot{q}). \quad (2.8.37)$$

Then, using (2.8.32) and this new choice of constraint functions the equations of motion for the $\tilde{q}$ become:

$$\frac{\delta S_0}{\delta \tilde{q}^\alpha} = -\lambda_\beta \frac{\partial C'^\beta}{\partial \dot{\tilde{q}}^\alpha} = -\lambda_\beta \delta_\alpha^\beta = -\lambda_\alpha. \quad (2.8.38)$$

Hence by solving for some of the velocities, it automatically determines the λ_α . Using these values of the λ_α

in (2.8.32) the equations of motion for the q become:

$$\frac{\delta S_0}{\delta q^\mu} = -\lambda_\alpha \frac{\partial C^\alpha}{\partial \dot{q}^\mu} = \frac{\delta S_0}{\delta \tilde{q}^\alpha} \left(-\frac{\partial f^\alpha}{\partial \dot{q}^\mu} \right) \quad (2.8.39)$$

$$\implies \frac{\delta S_0}{\delta q^\mu} + \frac{\partial f^\alpha}{\partial \dot{q}^\mu} \frac{\delta S_0}{\delta \tilde{q}^\alpha} = 0. \quad (2.8.40)$$

If we now consider the variation of the original action:

$$\delta S = \int_{t_0}^{t_f} \frac{\delta S}{\delta Q^a} \delta Q^a dt = \int_{t_0}^{t_f} \left(\frac{\delta S}{\delta q^\mu} \delta q^\mu + \frac{\delta S}{\delta \tilde{q}^\alpha} \delta \tilde{q}^\alpha \right) dt \quad (2.8.41)$$

then we can see if we take the variations $\delta \tilde{q}^\alpha$ to be constrained as:

$$\delta \tilde{q}^\alpha = \frac{\partial f^\alpha}{\partial \dot{q}^\mu} \delta q^\mu \quad (2.8.42)$$

then the action's constrained variation becomes:

$$\delta S = \int_{t_0}^{t_f} \left(\frac{\delta S_0}{\delta q^\mu} + \frac{\partial f^\alpha}{\partial \dot{q}^\mu} \frac{\delta S_0}{\delta \tilde{q}^\alpha} \right) \delta q^\mu. \quad (2.8.43)$$

Hence, by equation (2.8.40) the requirement that the action be stationary under such constrained variations reproduces the correct nonholonomic equations of motion (2.8.32). This all gives us:

Theorem 2.15: Velocity Constraint Theorem

If a system with configuration Q whose unconstrained dynamics are given by the stationary variation of the action $S_0[Q]$ is constrained by the velocity constraints:

$$C^\alpha(t, Q, \dot{Q}) = 0 \quad (2.8.44)$$

then the constrained dynamics are given by:

$$\frac{\delta S_0}{\delta Q^a} = -\lambda_\alpha(t) \frac{\partial C^\alpha_a}{\partial \dot{Q}^a} \quad (2.8.45)$$

for some functions $\lambda_\alpha(t)$. If some of the velocities are solved for using the constraints, calling $\tilde{q}^\alpha$ the coordinates whose velocities are solved for and the rest of the coordinates q^μ , then the constraints can be reexpressed as:

$$\dot{\tilde{q}}^\alpha = f^\alpha(t, q, \tilde{q}, \dot{q}) \quad (2.8.46)$$

for some functions f^α . Then, the equations of motion of the constrained dynamics can be rewritten as:

$$\frac{\delta S_0}{\delta q^\mu} + \frac{\partial f^\alpha}{\partial \dot{q}^\mu} \frac{\delta S_0}{\delta \tilde{q}^\alpha} = 0. \quad (2.8.47)$$

These exact same techniques can be generalized to constraints on higher derivatives of the coordinates. We will have no application for this but it is accomplished in [29].

2.8.3 (2nd Pass) Phase Space Constraints

The final class of equality constraints is to have constraints which are general functions of t, Q, P (that is, the constraints are formulated on the phase space instead of configuration space). This class of constraints was studied in detail by Dirac and so they are sometimes called Dirac constraints. It can be quite difficult to find literature on this topic, though it is an important subject. For further reading, I suggest [23], [22], [43]. The most common way phase space constraints will arise for us is that we will sometimes have a Lagrangian for which the Legendre transform to the Hamiltonian cannot be completed. This is because the momenta as computed from the Lagrangian for such a system will not be enough data to solve for the coordinate velocities. Because there are an equal number of momenta to the number of coordinate velocities, this is generically possible if some of the momenta are interrelated. These interrelations can then be written as constraints of the form $C^\alpha(t, Q, P) \stackrel{!}{=} 0$. (For a concrete example that will become relevant later on, consider the arclength Lagrangian $\mathcal{L} = |\dot{\vec{x}}|$. The momentum satisfies $|\vec{p}| = 1$ which is a phase space constraint and the Legendre transformation cannot be completed.)

When writing the action in Hamiltonian form as in theorem 1.4, we vary with respect to Q^a and P_a

independently:

$$S[Q, P] = \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}(t, Q, P)) dt. \quad (2.8.48)$$

Then, if we have constraint functions $C^\alpha(t, Q, P)$ which are to equal 0 for the allowed positions in phase space, we have the same mathematical structure to the problem as when we studied holonomic constraints with the configuration space directly replaced by the phase space. So, we should vary this action according to variations preserving the constraints and by the same line of argumentation as in equations (2.8.1)-(2.8.8) we have that this is equivalent to using the action:

$$S[\lambda, Q, P] = \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}(t, Q, P) + \lambda_\alpha(t) C^\alpha(t, Q, P)) dt \quad (2.8.49)$$

where the time dependent Lagrange multipliers $\lambda_\alpha(t)$ are to be varied independently along with the unconstrained variations of the coordinates and momenta. It may seem that now that we have this action we can use it to find equations of motion and we are simply at the end of the story. However, there are some subtleties to discuss. In the presence of the Lagrange multipliers λ_α , Hamilton's equations are modified to:

$$\frac{\delta S}{\delta P_a} = \dot{Q}^a - \frac{\partial \mathcal{H}}{\partial P_a} + \lambda_\alpha \frac{\partial C^\alpha}{\partial P_a} \stackrel{!}{=} 0 \implies \dot{Q}^a = \frac{\partial \mathcal{H}}{\partial P_a} - \lambda_\alpha \frac{\partial C^\alpha}{\partial P_a} \quad (2.8.50)$$

$$\frac{\delta S}{\delta Q^a} = -\dot{P}_a - \frac{\partial \mathcal{H}}{\partial Q^a} + \lambda_\alpha \frac{\partial C^\alpha}{\partial Q^a} \stackrel{!}{=} 0 \implies \dot{P}_a = -\frac{\partial \mathcal{H}}{\partial Q^a} + \lambda_\alpha \frac{\partial C^\alpha}{\partial Q^a}. \quad (2.8.51)$$

Because Hamilton's equations are different, the time derivative of a function $f(t, Q, P)$ on extended phase space is also given by a different than typical formula:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \dot{Q}^a + \frac{\partial f}{\partial P_a} \dot{P}_a = \frac{\partial f}{\partial t} \quad (2.8.52)$$

$$= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \left(\frac{\partial \mathcal{H}}{\partial P_a} - \lambda_\alpha \frac{\partial C^\alpha}{\partial P_a} \right) + \frac{\partial f}{\partial P_a} \left(-\frac{\partial \mathcal{H}}{\partial Q^a} + \lambda_\alpha \frac{\partial C^\alpha}{\partial Q^a} \right) \quad (2.8.53)$$

$$= \frac{\partial f}{\partial t} + \{f, \mathcal{H}\} - \lambda_\alpha \{f, C^\alpha\}. \quad (2.8.54)$$

Hence, the original Poisson bracket of the unconstrained theory does not serve as the effective Poisson bracket of the constrained theory (due to the extra term here) and in the constrained theory the phase space (Q, P) is not exactly the right set of variables (we also have the variables λ_α and cannot access all values of (Q, P) due to the constraints).

Going forward it is useful to introduce some notation which we will use in this section only unless explicitly reintroduced. When dealing with these constraints there are three different notions of equivalence for functions $f(t, Q, P)$ and $g(t, Q, P)$ on the phase space. First, there is standard equality written for two functions as $f = g$ if the functions $f(t, Q, P)$ and $g(t, Q, P)$ are exactly the same function independently of any further information about the values of (Q, P) (and thus independently of whether the constraints are applied). Second, there is weak equality written for two functions as $f(t, Q, P) \approx g(t, Q, P)$ if the functions f and g always take the same value for values of (Q, P) which satisfy all the constraints. Finally, there is strong equality written for two functions as $f(t, Q, P) \equiv g(t, Q, P)$ if the two functions f and g and their first derivatives always take the same values for values of (Q, P) which satisfy the constraints. In this notation the constraint functions satisfy $C^\alpha(t, Q, P) \approx 0$ but $C^\alpha(t, Q, P) \neq 0$ and $C^\alpha(t, Q, P) \not\equiv 0$. Because the Poisson brackets only take first derivatives, anything which is strongly equal to 0 has vanishing Poisson bracket with any other function once constraints are applied. If something is only weakly equal to 0, its first derivatives will not be weakly equal to 0 and it may have non-trivial Poisson brackets with other quantities. So, if $f \equiv g$ then g may be replaced by f in a Poisson bracket but if g only satisfies $f \approx g$ that replacement cannot be made.

The Dirac Algorithm

The constraint functions must vanish at all times by definition of the constrained system and so for values of the coordinates and momenta which satisfy the constraints, $\frac{dC^\alpha}{dt}$ must be 0. Thus we need $\frac{dC^\alpha}{dt} \approx 0$. Combining this with equation (2.8.54):

$$\frac{dC^\alpha}{dt} \approx 0 \implies \frac{\partial C^\alpha}{\partial t} + \{C^\alpha, \mathcal{H}\} - \lambda_\beta \{C^\alpha, C^\beta\} \approx 0. \quad (2.8.55)$$

This is in general a non-trivial property which must be checked for each constraint function if the combination

of the constraints and equations of motion are to be consistent. Explicitly computing, simplifying, and requiring the above to be weakly equal to 0 can lead to four different scenarios:

- (1) The result gives some linear equation of the λ_β which must hold with weak equality. The set of these then defines some of the λ_β by solving these equations.
- (2) The result is independent of the λ_β but does not vanish automatically and the left-hand side is not simply a constant. This gives some function D and condition of the form $D(t, Q, P) \approx 0$.
- (3) The result is independent of the λ_β and vanishes automatically (one arrives at $0 \approx 0$). This is consistent but tells you nothing.
- (4) The result is independent of the λ_β but does not vanish automatically and the left-hand side is a constant. It then becomes constant ≈ 0 for a nonzero constant, which is a contradiction. Then, the constraints and Hamiltonian are inconsistent with each other and there are no values of the Lagrange multipliers which can make the equations of motion true while satisfying the constraints. This is generally a bug of overly simple systems and not of concern for real systems of physical interest. In the case this scenario happens the theory is just wrong and must be modified somehow to get anything mathematically sensible.

Each time we encounter scenario (2) it gives a new independent function $D(t, Q, P)$ which is required to weakly vanish for consistency (if it were not independent it would vanish automatically and be scenario (3)). Let us call the list of these functions $D^\mu(t, Q, P)$ with μ running over all these new constraints. These D^μ are “hidden” initially; they are only revealed as constraints by combining the equations of motion and C^α constraints self-consistently. Because we now have two sets of constraints, the C^α are called primary constraints and the D^μ are called secondary constraints. Now not only do we take our full list of constraints to be the combined list of C^α and D^μ , but we also need to check that the D^μ remain weakly 0 under the equations of motion for consistency just like we did with the C^α . As well, because these constraints are required for consistency it means we did not correctly write down the variational principle in (2.8.49). If we had known about these necessary constraints, we would have included Lagrange multipliers $\lambda_{2\mu}(t)$ for them. Adding these, we must require:

$$\frac{dD^\mu}{dt} \approx 0 \implies \frac{\partial D^\mu}{\partial t} + \{D^\mu, \mathcal{H}\} - \lambda_\alpha \{D^\mu, C^\alpha\} - \lambda_{2\nu} \{D^\mu, D^\nu\} \approx 0. \quad (2.8.56)$$

We do this for each μ . Each of these will then fall exactly into one of the same 4 scenarios as could occur with the C^α . Assuming we have no inconsistencies, we will again have some scenario (1)’s which then can be used to determine more of the Lagrange multipliers and some scenario (2)’s which will then produce even more constraint functions, now tertiary constraints. We must then iterate once more, and then again, and so on provided no inconsistencies appear until no scenario (1)’s or (2)’s occur. That is, we go until all of the last constraints we would have give scenario (3) and are automatically constant under the tower of constraints before them. With a $2N$ dimensional phase space we cannot possibly have more than $2N$ independent and self-consistent constraints on those variables and so this process will terminate after a finite number of iterations¹¹. After doing this we will have some list of all the constraints primary, secondary, tertiary, and so on. Call this complete list $C_{\text{all}}^\alpha(t, Q, P)$ with α running over all of the constraints (so it will go from 1 to the total number of constraints whether primary, secondary, tertiary, ...).

It is the list $C_{\text{all}}^\alpha(t, Q, P)$ which truly gives all of the restrictions on the phase space. If we had been smart enough to see all of them initially, we could have started with this list as the full list of constraints and thus we would have had the action:

$$S[\lambda^{\text{all}}, Q, P] = \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}(t, Q, P) + \lambda_\alpha^{\text{all}} C_{\text{all}}^\alpha(t, Q, P)) dt. \quad (2.8.57)$$

This gives identical equations of motion to our original action in equation (2.8.49) if we set all of the Lagrange multipliers on the non-primary constraints to 0. So, this is at least as general as that action. Earlier when we deduced the equations of motion from the equation (2.8.49) action we were to assume that the variations δQ^a and δP_a we considered were consistent with the necessary constraints. However, we saw that for consistency they in fact not only need to be consistent with the C^α we started with but the whole set of C_{all}^α . Thus, each of the C_{all}^α provides a linearly independent restriction on δQ^a and δP_a and warrants its own Lagrange multiplier. d’Alembert’s principle requires that we consider all variations consistent with all the constraints and this is only true if we attach a Lagrange multiplier to each of this

¹¹Later we will deal with systems with an infinite dimensional phase space and in principle in that case one has no such guarantee. However, for the known systems of physical interest we can show the process terminates explicitly by just calculating.

full set of constraints. This algorithm we have performed to construct equation (2.8.57), known as the Dirac algorithm, essentially then reveals all the constraints which were implied but not originally written and the full application of d'Alembert's principle means that we should consider only variations consistent with that full set of constraints. This gives those previously hidden constraints (the secondary, tertiary, and so on) the additional Lagrange multipliers present in equation (2.8.57). Thus, the action in equation (2.8.57) is the actual fully correct action to use when one has phase space constraints.

Constraint Function Redefinition

The constraint functions in equation (2.8.57) are not unique (constraint functions never are). If $\hat{W}(t, Q, P)$ is a matrix (with components W^α_β) which is invertible when all the constraints are satisfied then the new constraints C'^α defined by:

$$C'_{\text{all}}{}^\alpha(t, Q, P) = W^\alpha_\beta(t, Q, P)C_{\text{all}}^\beta(t, Q, P) \quad (2.8.58)$$

are equivalent as they weakly vanish if and only if the original constraints do and due to the invertibility of $\hat{W}$ they also have linearly independent variations. This amounts to also redefining the Lagrange multipliers to:

$$\lambda'^{\text{all}}_\alpha = (\hat{W}^{-1})^\beta_\alpha \lambda^{\text{all}}_\beta \quad (2.8.59)$$

as this keeps the Lagrange multiplier pieces in the action unchanged:

$$\lambda'^{\text{all}}_\alpha C'_{\text{all}}{}^\alpha = \lambda^{\text{all}}_\alpha C_{\text{all}}^\alpha. \quad (2.8.60)$$

Identifying First and Second Class Constraints

Let us assume now we have found all of the constraints and constructed the action in equation (2.8.57). Then in this action all of the constraints are primary constraints (so, the distinction between primary, secondary, tertiary, and so on constraints is purely procedural and not fundamental) and when we study the consistency condition equation (2.8.55) we must always either run into scenarios (1) or (3). Each time we encounter scenario (1) provides a new independent linear relation among the Lagrange multipliers (if it were not independent, it would have counted as encountering scenario (3)). Thus, we can solve for one Lagrange multiplier for each time we encounter scenario (1). After doing so there are usually still some undetermined Lagrange multipliers. Let the undetermined Lagrange multipliers be called $v_A(t)$ with A running as an index over all such multipliers (the total number of which is now less than or equal to the total number of constraints). Then, solving these linear conditions will give:

$$\lambda^{\text{all}}_\alpha(t) \approx U_\alpha(t, Q, P) + V_\alpha^A(t, Q, P)v_A(t) \quad (2.8.61)$$

for some functions $U_\alpha(t, Q, P)$ and $V_\alpha^A(t, Q, P)$ which are just the coefficients from solving the linear equations and which in particular depend on which Lagrange multipliers one solves for in terms of which others. This is by definition the most general solution of all the conditions placed on the Lagrange multipliers and so these $v_A(t)$ remain completely undetermined. For a general function on the phase space then:

$$\frac{df}{dt} \approx \frac{\partial f}{\partial t} + \{f, \mathcal{H}\} - (U_\alpha + V_\alpha^A v_A)\{f, C_{\text{all}}^\alpha\}. \quad (2.8.62)$$

Using the Leibniz property of the Poisson bracket:

$$\{f, (U_\alpha + V_\alpha^A v_A)C_{\text{all}}^\alpha\} = \{f, U_\alpha + V_\alpha^A v_A\}C_{\text{all}}^\alpha + (U_\alpha + V_\alpha^A v_A)\{f, C_{\text{all}}^\alpha\} \quad (2.8.63)$$

$$\approx 0 + (U_\alpha + V_\alpha^A v_A)\{f, C_{\text{all}}^\alpha\}. \quad (2.8.64)$$

Thus:

$$\frac{df}{dt} \approx \frac{\partial f}{\partial t} + \{f, \mathcal{H} - U_\alpha C_{\text{all}}^\alpha\} - v_A \{f, V_\alpha^A C_{\text{all}}^\alpha\}. \quad (2.8.65)$$

This is exactly of the form of equation (2.8.54) but with the new Hamiltonian:

$$\mathcal{H}_1(t, Q, P) = \mathcal{H}(t, Q, P) - U_\alpha(t, Q, P)C_{\text{all}}^\alpha(t, Q, P) \quad (2.8.66)$$

(which is weakly equal to the original Hamiltonian) and a new reduced set of constraint functions:

$$\gamma^A(t, Q, P) = V_\alpha^A(t, Q, P)C_{\text{all}}^\alpha(t, Q, P). \quad (2.8.67)$$

Thus:

$$\frac{df}{dt} \approx \frac{\partial f}{\partial t} + \{f, \mathcal{H}_1\} - v_A \{f, \gamma^A\}. \quad (2.8.68)$$

However, we still need to apply all of the constraints C_{all}^α , not just the γ^A . These γ^A constraints are usually not equivalent to all of the C_{all}^α constraints. Instead, some of the full set of constraints can be expressed

as linear combinations of the γ^A while some cannot. The remaining constraints among the C_{all}^α which cannot be written as linear combinations of the γ^A are called $\chi^k(t, Q, P)$. The range of the index k plus the range of the index A must then equal the total number of constraints. So, these γ^A and χ^k form a basis for our full set of constraints C_{all}^α . In that way we can simply take the full set of constraints to be the combined list of γ^A and χ^k as they are all 0 if and only if the C_{all}^α are all 0. This is a change of basis of constraint functions as done in equation (2.8.58) with γ^A and χ^k now acting as our set of new constraint functions. The action in equation (2.8.57) can now be rewritten:

$$S[v, Q, P] = \int_{t_0}^{t_f} (P_a \dot{Q}^a - \mathcal{H}_1(t, Q, P) + v_A(t) \gamma^A(t, Q, P)) dt \quad (2.8.69)$$

where the variations considered must satisfy the γ^A and χ^k constraints.

These γ^A and χ^k constraints we have constructed are special. We see that by construction the general solution to the conditions on their Lagrange multipliers is that all of the v_A Lagrange multipliers associated to the γ^A are completely undetermined by the consistency conditions and all of the Lagrange multipliers associated to the χ^k are exactly 0 as they automatically do not appear in equation (2.8.68) or (2.8.69). We could write equation (2.8.68) with Lagrange multipliers w_k for the χ^k as:

$$\frac{df}{dt} \approx \frac{\partial f}{\partial t} + \{f, \mathcal{H}_1\} - v_A \{f, \gamma^A\} - w_k \{f, \chi^k\}. \quad (2.8.70)$$

However, because equation (2.8.68) is the most general consistent solution by construction the consistency conditions must set all of the w_k to 0. That is, there cannot be any non-zero Lagrange multipliers for the χ^k due to all of the conditions from scenario (1)'s. If we return now to the consistency condition on γ^A :

$$\frac{d\gamma^A}{dt} \approx 0 \implies \frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_1\} - v_B \{\gamma^A, \gamma^B\} \approx 0. \quad (2.8.71)$$

We know that by construction these consistency conditions no longer restrict the values of $v_B(t)$ at all. Therefore this weak equality must hold for all values of v_B and so each term multiplied by a v_B must weakly vanish individually. So:

$$\{\gamma^A, \gamma^B\} \approx 0, \quad \frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_1\} \approx 0. \quad (2.8.72)$$

Similarly, if we look at the consistency conditions on χ^k :

$$\frac{d\chi^k}{dt} \approx 0 \implies \frac{\partial \chi^k}{\partial t} + \{\chi^k, \mathcal{H}_1\} - v_A \{\chi^k, \gamma^A\} \approx 0. \quad (2.8.73)$$

Again this cannot restrict the values of v_A at all and so must hold for all values of v_A giving similarly:

$$\{\chi^k, \gamma^A\} \approx 0, \quad \frac{\partial \chi^k}{\partial t} + \{\chi^k, \mathcal{H}_1\} \approx 0. \quad (2.8.74)$$

Combining equations (2.8.72) and (2.8.74) we see that the γ^A must have weakly vanishing Poisson brackets with all of the constraints, either the γ^B or the χ^k . Because they have weakly vanishing Poisson brackets with all constraints, the γ^A constraints are called “first-class constraints”. In general, any function which has weakly vanishing brackets with all of the constraints is called a first-class function. Any other function is called a second-class function. (Meaning there is at least one constraint a second class function has weakly non-vanishing Poisson bracket with.) What about the χ^k ? Do they have weakly vanishing Poisson brackets with all for the other constraints? Are they first or second class? We see in equation (2.8.74) that the χ^k do have weakly vanishing Poisson brackets with γ^A , but what about each other? Consider a general linear combination of the χ^k with coefficients of linear combination $g_k(t, Q, P)$ and call this combination $\zeta(t, Q, P)$:

$$\zeta(t, Q, P) = g_k(t, Q, P) \chi^k(t, Q, P). \quad (2.8.75)$$

Suppose there exists such a linear combination which has weakly vanishing Poisson bracket with all of the χ^k . Then:

$$0 \approx \{\zeta, \chi^k\} = \{g_l \chi^l, \chi^k\} = g_l \{\chi^l, \chi^k\} + \chi^l \{g_l, \chi^k\} \approx g_l \{\chi^l, \chi^k\} \quad (2.8.76)$$

$$\implies g_l \{\chi^l, \chi^k\} \approx 0. \quad (2.8.77)$$

Consider now setting the values of the Lagrange multipliers w_k in equation (2.8.70) to these g_k :

$$w_k = g_k. \quad (2.8.78)$$

Then, with these new w_k the γ^A still pass all of their consistency by using equations (2.8.72) and (2.8.74):

$$\frac{d\gamma^A}{dt} \approx \frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_1\} - v_B \{\gamma^A, \gamma^B\} - w_k \{\gamma^A, \chi^k\} \approx 0. \quad (2.8.79)$$

As well, with these particular values of w_k the χ^k also pass their consistency checks by using equation (2.8.77):

$$\frac{d\chi^k}{dt} \approx \frac{\partial \chi^k}{\partial t} + \{\chi^k, \mathcal{H}_1\} - v_A \{\chi^k, \gamma^A\} - w_l \{\chi^k, \chi^l\} \approx -g_l \{\chi^k, \chi^l\} \approx 0. \quad (2.8.80)$$

Hence, if the g_k are non-zero this means there are consistent nonzero values of w_k which would be a contradiction. Thus, the g_k must be zero and so there can be no nonzero linear combination of the χ^k which have weakly vanishing Poisson brackets with all of the other χ^k . In particular this means that no individual χ^k can have weakly vanishing Poisson bracket with all of the other χ^l . None of the χ^k can be first class; instead they are all second class.

Define the matrix $\hat{M}$ with components $M^{kl}(t, Q, P)$ by:

$$M^{kl}(t, Q, P) = \{\chi^k, \chi^l\}. \quad (2.8.81)$$

We found that there can be no nonzero g_k satisfying equation (2.8.77), equivalently:

$$g_k M^{kl} \approx 0. \quad (2.8.82)$$

This is simply a matrix equation in which the vector with components g_k is multiplied onto the left of the matrix $\hat{M}$. Because no nonzero solutions of this matrix equation exist, the matrix $\hat{M}$ sends no vector to 0 and thus is invertible. Therefore the determinant of $\hat{M}$ is nonzero. By definition $\hat{M}$ is antisymmetric because the Poisson bracket is. Any antisymmetric matrix of odd dimension has determinant zero¹². Therefore, we cannot have an odd number of second-class constraints χ^k . **There will always be an even number of second class constraints.** That is, $\hat{M}$ is an even dimensional antisymmetric invertible matrix. Let the inverse be called $\hat{M}^{-1}$ and have components written as M_{kl}^{-1} . The inverse condition then reads:

$$\hat{M}^{-1} \hat{M} = \mathbb{1} \implies M_{km}^{-1} M^{ml} = \delta_k^l \quad (2.8.83)$$

$$\hat{M} \hat{M}^{-1} = \mathbb{1} \implies M^{km} M_{ml}^{-1} = \delta_l^k. \quad (2.8.84)$$

Interpretation of First Class Constraints

There is a nice interpretation both for the first class constraints and the second class constraints. After we have put the time evolution into the form of equation (2.8.68) we see that the time evolution of a general function still depends on the completely undetermined functions of time $v_A(t)$ about which we get no information from the consistency conditions and there is one v_A associated to each first class constraint γ^A . The $v_A(t)$ have no equation of motion and can be set to anything. This seems very weird; in a theory which has first class constraints the equations of motion are partly indeterminate and there is one arbitrary function of time for each such first class constraint. Because of this indeterminacy anything “directly experimentally observable” cannot depend on these indeterminate functions. Therefore, we can study shifts of these $v_A(t)$ and under such shifts anything “directly experimentally observable” must be invariant. Suppose at time t we consider the Lagrange multipliers to have either the values $v_A(t)$ or the values $v_A(t) + \delta v_A(t)$. Then, at a slightly later time δt the difference ΔF in the value of a quantity F in time is:

$$\Delta F = F(t + \delta t)|_{v+\delta v} - F(t + \delta t)|_v = F(t) + \delta t \left. \frac{dF}{dt} \right|_{v+\delta v} - F(t) - \delta t \left. \frac{dF}{dt} \right|_v + \mathcal{O}(\delta t^2) \quad (2.8.85)$$

$$\approx \delta t \frac{\partial F}{\partial t} + \delta t \{F, \mathcal{H}_1\} - \delta t (v_A + \delta v_A) \{F, \gamma^A\} - \delta t \frac{\partial F}{\partial t} - \delta t \{F, \mathcal{H}_1\} + \delta t v_A \{F, \gamma^A\} + \mathcal{O}(\delta t^2) \quad (2.8.86)$$

$$\approx -\delta t \delta v_A \{F, \gamma^A\} + \mathcal{O}(\delta t^2). \quad (2.8.87)$$

We see that the value of F is shifted in a way determined by its weak Poisson bracket with $\{f, \gamma^A\}$. This looks like varying F under a continuous transformation with γ^A acting as the generator with a time dependent transformation parameter (because $\delta v_A(t)$ depends on time) and an unchanged Hamiltonian $\mathcal{H}_1$. Because the value of the $v_A(t)$ are indeterminate, F and $F + \Delta F$ should be “experimentally equivalent”. Therefore, we think this transformation should be a continuous symmetry of the system. We can formalize this idea by looking at the generator:

$$G(t, Q, P) = u_A(t) \gamma^A(t, Q, P) \quad (2.8.88)$$

¹²The determinant of a matrix is equal to the determinant of its transpose and the determinant of a product of matrices is equal to the product of determinants. Therefore for an antisymmetric matrix $\hat{A}$ of dimension n , $\det(\hat{A}) = \det(\hat{A}^T) = \det(-\hat{A}) = \det(-1) \det(\hat{A}) = (-1)^n \det(\hat{A})$. If n is odd it immediately follows that $\det(\hat{A}) = 0$.

for some functions $u_A(t)$. Treating G as the generator of a canonical transformation in which $t' = t$:

$$\mathcal{D}Q^a = \left. \frac{dQ^a}{d\varepsilon} \right|_{\varepsilon=0} = \{Q^a, G\} = u_A \frac{\partial \gamma^A}{\partial P_a} \quad (2.8.89)$$

$$\mathcal{D}P_a = \left. \frac{dP_a}{d\varepsilon} \right|_{\varepsilon=0} = \{P_a, G\} = -u_A \frac{\partial \gamma^A}{\partial Q^a}. \quad (2.8.90)$$

The surface term $f(\varepsilon, t, Q, P)$ produced by the transformation is given by (1.10.30)

$$\mathcal{D}f = P_a \mathcal{D}Q^a - \mathcal{H} \mathcal{D}t - G = u_A P_a \frac{\partial \gamma^A}{\partial P_a} - u_A \gamma^A \quad (2.8.91)$$

$$\implies f(\varepsilon, t, Q, P) = \varepsilon \mathcal{D}f + \mathcal{O}(\varepsilon^2) = \varepsilon u_A \left(P_a \frac{\partial \gamma^A}{\partial P_a} - \gamma^A \right) + \mathcal{O}(\varepsilon^2). \quad (2.8.92)$$

Let us now study the integrand of the action with this surface term. After a bit of algebra:

$$\begin{aligned} P_a \dot{Q}^a - \mathcal{H}_1(t, Q, P) + v_A(t) \gamma^A(t, Q, P) + \frac{df}{dt} \\ = P_a \dot{Q}^a - \mathcal{H}_1(t, Q, P) + v_A \gamma^A(t, Q, P) + \varepsilon \frac{d}{dt} \left(u_A \left(P_a \frac{\partial \gamma^A}{\partial P_a} - \gamma^A \right) \right) + \mathcal{O}(\varepsilon^2) \end{aligned} \quad (2.8.93)$$

$$= P'_a \dot{Q}'^a - \mathcal{H}_1(t, Q', P') + (v_A - \varepsilon \dot{u}_A) \gamma'^a - \varepsilon u_A \left(\frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_1\} - v_B \{\gamma^A, \gamma^B\} \right) + \mathcal{O}(\varepsilon^2). \quad (2.8.94)$$

For this to be a canonical transformation we need the form of the integrand to be unchanged:

$$P_a \dot{Q}^a - \mathcal{H}_1 + v_A \gamma^A + \frac{df}{dt} = P'_a \dot{Q}'^a - \mathcal{H}'_1 + v'_A \gamma'^A. \quad (2.8.95)$$

Therefore we see that if we transform the Lagrange multipliers by:

$$v'_A = v_A - \varepsilon \dot{u}_A + \mathcal{O}(\varepsilon^2) \implies \mathcal{D}v_a = -\dot{u}_A \quad (2.8.96)$$

then the Hamiltonian is changed by:

$$\mathcal{H}'_1(t, Q', P') = \mathcal{H}_1(t, Q', P') - \varepsilon u_A \left(\frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_1\} - v_B \{\gamma^A, \gamma^B\} \right) + \mathcal{O}(\varepsilon^2). \quad (2.8.97)$$

The expression in parentheses is the total time derivative of γ^A by equation (2.8.72) which is weakly 0 by the consistency conditions. So, $\mathcal{H}'_1$ is weakly equal to $\mathcal{H}_1$ evaluated at the transformed point and thus the functional form of $\mathcal{H}_1$ is changed by a term which is weakly 0. So, we in fact do have symmetry under this transformation for any choice of functions $u_A(t)$ in that an equal and equivalent Hamiltonian exists before and after the transformation. Because we have a family of symmetry transformations determined by *functions* instead of simply numbers, this is a gauge symmetry. Consequently, **first class constraints generate gauge transformations** under which the constrained system has symmetry. Noether's theorem requires that because we have a continuous symmetry the generator is conserved. This is trivially true because the generator $u_A \gamma^A$ is automatically 0 when the constraints are satisfied and it remains 0 because the dynamics preserve the constraints.

Because the indeterminant $v_A(t)$ can be set arbitrarily using the above transformation, **all experimental predictions must be unchanged by the gauge transformations generated by the first class constraints**. That just requires having weakly vanishing Poisson bracket with each of the γ^A and this is equivalent to being independent of the choice of v_A . So:

$$f \text{ experimentally observable} \implies \{f, \gamma^a\} \approx 0. \quad (2.8.98)$$

A subtlety here is that many quantities which do depend on $v_A(t)$ may be interesting and important; they will generally not have weakly vanishing bracket with the first class constraints but they can still be determined meaningfully *up to a well defined transformation property under these gauge transformations*. We will see that this is precisely the case with the scalar and vector potentials. We will see in chapter 4 that the scalar potential is literally an example of $v_A(t)$ and that the gauge transformation of the potentials is exactly generated by a first class constraint. But, while the potentials are not uniquely defined, they are completely well defined up to a gauge function that systematically described their redundancy. The experimental predictions made by the potentials do not depend on that redundancy (the gauge function).

The gauge transformation is like a choice of coordinates. The definitions of Q^a and P_a are generally changed by the gauge transformation as shown in equations (2.8.89) and (2.8.90) but through this systematic

way of redefining coordinates there happen to be some quantities (functions which weakly have vanishing Poisson bracket with all the first class constraints) that are independent of these coordinate choices. Only those quantities are directly observable. This is exactly analogous (and a mere generalization of) the logic behind any ordinary symmetry. Choosing different coordinate axes chooses different x , y , and z directions. The components of any vector or other quantity have to be systematically transformed when a choice of coordinates is made. However, the choice of coordinates must always drop out of the final predictions of the theory because the choice of coordinates was an artifact of description, not a genuine part of the system. In the exact same way, a choice of gauge (fixing particular choices for what the $v_A(t)$ should be) is an artifact of description, not a genuine part of the system and all predictions must be independent of such a choice.

Experimentally Equivalent Functions

There is somewhat of a subtle issue we should confront. In any sort of experiment whatever constraints apply to a system are always present. Therefore, for experimental purposes, two functions $f(t, Q, P)$ and $f'(t, Q, P)$ which are weakly equal can't be distinguished from each other and define some kind of experimental equivalence class. However, we should take care to see if such f and f' might have meaningful theoretical differences from each other. Suppose we have two such functions f and f' which are weakly equal. Then, their difference is weakly equal to 0:

$$f' \approx f \implies f' - f \approx 0 \quad (2.8.99)$$

as when the constraints are applied $f' = f$ and so when the constraints are applied $f' - f = 0$. Let us define $h(t, Q, P) = f' - f$ and study how it may differ from 0 when the constraints are not applied. Because $h \approx 0$ for any values of Q, P which satisfy the constraints, under variation of the Q and P by variations δQ and δP which preserve the constraints, the variation of h must be 0:

$$\delta h = \frac{\partial h}{\partial Q^a} \delta Q^a + \frac{\partial h}{\partial P_a} \delta P_a \approx 0 \text{ (under variations which preserve the constraints)}. \quad (2.8.100)$$

Because the list C_{all}^α of all the constraints defines the full set of linear relations among the variations of δQ and δP by definition, any generally vanishing linear combination of the δQ and δP must be expressible as a linear combination of those implied by the constraints. That is, $C^\alpha \stackrel{!}{=} 0$ and consequently $\delta C^\alpha \stackrel{!}{=} 0$ give the full set of conditions on the variations δQ and δP . Therefore, for some functions $\kappa_\alpha^{\text{all}}(t, Q, P)$ it must be the case that:

$$\delta h \approx 0 \text{ (under constrained variations)} \implies \delta h \approx \kappa_\alpha^{\text{all}} \delta C_{\text{all}}^\alpha \text{ (under all variations)}. \quad (2.8.101)$$

(The reasoning for why this is true is identical to the reasoning that leads to equation (2.8.3) but phrased on the phase space.) However, this linear combination can be rewritten as:

$$\kappa_\alpha^{\text{all}} \delta C_{\text{all}}^\alpha = \delta(\kappa_\alpha^{\text{all}} C_{\text{all}}^\alpha) - C_{\text{all}}^\alpha \delta \kappa_\alpha^{\text{all}} \approx \delta(\kappa_\alpha^{\text{all}} C_{\text{all}}^\alpha). \quad (2.8.102)$$

This allows us to rewrite the variation of h as:

$$\delta h \approx \delta(\kappa_\alpha^{\text{all}} C_{\text{all}}^\alpha) \quad (2.8.103)$$

for any variations of Q and P . Because h and $\kappa_\alpha C_{\text{all}}^\alpha$ both vanish with the constraints applied, they are weakly equal. As well, we see here that their arbitrary variations and thus first derivatives match when all the constraints are applied at the end. Therefore, h is strongly equal to this linear combination of the constraints:

$$h(t, Q, P) \equiv \kappa_\alpha^{\text{all}}(t, Q, P) C_{\text{all}}^\alpha(t, Q, P). \quad (2.8.104)$$

So, a function is weakly 0 if and only if it is strongly a linear combination of the constraint functions and consequently two functions are weakly equal if and only if they strongly differ by a linear combination of constraint functions:

$$f'(t, Q, P) \approx f(t, Q, P) \implies \exists \kappa_\alpha^{\text{all}}(t, Q, P) \mid f'(t, Q, P) \equiv f(t, Q, P) + \kappa_\alpha^{\text{all}}(t, Q, P) C_{\text{all}}^\alpha(t, Q, P). \quad (2.8.105)$$

This means that the most general way a function $f(t, Q, P)$ on phase space can be modified so that its value when the constraints are applied is unchanged is by adding to it some linear combination of the constraint functions. We can write this explicitly in terms of the first and second class constraints as:

$$f'(t, Q, P) \approx f(t, Q, P) \implies f'(t, Q, P) \equiv f(t, Q, P) + \rho_A(t, Q, P) \gamma^A(t, Q, P) + \sigma_k(t, Q, P) \chi^k(t, Q, P). \quad (2.8.106)$$

Here ρ_A and σ_k are just some unspecified functions which would be fixed by knowing f and f' . While f' and f coincide under their constraints, they may behave differently under Poisson brackets. First, let us consider

the Poisson bracket of $f'(t, Q, P)$ with the first class constraints:

$$\{f', \gamma^A\} \approx \{f + \rho_B \gamma^B + \sigma_k \chi^k, \gamma^A\} \quad (2.8.107)$$

$$\approx \{f, \gamma^A\} \quad (2.8.108)$$

where we have used equations (2.8.72) and (2.8.74). So, f' and f behave identically under Poisson brackets with the first class constraints. Now let us consider the Poisson bracket of $f'(t, Q, P)$ with the second class constraints:

$$\{f', \chi^k\} \approx \{f + \rho_A \gamma^A + \sigma_l \chi^l, \chi^k\} \quad (2.8.109)$$

$$\approx \{f, \chi^k\} + \sigma_l M^{lk} \quad (2.8.110)$$

where we have again used equation (2.8.74) and now also equation (2.8.81). Importantly, the Poisson bracket of two weakly equal functions with the second class constraints may not be the same. In fact, we can always make such an f' above which is weakly equal to f but which has weakly vanishing Poisson bracket with every second class constraint. To see this, suppose we choose:

$$\sigma_k = -M_{lk}^{-1} \{f, \chi^l\}. \quad (2.8.111)$$

Then:

$$\{f', \chi^k\} \approx \{f, \chi^k\} - M_{nl}^{-1} \{f, \chi^n\} M^{lk} = \{f, \chi^k\} - \delta_n^k \{f, \chi^n\} = 0. \quad (2.8.112)$$

Because this construction will continue to be useful, define for any function f the function f_D by:

$$f_D(t, Q, P) = f(t, Q, P) - \{f, \chi^l\} M_{lk}^{-1} \chi^k \implies \{f_D, \chi^k\} \approx 0. \quad (2.8.113)$$

f_D is known as the Dirac version of f .

Interpretation of Second Class Constraints

How should we interpret such the Dirac version f_D of a function f ? As we already established, each χ^k fails to have weakly vanishing Poisson bracket with at least one other χ^l . We know that the only independent variable a coordinate or momentum fails to have weakly vanishing Poisson bracket with is its conjugate variable (momentum or coordinate). So, if we make a canonical transformation so that χ^k is a coordinate, then its conjugate variable must be present among some combination of the other χ^l due to the non-vanishing weak Poisson bracket. In principle then we can (locally) perform a canonical transformation so that half of the χ^k are canonical coordinates and the other half are the corresponding canonical momenta to those coordinates. After doing so, the condition that f_D has weakly vanishing Poisson bracket with all of the χ^k just means that f_D is not a function of any of those canonical coordinates or momenta and thus is defined as a function on the reduced phase space of only the coordinates and momenta which are not constrained by the second class constraints. This is analogous to eliminating variables through explicitly solving holonomic constraints. So, the interpretation of f_D is that for all purposes experimentally it is equal to f but it is theoretically written in a way so that it only depends on the reduced phase space coordinates which remain after the second class constraints are imposed. Thus, f_D already has the second class constraints “built-in” and the second class constraints can be viewed as providing a reduction in the dimension of the phase space.

The second class constraints do not and cannot generate any sort of gauge symmetry. Using a second class constraint as the generator of a canonical transformation in the way we did for the first class constraints will end up, after following the same logic, requiring the Lagrange multipliers w_k to be varied (just as the v_A were varied). However, we know that the only consistent values for these are 0; they cannot be made nonzero while consistently preserving the constraints. Thus, the second class constraints do not generate any sort of gauge transformations which preserve the theory.

There is more to the idea of fully building in the second class constraints. Consider a function f and how it changes under a general transformation with parameter β and generator g . Then, with the local coordinates just discussed, there will be some changes in f due to changes in the reduced phase space coordinates (which don't affect the values of the χ^k) and some changes in f due to changes of the χ^k . Let ξ_k be the coordinate to which χ^k is conjugate. Then, explicitly in the chain rule:

$$\frac{df}{d\beta} = \left. \frac{df}{d\beta} \right|_{\chi=0} + \frac{\partial f}{\partial \xi_k} \frac{d\xi_k}{d\beta} \quad (2.8.114)$$

where the first term gives the changes in f on the reduced phase space on which the second class constraints are enforced and the the second terms give the change in f with respect to each of the second class constraints changing. (By our previous reasoning, χ^k for a particular k and its conjugate must be able to be written of

some function of the full set of χ 's. Thus, each of χ^k coordinates can be found among the ξ_k .) Rewriting the derivatives in Poisson brackets we have:

$$\{f, g\} = \{f, g\}|_{\chi=0} + \{f, \chi^k\}\{\varepsilon_k, g\}. \quad (2.8.115)$$

We have already established that the function g_D defined just like before as:

$$g_D(t, Q, P) = g(t, Q, P) - \{g, \chi^l\}M_{lk}^{-1}\chi^k \quad (2.8.116)$$

doesn't depend on the phase space variables eliminated by the second class constraints. Therefore, it must have weakly vanishing Poisson bracket with all of their conjugate variables:

$$\{\varepsilon_k, g_D\} \approx 0 \implies 0 \approx \{\varepsilon_k, g\} - \{\varepsilon_k, \{g, \chi^l\}M_{ln}^{-1}\chi^n\}. \quad (2.8.117)$$

Using the Leibniz property of the Poisson bracket:

$$\{\varepsilon_k, g\} \approx \{\varepsilon_k, \{g, \chi^l\}M_{ln}^{-1}\chi^n + \{\varepsilon_k, \chi^n\}\{g, \chi^l\}M_{ln}^{-1} \approx \{\varepsilon_k, \chi^n\}\{g, \chi^l\}M_{ln}^{-1}. \quad (2.8.118)$$

Because ε_k is by definition the coordinate to which χ^k is the conjugate momentum:

$$\{\varepsilon_k, \chi^l\} = \delta_k^l \implies \{\varepsilon_k, g\} \approx \{g, \chi^l\}M_{lk}^{-1}. \quad (2.8.119)$$

Now returning these results to equation (2.8.115) we have:

$$\{f, g\}|_{\chi=0} = \{f, g\} - \{f, \chi^k\}M_{kl}^{-1}\{\chi^l, g\}. \quad (2.8.120)$$

Therefore, we can define an effective Poisson bracket which is just the Poisson bracket on reduced phase space (the surface in phase space on which all of the second class constraints are applied) to be this bracket above. It is called the Dirac bracket:

$$\{f, g\}_D \stackrel{\text{def}}{=} \{f, g\} - \{f, \chi^k\}M_{kl}^{-1}\{\chi^l, g\}. \quad (2.8.121)$$

One can check by explicit computation that it inherits all of the properties of anti-symmetry, bilinearity, the Jacobi identity, and the Leibniz property of the ordinary Poisson bracket. This should not be surprising because by construction it is just the Poisson bracket for the coordinates and momenta that remain after the second class constraints are applied (the reduced phase space). Because of that, one would expect that the Dirac bracket and full Poisson bracket should coincide for functions which do not depend on the second class constraint variables, meaning the functions f_D and g_D defined before. In fact, one can check directly by calculation that:

$$\{f_D, g_D\} \approx \{f_D, g_D\}_D \approx \{f, g\}_D. \quad (2.8.122)$$

So, second class constraints can be viewed as providing a reduction in the size of phase space and the Dirac bracket can be viewed as explicitly subtracting out anything not in that reduced phase space. The variables the second class constraints eliminate can be removed from a function f by using its Dirac version f_D and/or by using the Dirac bracket $\{\cdot, \cdot\}_D$ when computing evolution under a transformation. Because of this, when using the Dirac bracket, one can take the second class constraints to be applied strongly, not weakly (as in whether one applies the second class constraints before or after using the Dirac bracket does not matter).

We have now seen that two functions f' and f which are weakly equal have the same Poisson brackets with the first class constraints and different Poisson brackets with the second class constraints. We can fix this by using the Dirac bracket so that then they have the same Dirac brackets with both the first and second class constraints. However, do they have the same Dirac brackets with general functions? Consider f' and g' which are weakly equal to f and g and so must be related to their Dirac versions by:

$$f'(t, Q, P) \equiv f_D(t, Q, P) + \rho_A^{(f)}(t, Q, P)\gamma^A(t, Q, P) + \sigma_k^{(f)}(t, Q, P)\chi^k(t, Q, P), \quad (2.8.123)$$

$$g'(t, Q, P) \equiv g_D(t, Q, P) + \rho_A^{(g)}(t, Q, P)\gamma^A(t, Q, P) + \sigma_k^{(g)}(t, Q, P)\chi^k(t, Q, P) \quad (2.8.124)$$

for some functions $\rho_A^{(f)}, \sigma_k^{(f)}, \rho_A^{(g)}, \sigma_k^{(g)}$. Then, their Dirac bracket is:

$$\{f', g'\}_D = \{f_D + \rho_A^{(f)}\gamma^A + \sigma_k^{(f)}\chi^k, g_D + \rho_A^{(g)}\gamma^A + \sigma_k^{(g)}\chi^k\}_D \quad (2.8.125)$$

$$\approx \{f, g\}_D + \rho_A^{(f)}\{\gamma^A, g_D\} + \rho_A^{(g)}\{f_D, \gamma^A\}. \quad (2.8.126)$$

Therefore, we see that the $\{f', g'\}_D$ and $\{f, g\}_D$ only coincide in general if the Poisson brackets of both f_D and g_D with the all the first class constraints are 0. By construction f_D and g_D have vanishing Poisson brackets with all of the second class constraints. So, this condition becomes equivalent to requiring f_D and g_D to have weakly vanishing Poisson bracket with all of the constraints and thus for them to be first

class functions. As well, by the logic leading to equation (2.8.98) this means equivalently that f_D and g_D must be gauge invariant if we want $\{f', g'\}_D$ to coincide with $\{f, g\}_D$ in general. So, the Dirac bracket allows us to define a well-defined bracket between all quantities with respect to changing them by terms proportional to the second class constraints. But, a well-defined bracket with respect to changing quantities by terms proportional to first class constraints is only possible for gauge invariant quantities. The bracket is “well-defined” in the sense that all gauge invariant functions which are weakly equal (and thus experimentally indistinguishable) behave the same under the Dirac bracket. It is not an issue that the Dirac bracket is only unique and well-defined for gauge invariant quantities because quantities which are not gauge invariant do not have experimentally well defined values by the logic leading to (2.8.98). Regardless of if one is considering gauge invariant functions, one can always form the Dirac version of a function so that it has weakly vanishing Poisson bracket with the second class constraints and so the second class constraints can be applied strongly.

Theorem 2.16: Phase Space Constraints

If a system with Hamiltonian $\mathcal{H}$ on a phase space of dimension $2N$ is subject to a consistent set of naive constraints $C_{\text{primary}}^\alpha(t, Q, P) \stackrel{!}{=} 0$ then the appropriate primary action to use is:

$$S_{\text{primary}}[\lambda, Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H} + \lambda_\alpha C_{\text{primary}}^\alpha \right) dt. \quad (2.8.127)$$

The equations of motion implied by this action generally will not automatically conserve the constraints. Explicitly requiring the conservation of the primary constraints will typically imply additional necessary constraints, known as secondary constraints. Explicitly requiring their conservation may require tertiary constraints and so on. Eventually, explicitly requiring the conservation of all such generated constraints will not require any more constraints for finite N . This full set of required constraints is then called C_{all}^α . Once the set of all constraints is known, the full self-consistent action for the constrained system is given by:

$$S[\lambda, Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H} + \lambda_\alpha C_{\text{all}}^\alpha \right) dt. \quad (2.8.128)$$

It is possible to define a new set of constraint functions from linear combinations of the C_{all}^α so that the constraints split into two classes, the first class constraints $\gamma^A(t, Q, P)$ which weakly Poisson commute with all the constraints and the second class constraints $\chi^k(t, Q, P)$ of which there is always an even number and for which the matrix with components $\{\chi^k, \chi^l\}$ is invertible. If the number of second class constraints is $2K$ then it is possible to perform a canonical transformation so that the second class constraints can be written in terms of only K coordinates and their corresponding momenta and that these are set to 0 by the constraints. After this canonical transformation it is self-consistent to set all of those coordinates and momenta to 0 in all other quantities so that the remaining system is formulated on a reduced phase space of dimension $2N - 2K$. On the reduced phase space, all the remaining constraints are first class and there exists a Dirac Hamiltonian $\mathcal{H}_D$ which is weakly equal to the original Hamiltonian $\mathcal{H}$ but which satisfies:

$$\frac{\partial \gamma^A}{\partial t} + \{\gamma^A, \mathcal{H}_D\} \approx 0. \quad (2.8.129)$$

In terms of the Dirac Hamiltonian, the action becomes:

$$S[v, Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - \mathcal{H}_D + v_A \gamma^A(t, Q, P) \right) dt \quad (2.8.130)$$

where the coordinates and momenta here are the coordinates and momenta only on the reduced phase space and v_A are the Lagrange multipliers associated to the first class constraints. The v_A are completely undetermined by the consistency conditions or equations of motion. They can be chosen arbitrarily. Making a particular choice is known as “gauge fixing”. The remaining theory has symmetry under the continuous gauge transformation generated by:

$$G(t, Q, P) = u_A(t) \gamma^A(t, Q, P) \quad (2.8.131)$$

for all smooth functions $u_A(t)$. Under that transformation the various quantities of the theory change

by:

$$\mathcal{D}v_A = -\dot{u}_A, \quad \mathcal{D}Q^a = u_A \frac{\partial \gamma^A}{\partial P_a}, \quad \mathcal{D}P_a = -u_A \frac{\partial \gamma^A}{\partial Q^a}. \quad (2.8.132)$$

All experimentally well defined quantities must be weakly gauge invariant under these transformations (meaning they weakly Poisson commute with G ; this is the same as being independent of the choice of $v_A(t)$).

2.8.4 Inequality Constraints

Inequality constraints don't come up that often and are straightforward to handle, so we will go quickly. They can be handled using the strong spring method described earlier. That is, we add an external force which is only nonzero when the inequality is not satisfied and put some coefficient out front whose value we can select, compute the dynamics as a function of this parameter, then at the end take the limit that the coefficient goes to infinity (thus making the penalty for not satisfying the inequality arbitrarily large, guaranteeing it is satisfied in the limit). As an example, suppose we have an inequality constraint: $a \leq F(t, Q) \leq b$ where a, b and $F(t, Q)$ are given by the setup (such as the particle being stuck inside a box). Then, let $R(F)$ be any smooth function which is zero on the interval (a, b) and positive outside of that interval. By taking the action:

$$S_k[Q] = S_0[Q] - k \int_{t_0}^{t_f} R(F(t, Q)) dt \quad (2.8.133)$$

for some constant k where S_0 is the unconstrained action of the theory, we can take the variation to get equations of motion which in the limit $k \rightarrow \infty$ produce the inequality constrained dynamics. For finite k , this action corresponds to a box which is hard to penetrate but can be broken through with enough energy¹³. Essentially, the added term does nothing except reflect the coordinate back in the allowed direction when it comes up against the boundary of the allowed region. At each k one gets an equation of motion and the fully constrained dynamics are given by taking $k \rightarrow \infty$ at the end. An example of this is done in the homework.

Exercises

Problem 2.37: Recovering Holonomic as a special case of Velocity constraints. The holonomic constraints $C^\alpha(t, Q) = 0$ seem at first glance like just a special case of velocity constraints $C^\alpha(t, Q, \dot{Q}) = 0$ where the constraint functions just don't depend on the velocity. This is true, but when we applied velocity constraints we assumed they were sufficient to solve for some of the velocities in terms of the others. This is not true if the constraint function are written in a way that doesn't depend on the velocity.

- (a) Show that if we have holonomic constraints $C^\alpha(t, Q) = 0$ then it implies as well that $\frac{dC^\alpha}{dt} = 0$ and that using the new constraint functions $C'^\alpha(t, Q, \dot{Q}) = \frac{dC^\alpha}{dt} = 0$ gives velocity constraints which produce the same equations of motion as the original C^α when the theory of velocity constraints is used. Hence, conclude that it is true that holonomic constraints are just a special case of velocity constraints. Unsurprisingly, this special case structure repeats itself at each higher order of differentiation.
- (b) Show that if one uses the action:

$$S_\lambda[\lambda, Q] = S_0[Q] + \int_{t_0}^{t_f} \lambda_\alpha(t) C'^\alpha(t, Q, \dot{Q}) dt$$

where $C'^\alpha = \frac{dC^\alpha}{dt}$ just as in the previous part, then the stationary variation of this action actually does produce the correct equations of motion for Q^α even though the Lagrange multiplier method is not correct for a general velocity constraint. Thus, for a velocity constraint which is integrable to being just a holonomic constraint, the Lagrange multiplier method is correct.

Problem 2.38: The Planar Pendulum. Consider a mass m hanging on a string (which you may take to be essentially massless) of fixed length l from a fixed point so that the system forms a pendulum. This pendulum is allowed to swing only in a plane. Assume the string always remains taut.

- (a) Write the constraint function imposed by the string for this system.

¹³Technically a better model for a penetrable box would be to choose the function R so that it is 0 inside the box, 0 outside of the wall of the box, and nonzero in the thickness of the wall of the box.

- (b) Write the Lagrangian for the unconstrained mass experiencing gravity (you may reference the result of problem 2.21) and add the constraint function as a Lagrange multiplier.
- (c) Find the equations of motion implied by the Lagrangian in the previous part and find an expression for the constraint force on the mass. A constraint force which resists a string/rod from extending is called tension.
- (d) Switch to polar coordinates where r is the distance of the mass from the pivot point and θ is the angle the pendulum is away from hanging vertically downward. Write the Lagrangian and constraint function in terms of these coordinates.
- (e) Directly apply the constraint to the Lagrangian (it is holonomic!) and find the resulting equation of motion for θ .
- (f) From the full equation of motion found in the previous part, find the approximate equation of motion for small θ and solve it. You should find it is a harmonic oscillator with angular frequency $\omega = \sqrt{\frac{g}{l}}$ (and thus period $\tau = 2\pi\sqrt{\frac{l}{g}}$).
- (g) For this part, you may want to reference problem 1.8. Let α be the maximum angle that the pendulum reaches off of vertical in its motion. Integrate the exact equation of motion once to show that:

$$\frac{1}{2}\dot{\theta}^2 - \frac{g}{l}\cos\theta = -\frac{g}{l}\cos\alpha.$$

- (h) The equation found in the previous part is a separable differential equation. Separate and manipulate it to find:

$$dt = \frac{1}{2}\sqrt{\frac{l}{g}} \frac{d\theta}{\sqrt{\sin^2\frac{\alpha}{2} - \sin^2\frac{\theta}{2}}}.$$

- (i) Using the results of the previous parts, identify that one full swing of the pendulum consists of swinging from α to 0, 0 to $-\alpha$, $-\alpha$ back to 0, and 0 back to α and that each of those take equal time. From this conclude that the period of the motion is given by:

$$\tau = 2\sqrt{\frac{l}{g}} \int_0^\alpha \frac{d\theta}{\sqrt{\sin^2\frac{\alpha}{2} - \sin^2\frac{\theta}{2}}}.$$

- (j) Make the change of variables in the integral $\sin\varphi = \frac{\sin\frac{\theta}{2}}{\sin\frac{\alpha}{2}}$ and show that the resultant expression for the period is:

$$\tau = 4\sqrt{\frac{l}{g}} \int_0^{\frac{\pi}{2}} \frac{d\varphi}{\sqrt{1 - \sin^2\frac{\alpha}{2}\sin^2\varphi}}.$$

- (k) The previous part shows that the period of a pendulum depends on its amplitude α , unlike a simple harmonic oscillator. Taylor expand the integrand above in powers of α to find the lowest non-zero correction to the period to find how the period changes at lowest order for small α . Use this to find the lowest order correction to the angular frequency as well.
- (l) Using the exact expression for the period, show that the period diverges as the amplitude goes to π (if a pendulum has precisely enough energy to get upright, it will take forever to do so). As well, consider the pendulum to have amplitude $\alpha = \pi - \varepsilon$ and find the lowest order expression for the amplitude in terms of ε . (Instead of the familiar “small angle approximation”, this is a “very-large angle approximation”.) To do so, the following asymptotic formula [40], valid for k close to 1, will be useful:

$$\int_0^{\frac{\pi}{2}} \frac{d\varphi}{\sqrt{1 - k^2\sin^2\varphi}} = \ln\left(\frac{4}{\sqrt{1 - k^2}}\right) + \mathcal{O}\left((1 - k^2)\ln\left(\frac{5 - k^2}{1 - k^2}\right)\right).$$

Problem 2.39: The Spherical Pendulum. Consider a mass m hanging on a string of fixed length l from a fixed point so that the system forms a pendulum. This pendulum is allowed to swing in any direction in space. Assume the string remains taut.

- (a) Write the Lagrangian for this system in spherical coordinates, keeping θ as the angle away from hanging vertically as before and with φ as the azimuthal angle.
- (b) Find the equations of motion implied by this Lagrangian.
- (c) Show that the azimuthal symmetry of this Lagrangian implies that the quantity $ml^2\dot{\varphi}\sin^2\theta$ is conserved. Show that this quantity matches the component of the angular momentum of the mass in the vertical

direction and explain how this was predicted by Noether's theorem.

- (d) Using the conservation law of the previous part, show that φ can be eliminated from the equation of motion for θ and that the result gives:

$$\ddot{\theta} + \omega_0^2 \sin \theta - \gamma^2 \frac{\cos \theta}{\sin^3 \theta} = 0$$

for some constants ω_0 and γ . Determine these two parameters from the given information in your calculation.

- (e) Show that the equation of motion in the previous part has a new equilibrium value of $\theta_{\text{eq}} \neq 0$ and find an implicit equation for it.
- (f) For $\gamma = 0$, $\theta_{\text{eq}} = 0$ as this is simply the planar pendulum case. Find the lowest order expression for θ_{eq} for small γ .
- (g) Do not assume γ is small. Consider θ which deviates slightly from θ_{eq} as $\theta = \theta_{\text{eq}} + \delta\theta$. Keeping only terms which are first order in $\delta\theta$, find the equation of motion for small $\delta\theta$.
- (h) Describe the motion of this system near θ_{eq} geometrically based on the previous results of this question.

Problem 2.40: Mass on a track. Consider a mass m in two dimensions with position $(x(t), y(t))$ which moves on a track for which the height of the track at a particular value of x is given by some function $y(x)$.

- (a) Write the constraint function for this system and write its Lagrangian with the constraint function as a Lagrangian multiplier.
- (b) Use the Lagrangian found in the previous part to find the constraint force on the system. Show that the constraint force is perpendicular to the tangent of the track at any point. Because the constraint force holding a variable in place always acts normally to surfaces of constant value of that variable, such a constraint force is often called a “normal force” (as normal can be used to mean perpendicular).
- (c) Use the constraint to reduce the system to 1 independent variable. Find the Lagrangian, equations of motion, and conserved energy of the single variable system.
- (d) Using the one variable description, assume the system is near stable equilibrium. Show that a stable equilibrium of this system corresponds to a local minimum of the track, that the dynamics near stable equilibrium are a harmonic oscillator, and that the angular frequency of oscillation is $\omega = \sqrt{\frac{g}{R}}$ where R is the radius of curvature of the track at the minimum.

Problem 2.41: Brachistochrone Problem. This is a classic and challenging problem. In the previous problem we found the general Lagrangian for a mass on a track. In this problem we will find which track shape causes a mass to reach the bottom the fastest. As such, this is called the brachistochrone problem (brachisto for shortest, chrone for time). Consider a track which begins at $(x, y) = (0, h)$ and ends at $(x, y) = (l, 0)$ where $l > 0$ and $h > 0$ and a mass m which begins at the top of the track at rest.

- (a) Show using the energy found in the previous question and the parameters given in the preamble that the horizontal position $x(t)$ of the mass on the track satisfies:

$$\frac{1}{2}(1 + y'(x)^2) \left(\frac{dx}{dt} \right)^2 + gy(x) = gh.$$

Here $y'(x) = \frac{dy}{dx}$.

- (b) Use the previous result to show that the time taken to reach the end of the track as a functional of the track shape $y(x)$ is given by:

$$t[y] = \int_0^l \sqrt{\frac{1 + y'(x)^2}{2g(h - y(x))}} dx.$$

- (c) Now that we have the time to travel down the track as a functional of the track path, we could find the fastest track shape by taking the functional derivative and setting the result to 0. This is true but for the above functional is somewhat computationally messy. We can save some work by proving another fact first. Let the function $f(y, y')$ be the integrand above:

$$t[y] = \int_0^l f(y, y') dx, \quad f(y, y') = \sqrt{\frac{1 + y'(x)^2}{2g(h - y(x))}}.$$

Without using the specific expression for $f(y, y')$ show that the vanishing variation of t with respect to

y implies that for some constant C :

$$y' \frac{\partial f}{\partial y'} - f(y, y') = C.$$

This result is known as the Beltrami identity. Notice that it is true because f does not depend explicitly on x . This is mathematically analogous to the theorem that energy is conserved when the Lagrangian does not depend explicitly on time as this functional $t[y]$ is acting in this analogy as our action, y as our path, x as our time, f as our Lagrangian, and the expression appearing on the left hand side of the Beltrami identity as our energy.

- (d) Using the Beltrami identity, show that the condition $\frac{\delta t}{\delta y} = 0$ implies that for some positive constant R :

$$(h - y(x))(1 + y'(x)^2) = 2R.$$

- (e) Separate the differential equation found in the previous part to derive the following integral relationship between x and y ($x(y)$ indicates the inverse function of $y(x)$):

$$x(y) = \int_y^h \sqrt{\frac{h - y_1}{2R - h + y_1}} dy_1.$$

Here y_1 is used as the name of the integration variable to avoid ambiguities with the meanings of y and y' .

- (f) The above integral is quite difficult to do without the right u-substitution. Use the u-substitution $y = h - R(1 - \cos \theta)$ to perform the integral in terms of θ and show that:

$$x = R(\theta - \sin \theta).$$

- (g) Show that the above solution is a cycloid of radius R and that the conditions on the track that the initial point is $(0, h)$ and final point is $(l, 0)$ imply that R is implicitly determined by:

$$l = R \arccos \left(1 - \frac{h}{R} \right) - \sqrt{2hR - h^2}.$$

- (h) Show then that no matter where the mass starts on the track from rest it actually takes the same amount of time to reach the lowest point of the track. Thus, not only is the cycloid the brachistochrone curve (curve of shortest time) but also an isochrone curve (curve of same time).

Problem 2.42: ★ Huygens' Pendulum. In studying the planar pendulum we found that the period of that pendulum depends on the amplitude of its swinging. This dependence makes it difficult to use an ordinary planar pendulum as a time keeping device. If instead the pendulum's period was independent of the amplitude, then time could be kept by counting the number of full swings, regardless of the amplitude of that swing. Christiaan Huygens (1629-1695, Dutch) discovered that if we place a correctly shaped wooden carving at the top of the pendulum string so that the string must conform to the shape of the carving, then the resulting pendulum can have this property.

- (a) Let the pivot point of the pendulum be the origin of our coordinate system and the edge of the wooden carving be given by the function $(u(s), v(s))$ where s is the arclength traveled from the pivot point along the wooden carving to the point in question. While swinging, the pendulum string (which always has fixed length l) conforms to the shape of the wood up to some point along the carving beyond which the string is a straight line (as it no longer is experiencing the constraint of the wood) until the mass m at the end is reached. Let $(x(s), y(s))$ be the position of the mass when the string makes contact with the wood up to arclength s . Show that $(x(s), y(s))$ are given in terms of $(u(s), v(s))$ by:

$$(x(s), y(s)) = (u(s) + (l - s)u'(s), v(s) + (l - s)v'(s)).$$

- (b) The above gives a parametric equation for the position of the mass (x, y) . Let z be the arclength traveled by the mass along whatever curve it traces out when displaced from hanging vertically. That is:

$$dz^2 = dx^2 + dy^2.$$

Then, we can use the arclength parameterization of a curve to define $(x(z), y(z))$, the position of the mass when it is an arclength z from hanging vertically. The position of the mass in time is thus specified by $z(t)$. Show that the Lagrangian for z is:

$$\mathcal{L} = \frac{1}{2}m\dot{z}^2 - mgy(z).$$

- (c) We know that the simple harmonic oscillator has a frequency which is independent of its amplitude and is given by a quadratic potential. Thus, we can make the Lagrangian in the previous part have oscillations which are isochronous (frequency is independent of amplitude) if we choose our curve so that y is quadratic in z . Show, using the conditions that $z = 0$ is defined as when the pendulum is hanging vertically, that hanging vertically is a stable equilibrium, and that we already know what the angular frequency of small oscillations is (from our study of the planar pendulum) that if y is quadratic in z it must be given by:

$$y(z) = -l + \frac{z^2}{2l}.$$

- (d) Use the above result and the definition of z to show that:

$$\frac{dx}{dz} = \sqrt{1 - \frac{z^2}{l^2}}.$$

- (e) The above can be integrated more easily if one makes the change of variables $z = l \sin \frac{\theta}{2}$. Use this to derive:

$$x = \frac{l}{4}(\theta + \sin \theta), \quad y = -\frac{3}{4}l - \frac{l}{4} \cos \theta.$$

Thus, conclude that the path the mass traces out must be a cycloid with radius $l/4$.

- (f) We now know the path x and y . Inverting to find the shape the wood must be to make this path can be challenging. However, an old theorem of geometry is helpful. When two curves are related the way we have related (x, y) and (u, v) , the (x, y) curve is called the “evolute” of (u, v) and it is a classic theorem that the evolute of a cycloid is a cycloid. Thus, we already know the curve (u, v) will also be a cycloid and simply have to find its parameters. So, (u, v) can be written as:

$$u = a + R(\theta + \alpha - \sin(\theta + \alpha)), \quad v = b - R(1 - \cos(\theta + \alpha)).$$

Use the results of (a) and (e) to determine the parameters a , b , α , and R and thus finally find the simplified functions $u(\theta)$ and $v(\theta)$ which define the necessary shape of the wood carving to make an isochronous pendulum. Huygens’ isochronous pendulum was used to design the pendulum clock, which was the most precise timekeeping device in the world from his invention in 1656 until the 1930’s [71].

Problem 2.43: Non-holonomic Bicycle. Consider a bicycle on flat ground, going without slipping, with wheels of radius R and distance l from the center of the back wheel to the center of the front wheel. When a bicycle turns, the back wheel points along the line between the front and back wheels while the front wheel turns from side to side without the center of the front wheel moving.

- (a) Let the xy plane be the plane of the ground. Let θ be the angle the line pointing from the back wheel to the front wheel makes with the x -axis. Let $\vec{x}_b$ be the position of the back wheel and $\vec{x}_f$ be the position of the front wheel. Show that:

$$\vec{x}_f - \vec{x}_b = l(\cos \theta, \sin \theta).$$

- (b) Let v_b be the speed of the center of the back wheel with respect to the ground, v_f be the speed of the center of the front wheel with respect to the ground, and α be the turn angle of the front wheel (the angle the direction of the front wheel makes with respect to the line between the back and front wheel). Show that:

$$\dot{\vec{x}}_b = v_b(\cos \theta, \sin \theta) \quad \text{and} \quad \dot{\vec{x}}_f = v_f(\cos(\theta + \alpha), \sin(\theta + \alpha)).$$

- (c) Use the results of the previous two parts together to show that:

$$v_f = \frac{v_b}{\cos \alpha} \quad \text{and} \quad \dot{\theta} = \frac{v_b}{l} \tan \alpha.$$

Thus, we see that riding a bicycle involves a linear non-holonomic constraint relating the speed of the front wheel to back wheel as well as a linear non-holonomic constraint relating the rate of change of the orientation of the bicycle to the speed of the back wheel. The speed of the back wheel is controlled by the rider (pedaling provides an external force to the back wheel) and so is the turn angle (by hands on the handles) and so $\alpha(t)$ and $v_b(t)$ are determined by the forces the rider provides. Explain how given this data this is sufficient to determine the path followed by the bicycle.

Problem 2.44: Particle hitting an impenetrable wall. Consider a particle of mass m for which $x > 0$

heading toward a wall on the yz plane at $x = 0$. The wall being impenetrable acts as an inequality constraint. We can study the effect of this constraint as in (2.8.16) by modeling the wall as being a spring and taking the limit that the stiffness of the spring goes to infinity.

- (a) Using our previous analysis of springs, the potential the wall produces is given by $U = \frac{1}{2}kx^2\vartheta(-x)$ where $\vartheta(x)$ is the Heaviside step function (1 for $x > 0$, 0 for $x < 0$ and $1/2$ for $x = 0$). The step function is because for $x > 0$ the mass does not compress the wall and so does not experience its springiness. Write the Hamiltonian for the mass incident on the wall and find the equations of motion for the mass.
- (b) Let the xy plane be the plane spanned by the normal vector to the wall and initial velocity vector of the particle before it hits the wall. Solve the equations of motion found in the previous part and show that the time the particle spends in contact with the wall is given by:

$$\tau = \pi\sqrt{\frac{m}{k}}$$

and the final velocity of the particle is given by:

$$\vec{v}_f = (v_{xf}, v_{yf}) = (-v_{x0}, v_{y0})$$

where v_{x0} and v_{y0} are the components of the initial velocity.

- (c) Show that the contact time goes to 0 as $k \rightarrow \infty$ (the wall becomes infinitely stiff means the bounce off the wall takes no time at all).
- (d) Explain how this derives that the “angle of incidence is the angle of reflection” where angle of incidence refers to the angle between the initial velocity and the normal vector to the wall and angle of reflection refers to the angle between the final velocity and the normal vector to the wall.
- (e) Explain how the limit of the potential as $k \rightarrow \infty$ is that $U = 0$ for $x > 0$ and $U = \infty$ for $x < 0$.

Problem 2.45: Particle hitting a penetrable wall. Consider a particle of mass m for which $x > 0$ heading toward a wall on the yz plane at $x = 0$. The wall being penetrable means that there is an energy cost ε to passing through the wall. If the particle is moving fast enough toward the wall, it will pass through. Otherwise, it will not. The exact potential corresponding to this scenario would be $U = \varepsilon\vartheta(-x)$ where $\vartheta(x)$ is the Heaviside step function defined in the previous problem.

- (a) The potential given in the preamble can be challenging to handle because the Heaviside step function is not differentiable. To be more careful, let $h_1(x)$ be a smooth monotonically increasing function which goes to 0 as x goes to $-\infty$ and which goes to 1 as x goes to ∞ . Show that:

$$\lim_{a \rightarrow 0^+} h_1\left(\frac{x}{a}\right) = \vartheta(x).$$

This allows us to use a nice function at all intermediate stages and then take the parameter $a \rightarrow 0^+$ at the end. One can think of a as the “thickness” of the wall in our problem (why?). If one needs an example of such an $h_1(x)$, consider:

$$h_1(x) = \frac{2}{\pi} \arctan(x).$$

- (b) Show that if the particle does not penetrate the wall then its final velocity is given by:

$$\vec{v}_f = (v_{xf}, v_{yf}) = (-v_{x0}, v_{y0})$$

and that again the angle of incidence is the angle of reflection.

- (c) Show that if the particle does penetrate the wall then its final velocity is given by:

$$(v_{xf}, v_{yf}) = \left(-\sqrt{v_{x0}^2 - \frac{2\varepsilon}{m}}, v_{y0} \right)$$

and that the angle of incidence θ_0 is related to the angle of transmission θ_t (the angle between the final velocity and the normal vector to the wall when the particle makes it through) by:

$$\tan \theta_t = \frac{\tan \theta_0}{\sqrt{1 - \frac{2\varepsilon}{mv_{x0}^2}}}.$$

- (d) Show that if the particle is transmitted with the minimum possible speed toward the wall then it comes out parallel to the wall. As well, show that as the speed of the particle goes to ∞ the angle of transmission limits to the angle of incidence (the particle just flies straight through the wall).

Problem 2.46: Loop-the-Loop Consider a mass m to be entering a vertical circular track of radius R at speed v at the bottom of the track. Let the origin be the center of the circle. Then, the track provides the inequality constraint $|\vec{x}| \leq R$.

- (a) Explain that while the mass is up against the track $|\vec{x}| = R$ and show that in coordinates $\vec{x} = (r \sin \theta, -r \cos \theta)$ the Lagrangian during this period can be taken to be:

$$\mathcal{L} = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + mgr \cos \theta + \lambda(r - R)$$

where λ is a Lagrangian multiplier to enforce the presence of the track.

- (b) Using the equations of motion of the Lagrangian, show that while the mass is against the track λ is given by:

$$\lambda = 2mg - \frac{mv^2}{R} - 3mg \cos \theta.$$

- (c) Explain that in order for the mass to fall off of the circular track, λ must drop to 0. As well, show that the minimum value of v so that the mass makes it all the way through the circular loop without falling off is $v = \sqrt{5gR}$.

2.9 Rigid Bodies

Certainly the objects of daily life are quite apparently not point particles. Instead, they seem to be made out of continuous distributions of matter. However, from our point particle model we can build up a theory of bodies of non-zero size. In principle, all of the mass elements which make up every day objects could move independently of each other and interact with each other. This allows significant complexity and leads to a discipline called **continuum mechanics**, which we will not be ready to discuss until chapter 6. For now, we will make the significant simplifying approximation that we are considering **rigid bodies**. A rigid body is a collection of masses in which the mass elements are constrained to move together in a way which keeps the geometry of the body fixed rather than allowing them to move independently. This is an appropriate assumption if the interactions between the mass elements is so strong as to keep them moving together without changing shape and so is good for most solids (when you don't hit them too hard) but obviously wrong for gases where the masses are essentially free from interacting with each other. For bodies which are deformable, one needs to study the theory of elastic bodies. For systems of particles which are not bound to a given shape at all, one needs to study a theory of fluids. All of these theories are simplifications of an underlying theory of interacting masses. Beyond rigid bodies will have to wait for now (until chapter 6).

A rigid body by definition has its mass distributed in a fixed way with a fixed shape. Let α be some label which identifies a unique mass element in the body and so to each α there is a position $\vec{x}_\alpha(t)$ which is the position of that mass element. Let $\vec{x}(t)$ be the position of a specially chosen reference point for the body (any point of the body can be chosen for now). We will call this arbitrarily chosen element the “center” (even though it need not be the geometric center or center in any other sense of the word). Because the shape of the body is fixed (it is rigid), the distance between any two mass elements of the body is fixed in time. So, once the position of the center $\vec{x}$ is known, the position of a mass element with label α , $\vec{x}_\alpha$, within the body must be on the sphere of a given radius (that radius is the fixed distance $|\vec{x}_\alpha - \vec{x}|$) and so it is specified up to a rotation about the center. Therefore, we can write that $\vec{x}_\alpha = \vec{x} + \hat{R}\vec{y}_\alpha$ where $\hat{R}$ is a rotation matrix and $\vec{y}_\alpha$ is the difference $\vec{x}_\alpha - \vec{x}$ in some “default” orientation of the body in which no rotation is applied (that default orientation is also arbitrary). Because the body is rigid, when we rotate one point about the center, all of the other points in the body are also rotated about the center by the same rotation. Hence, the rotation matrix $\hat{R}$ does not depend on α (which mass element we are looking at). A smart choice of labels α is just to label mass elements by where they would be relative to the center in the default orientation of the body. That is, $\vec{y}_\alpha = \vec{\alpha}$. As we found in section 2.4, a rotation matrix is specified by a vector $\vec{\theta}$ whose magnitude gives the angle of rotation and whose direction gives the axis of rotation. Therefore, the positions of mass elements within a rigid body are given by:

$$\boxed{\vec{x}_\alpha(t) = \vec{x}(t) + \hat{R}(\vec{\theta}(t))\vec{\alpha}.} \quad (2.9.1)$$

This is precisely a holonomic constraint on the positions of each mass element and so we can directly insert it into the Lagrangian for the unconstrained mass elements to find the Lagrangian for a rigid body. Thus, the theory of rigid bodies contains 6 variables: 3 variables for position of the body, $\vec{x}(t)$, and 3 variables for the orientation of the body, $\vec{\theta}(t)$.

2.9.1 The Axis-Angle Lagrangian for a Rigid Body

Because aside from the constraint of moving together each of the masses is independent of the others within the body we can use Theorem 2.10 to find the total Lagrangian by simply adding the individual Lagrangians for each mass. For N masses:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + q_n \vec{A}(t, \vec{x}_n) \cdot \dot{\vec{x}}_n - q_n \phi(t, \vec{x}) \right). \quad (2.9.2)$$

For a rigid body, this usually needs to be continuous (as mass would be distributed continuously throughout the body) which can be done by integrating (the continuum limit of summing) over all of the mass elements:

$$\mathcal{L} = \int_M \frac{1}{2} |\dot{\vec{x}}_\alpha|^2 dm(\vec{\alpha}) + \int_M \left(\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha - \phi(t, \vec{x}_\alpha) \right) dq(\vec{\alpha}). \quad (2.9.3)$$

The symbol M is used to indicate the set of all labels $\vec{\alpha}$ taken in the rigid body matter. This integral then is an integral over the whole body.

We have the constraint $\vec{x}_\alpha = \vec{x} + \hat{R}(\vec{\theta})\vec{\alpha}$ and would like to impose this in the Lagrangian. This constraint is holonomic and by the Holonomic Constraint Theorem, we can just direct insert this expression for $\vec{x}_\alpha$ into the unconstrained Lagrangian to get the constrained Lagrangian. This first term of (2.9.3), which we will call $\mathcal{L}_0$, can actually be simplified quite nicely for a rigid body. To do so, we will need the velocity $\dot{\vec{x}}_\alpha$:

$$\vec{x}_\alpha = \vec{x} + \hat{R}(\vec{\theta})\vec{\alpha} \implies \dot{\vec{x}}_\alpha = \dot{\vec{x}} + \frac{d\hat{R}}{dt}\vec{\alpha}. \quad (2.9.4)$$

The time derivative of the rotation matrix is a bit of a mess. Naively one might wish to apply the chain rule to the exponential representation of the rotation matrix to pull down a factor of $\dot{\vec{\theta}} \times$. However, it is not quite so simple because the matrices $\dot{\vec{\theta}} \times$ and $\vec{\theta} \times$ do not in general commute. So, we need to be a little more clever. Define the vector $\vec{\beta}(s)$:

$$\vec{\beta}(s) = \frac{d}{ds} \left(e^{s\vec{\theta} \times} \right) e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} \quad (2.9.5)$$

$$\implies \vec{\beta}(0) = 0, \quad \vec{\beta}(1) = \frac{d\hat{R}}{dt}\vec{\alpha}. \quad (2.9.6)$$

Using the fundamental theorem of calculus:

$$\frac{d\hat{R}}{dt}\vec{\alpha} = \vec{\beta}(1) = \vec{\beta}(0) + \int_0^1 \frac{d\vec{\beta}}{ds} ds = \int_0^1 \frac{d\vec{\beta}}{ds} ds. \quad (2.9.7)$$

Hence, we just need $\frac{d\vec{\beta}}{ds}$. Differentiating with respect to s , it is okay to use the chain rule here because $\vec{\theta} \times$ commutes with itself (as any matrix does):

$$\frac{d\vec{\beta}}{ds} = \frac{d}{ds} \left(e^{s\vec{\theta} \times} \vec{\theta} \times \right) e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} - \frac{d}{ds} \left(e^{s\vec{\theta} \times} \right) \vec{\theta} \times e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} \quad (2.9.8)$$

$$= \frac{d}{ds} \left(e^{s\vec{\theta} \times} \right) \vec{\theta} \times e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} + e^{s\vec{\theta} \times} \dot{\vec{\theta}} \times e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} - \frac{d}{ds} \left(e^{s\vec{\theta} \times} \right) \vec{\theta} \times e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} \quad (2.9.9)$$

$$= e^{s\vec{\theta} \times} \dot{\vec{\theta}} \times e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} \quad (2.9.10)$$

$$\implies e^{-s\vec{\theta} \times} \frac{d\vec{\beta}}{ds} = \dot{\vec{\theta}} \times \left(e^{-s\vec{\theta} \times} \hat{R}\vec{\alpha} \right). \quad (2.9.11)$$

Now using that $(\hat{R}\vec{u}) \times (\hat{R}\vec{v}) = \hat{R}(\vec{u} \times \vec{v})$ and applying the rotation matrix $e^{s\vec{\theta} \times}$ to all the vectors, we have:

$$\frac{d\vec{\beta}}{ds} = \left(e^{s\vec{\theta} \times} \dot{\vec{\theta}} \right) \times \left(\hat{R}\vec{\alpha} \right). \quad (2.9.12)$$

Thus (2.9.7) becomes:

$$\frac{d\hat{R}}{dt}\vec{\alpha} = \int_0^1 \left(e^{s\vec{\theta} \times} \dot{\vec{\theta}} \right) \times \left(\hat{R}\vec{\alpha} \right) ds = \left(\int_0^1 e^{s\vec{\theta} \times} ds \dot{\vec{\theta}} \right) \times \left(\hat{R}\vec{\alpha} \right). \quad (2.9.13)$$

The integral can in principle be done explicitly using (2.4.48), but the result will be useless to us. Instead, we will leave it unsimplified and define:

$$\hat{M}(\theta) = \int_0^1 e^{s\vec{\theta} \times} ds. \quad (2.9.14)$$

Thus because (2.9.13) holds for all $\vec{\alpha}$:

$$\frac{d\hat{R}}{dt} = \left(\hat{M}\dot{\vec{\theta}} \right) \times \hat{R} \quad (2.9.15)$$

$$\implies \dot{\vec{x}}_\alpha = \dot{\vec{x}} + (\hat{M}\dot{\vec{\theta}}) \times (\hat{R}\vec{\alpha}). \quad (2.9.16)$$

We need the magnitude $|\dot{\vec{x}}_\alpha|$ for the Lagrangian:

$$|\dot{\vec{x}}_\alpha|^2 = |\dot{\vec{x}}|^2 + 2\dot{\vec{x}} \cdot \left((\hat{M}\dot{\vec{\theta}}) \times (\hat{R}\vec{\alpha}) \right) + |(\hat{M}\dot{\vec{\theta}}) \times (\hat{R}\vec{\alpha})|^2. \quad (2.9.17)$$

Here we need the cyclicity of the triple product $\vec{A} \cdot (\vec{B} \times \vec{C}) = \vec{C} \cdot (\vec{A} \times \vec{B})$ and that the magnitude of the cross product is $|\vec{A} \times \vec{B}|^2 = |\vec{A}|^2 |\vec{B}|^2 - (\vec{A} \cdot \vec{B})^2$. With these and a little algebra:

$$|\dot{\vec{x}}_\alpha|^2 = |\dot{\vec{x}}|^2 + 2 \left(\dot{\vec{x}} \times (\hat{M}\dot{\vec{\theta}}) \right) \cdot \hat{R}\vec{\alpha} + (\hat{M}\dot{\vec{\theta}})^T \hat{R} (|\vec{\alpha}|^2 \mathbb{1} - \vec{\alpha}\vec{\alpha}^T) \hat{R}^T (\hat{M}\dot{\vec{\theta}}). \quad (2.9.18)$$

Computing $\mathcal{L}_0$ then:

$$\int_{\mathbf{M}} \frac{1}{2} |\dot{\vec{x}}_\alpha|^2 dm = \frac{1}{2} |\dot{\vec{x}}|^2 \int_{\mathbf{M}} dm + \left(\dot{\vec{x}} \times (\hat{M} \dot{\vec{\theta}}) \right) \cdot \hat{R} \int_{\mathbf{M}} \vec{\alpha} dm + \frac{1}{2} \dot{\vec{\theta}}^T \hat{M}^T \hat{R} \int_{\mathbf{M}} (|\vec{\alpha}|^2 \mathbb{1} - \vec{\alpha} \vec{\alpha}^T) dm \hat{R}^T \hat{M} \dot{\vec{\theta}}. \quad (2.9.19)$$

This first integral is simply the total mass of the object:

$$m = \int_{\mathbf{M}} dm. \quad (2.9.20)$$

We haven't ever specified any conditions on the definition of the center $\vec{x}$. We will now do so by defining the center so that the middle term vanishes. That is we want:

$$\int_{\mathbf{M}} \vec{\alpha} dm = 0. \quad (2.9.21)$$

Let's see that this is always possible. Suppose we pick one definition of the center and in that definition this integral doesn't vanish:

$$\int_{\mathbf{M}} \vec{\alpha} dm = \vec{u}. \quad (2.9.22)$$

Then, because it is the position of each element of the matter $\vec{x}_\alpha$ (and its time derivative) that enters the Lagrangian, we can shift the definitions of the center $\vec{x}$ and the deviation $\vec{\alpha}$ as long as we keep $\vec{x}_\alpha$ fixed. So, consider the redefined labels:

$$\vec{\alpha}' = \vec{\alpha} - \frac{\vec{u}}{m}. \quad (2.9.23)$$

Requiring that $\vec{x}_\alpha$ be unchanged:

$$\vec{x}_\alpha = \vec{x} + \hat{R} \vec{\alpha} = \vec{x}' + \hat{R} \vec{\alpha}' = \vec{x}' + \hat{R} \left(\vec{\alpha} - \frac{\vec{u}}{m} \right) \quad (2.9.24)$$

$$\implies \vec{x}' = \vec{x} + \frac{1}{m} \hat{R} \vec{u}. \quad (2.9.25)$$

Now under this redefinition of labels:

$$\int_{\mathbf{M}} \vec{\alpha}' dm = \int_{\mathbf{M}} \left(\vec{\alpha} - \frac{\vec{u}}{m} \right) dm = \int_{\mathbf{M}} \vec{\alpha} dm - \frac{\vec{u}}{m} \int_{\mathbf{M}} dm = \vec{u} - \frac{\vec{u}}{m} m = 0. \quad (2.9.26)$$

Hence it is always possible to make equation (2.9.21) true by the correct choice of the center as long as the total mass m is not 0. Conveniently, mass is always observed to be positive (which doesn't really have an explanation in our theory so far but we will show why much later) and so this is always possible. Considering this, we will require the second term in equation (2.9.19) to vanish by definition. In this scheme, we can now rightfully call the center the **center of mass** because it is literally the average position by mass:

$$\vec{x}_\alpha = \vec{x} + \hat{R} \vec{\alpha} \quad (2.9.27)$$

$$\implies \int_{\mathbf{M}} \vec{x}_\alpha dm = \int_{\mathbf{M}} \vec{x} dm + \int_{\mathbf{M}} \hat{R} \vec{\alpha} dm \quad (2.9.28)$$

$$\implies \vec{x} = \frac{1}{m} \int_{\mathbf{M}} \vec{x}_\alpha dm = \text{Mass weighted average position.} \quad (2.9.29)$$

It is entirely possible to study rigid bodies when the center is not chosen to be the center of mass of the body. However, the resulting equations of motion appear more complicated unnecessarily.

Turning our attention to the third term in equation (2.9.19), define the (body frame) **moment of inertia matrix**:

$$\hat{I} \stackrel{\text{def}}{=} \int_{\mathbf{M}} (|\vec{\alpha}|^2 \mathbb{1} - \vec{\alpha} \vec{\alpha}^T) dm. \quad (2.9.30)$$

Considering the mass density $\rho_m(\vec{\alpha})$ as the mass per unit volume in the default orientation of the body we can then write:

$$dm = \rho_m d^3 \vec{\alpha} \quad (2.9.31)$$

$$\implies \hat{I} = \int_{\mathbf{M}} \rho_m(\vec{\alpha}) (|\vec{\alpha}|^2 \mathbb{1} - \vec{\alpha} \vec{\alpha}^T) d^3 \vec{\alpha}. \quad (2.9.32)$$

Therefore the mass term in the Lagrangian becomes:

$$\int_M \frac{1}{2} |\dot{\vec{x}}_\alpha|^2 dm = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \dot{\vec{\theta}}^T \hat{M}^T \hat{R} \hat{I} \hat{R}^T \hat{M} \dot{\vec{\theta}}. \quad (2.9.33)$$

So all the necessary information about the geometry of the matter for computing this term is contained in the moment of inertia matrix. The interacting terms of the Lagrangian don't simplify as nicely in general and only become "nice" in select special cases. Thus, we have that the Lagrangian for a rigid body in Axis-Angle coordinates $(\vec{x}, \vec{\theta})$ is given by:

$$\mathcal{L}(t, \vec{x}, \dot{\vec{x}}, \vec{\theta}, \dot{\vec{\theta}}) = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \dot{\vec{\theta}}^T \hat{M}^T(\vec{\theta}) \hat{R}(\vec{\theta}) \hat{I} \hat{R}^T(\vec{\theta}) \hat{M}(\vec{\theta}) \dot{\vec{\theta}} + \int_M \left(\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha - \phi(t, \vec{x}_\alpha) \right) dq. \quad (2.9.34)$$

We then would get our equations of motion by the standard Euler-Lagrange equations applied to this Lagrangian for $\vec{x}$ and $\vec{\theta}$. However, doing so turns out to be quite a computational mess (due to the matrices $\hat{R}$ and $\hat{M}$) and not the most clear way of understanding what the body does. So, instead of going that route, we will explore more clever coordinates.

2.9.2 Angular Velocity and the Principal Axes

A useful additional variable for studying our system (and motivating better coordinates) will be the angular velocity, the rate at which the system rotates in time. Under a rotation of our system by angle vector $\vec{\varepsilon}$ the positions $\vec{x}_\alpha$ will be rotated to a new position $\vec{x}'_\alpha$:

$$\vec{x}'_\alpha(\vec{\varepsilon}) = \hat{R}(\vec{\varepsilon}) \vec{x}_\alpha = \hat{R}(\vec{\varepsilon})(\vec{x} + \hat{R}(\vec{\theta}) \vec{\alpha}) = \hat{R}(\vec{\varepsilon}) \vec{x} + \hat{R}(\vec{\varepsilon}) \hat{R}(\vec{\theta}) \vec{\alpha}. \quad (2.9.35)$$

This must give a new center $\vec{x}'(\vec{\varepsilon})$ and orientation $\vec{\theta}'(\vec{\varepsilon})$ after rotation:

$$\vec{x}'_\alpha(\vec{\varepsilon}) = \vec{x}'(\vec{\varepsilon}) + \hat{R}(\vec{\theta}'(\vec{\varepsilon})) \vec{\alpha}. \quad (2.9.36)$$

Matching the two, the α independent term tells us the center of mass rotates by:

$$\vec{x}'(\vec{\varepsilon}) = \hat{R}(\vec{\varepsilon}) \vec{x} \quad (2.9.37)$$

as we already knew. As well, the α dependent term tells us that the new rotation angle $\vec{\theta}'(\vec{\varepsilon})$ will satisfy:

$$\hat{R}(\vec{\theta}'(\vec{\varepsilon})) = \hat{R}(\vec{\varepsilon}) \hat{R}(\vec{\theta}). \quad (2.9.38)$$

The body rotates over time and so let $\vec{\omega}(t)$, the angular velocity of the body, be its rate of rotation at time t . The rate of rotation is defined so that in a time δt the body rotates by an angle vector $\vec{\omega}(t) \delta t + \mathcal{O}(\delta t^2)$. That is:

$$\hat{R}(\vec{\theta}(t + \delta t)) = \hat{R}(\vec{\omega}(t) \delta t + \mathcal{O}(\delta t^2)) \hat{R}(\vec{\theta}(t)). \quad (2.9.39)$$

Expanding both sides to order δt and using that $\hat{R}(\vec{\theta}) = e^{\vec{\theta} \times}$:

$$\hat{R}(\vec{\theta}(t)) + \delta t \frac{d\hat{R}(\vec{\theta}(t))}{dt} = (\mathbb{1} + \delta t \vec{\omega}(t) \times) \hat{R}(\vec{\theta}(t)) + \mathcal{O}(\delta t^2) \quad (2.9.40)$$

$$\implies \frac{d\hat{R}(\vec{\theta}(t))}{dt} = \vec{\omega}(t) \times \hat{R}(\vec{\theta}(t)). \quad (2.9.41)$$

By comparing to (2.9.15) (because it is true for all $\vec{\alpha}$) we see that:

$$\vec{\omega}(t) = \hat{M} \dot{\vec{\theta}}. \quad (2.9.42)$$

In a time δt the system rotates by an angle $\delta \vec{\Theta} = \vec{\omega} \delta t + \mathcal{O}(\delta t^2)$ and the angle coordinates $\vec{\theta}$ change by $\delta \vec{\theta} = \dot{\vec{\theta}} \delta t + \mathcal{O}(\delta t^2)$. Because this holds for arbitrary time dependence, we have that under a rotation of the system by $\delta \vec{\Theta}$, the angle coordinates are varied by $\delta \vec{\theta}$ give by:

$$\delta \vec{\Theta} = \hat{M} \delta \vec{\theta}. \quad (2.9.43)$$

Consequently, by (2.9.41) a general variation of the rotation matrix is given by:

$$\delta \hat{R} = \delta \vec{\Theta} \times \hat{R}. \quad (2.9.44)$$

If we apply a rotation by ε^a , then by definition $\delta \Theta^a = \varepsilon^a$. Similarly, letting $\mathcal{D}_b \theta^a$ be the change in θ^a with respect to ε^b near the identity, we have $\delta \theta^a = \varepsilon^b \mathcal{D}_b \theta^a$. Therefore:

$$\varepsilon^a = M^a_b \varepsilon^c \mathcal{D}_c \theta^b \implies M^a_b \mathcal{D}_c \theta^b = \delta^a_c \implies \mathcal{D}_b \theta^a = (\hat{M}^{-1})^a_b. \quad (2.9.45)$$

It will also be useful to define $\tilde{I}$, the spatial frame moment of inertia matrix. Viewing the body frame moment of inertia matrix $\hat{I}$ in components and applying the $\hat{R}$ and $\hat{R}^T$ factors which accompany it in our Lagrangian:

$$\tilde{I} \stackrel{\text{def}}{=} \hat{R} \hat{I} \hat{R}^T = \hat{R} I^{ab} \vec{t}_a \vec{t}_b^T \hat{R}^T = I^{ab} (\hat{R} \vec{t}_a) (\hat{R} \vec{t}_b)^T \quad (2.9.46)$$

we can see that $\tilde{I}$ is simply the new moment of inertia matrix after applying a rotation to the object. That is, $\hat{I}$ is defined in the default orientation of the body in which $\hat{R} = 1$ and $\tilde{I}$ is the version of the moment of the inertia matrix which rotates with the body as it is rotated. Then, our Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \vec{\omega}^T \tilde{I} \vec{\omega} + \int_M \left(\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha - \phi(t, \vec{x}_\alpha) \right) dq. \quad (2.9.47)$$

Through using $\vec{\omega}$, we can eliminate $\dot{\vec{\theta}}$ from directly appearing in the Lagrangian. Through introducing a rotating basis of vectors, we can eliminate $\vec{\theta}$ from directly appearing in the Lagrangian. The displacement of a mass element in the body from the center before rotation is by definition given by $\vec{\alpha}$. We can define a basis of vectors $\vec{t}_a$, thus allowing $\vec{\alpha}$ to be decomposed into components:

$$\vec{\alpha} = \alpha^a \vec{t}_a. \quad (2.9.48)$$

It will be convenient to choose this basis to be orthonormal and right-handed (for example, this basis could be that standard set of basis vectors for Cartesian coordinates):

$$\vec{t}_a \cdot \vec{t}_b = \delta_{ab}, \quad \text{Orthonormal} \quad (2.9.49)$$

$$\vec{t}^a \vec{t}_a^T = \mathbb{1}, \quad \text{Complete} \quad (2.9.50)$$

$$\vec{t}_a \times \vec{t}_b = \epsilon_{ab}{}^c \vec{t}_c, \quad \text{Right-Handed.} \quad (2.9.51)$$

Then, after the body is rotated, the new displacement from the center of mass is $\hat{R}\vec{\alpha}$. This rotation extends down to our basis vectors and allows us to define a rotated set of basis vectors:

$$\hat{R}\vec{\alpha} = \hat{R}\alpha^a \vec{t}_a = \alpha^a \hat{R}\vec{t}_a = \alpha^a \vec{\xi}_a \quad (2.9.52)$$

$$\vec{\xi}_a \stackrel{\text{def}}{=} \hat{R}\vec{t}_a \quad (2.9.53)$$

One can check by hand that the new basis $\vec{\xi}_a$ also satisfy the properties of orthonormality, completeness, and right-handedness. From (2.9.53), multiplying both sides by $\vec{t}_a^T$, summing over a , and using completeness:

$$\vec{\xi}^a \vec{t}_a^T = \hat{R} \vec{t}^a \vec{t}_a^T = \hat{R} \mathbb{1} = \hat{R}. \quad (2.9.54)$$

Hence, $\hat{R}$ can be recovered from the set of $\vec{\xi}_a$. Because $\vec{\theta}$ can be determined from $\hat{R}$, this means that $\vec{\theta}$ can be determined from the rotated set of basis vector $\vec{\xi}_a$. Hence, we can eliminate $\vec{\theta}$ from explicitly appearing in the Lagrangian in favor of expressing angle dependence in terms of the rotated basis $\vec{\xi}_a$. This change is only visual as the $\vec{\xi}_a$ are not independent variables, the underlying $\vec{\theta}$ are. To use the $\vec{\xi}_a$, we will need their equations of motion. This can be found directly from their definition:

$$\frac{d\vec{\xi}_a}{dt} = \frac{d}{dt} \hat{R} \vec{t}_a = \frac{d\hat{R}}{dt} \vec{t}_a = \vec{\omega} \times \hat{R} \vec{t}_a = \vec{\omega} \times \vec{\xi}_a. \quad (2.9.55)$$

Because the matrix $\hat{I}$ is real-symmetric, it is diagonalizable by a set of orthonormal normal eigenvectors with real eigenvalues. Since we already need an orthonormal basis, the most common choice of $\vec{t}_a$ are the orthonormal eigenvectors of $\hat{I}$. Then, the $\vec{\xi}_a$ are called the principal axes of the body and the eigenvalues I_a are called the principal moments of inertia. By the eigenvalue equation:

$$\hat{I} \vec{t}_a = I_a \vec{t}_a \quad (2.9.56)$$

Then, we can calculate $\hat{I}$ in terms of these eigenvectors and eigenvalues using the completeness relation:

$$\hat{I} = \hat{I} \mathbb{1} = \hat{I} \vec{t}^a \vec{t}_a^T = I_1 \vec{t}_1 \vec{t}_1^T + I_2 \vec{t}_2 \vec{t}_2^T + I_3 \vec{t}_3 \vec{t}_3^T. \quad (2.9.57)$$

Then $\tilde{I}$ becomes:

$$\tilde{I} = \hat{R} \hat{I} \hat{R}^T = I_1 \hat{R} \vec{t}_1 \vec{t}_1^T \hat{R}^T + I_2 \hat{R} \vec{t}_2 \vec{t}_2^T \hat{R}^T + I_3 \hat{R} \vec{t}_3 \vec{t}_3^T \hat{R}^T \quad (2.9.58)$$

$$= I_1 \vec{\xi}_1 \vec{\xi}_1^T + I_2 \vec{\xi}_2 \vec{\xi}_2^T + I_3 \vec{\xi}_3 \vec{\xi}_3^T. \quad (2.9.59)$$

So, then our basis $\vec{\xi}_a$ correspond to the eigenvectors of $\tilde{I}$, the moment of inertia matrix after the body is rotated (this is why they are called the principal axes). Because these $\vec{\xi}_a$ track the rotation of the body's

coordinates, they are called “body frame vectors” or “frame vectors” or just “the frame”.

In summary, now instead of expressing our Lagrangian as $\mathcal{L}(t, \vec{x}, \dot{\vec{x}}, \vec{\theta}, \dot{\vec{\theta}})$, we can eliminate $\vec{\theta}$ in favor of our rotating basis $\vec{\xi}_a$ and eliminate $\dot{\vec{\theta}}$ in favor of our angular velocity $\vec{\omega}$ to have the Lagrangian $\mathcal{L}(t, \vec{x}, \dot{\vec{x}}, \vec{\xi}, \vec{\omega})$. However, we have not yet established how to cleanly find the equations of motion of such a Lagrangian written in this way. It turns out the smart path is to go through the action as we can view the dependence of $\vec{\xi}$ and $\vec{\omega}$ on $\vec{\theta}$ and $\dot{\vec{\theta}}$ as constraints and use d’Alembert’s principle to compute equations of motion.

2.9.3 Rigid Body Action in Frame-Angular Velocity Coordinates

The motion of rigid bodies is captured very nicely by the action, even in frame-angular velocity coordinates. This is because the frame vectors are holonomically constrained by the value of θ , as they are just given by functions of θ , and the angular-velocity vector is non-holonomically constrained by the values of θ and $\dot{\vec{\theta}}$, as it is given by a function of them together. Thus, using d’Alembert’s principle we can find the equations of motion for these constrained variables from the action:

$$S = \int_{t_0}^{t_f} \mathcal{L}(t, \vec{x}, \dot{\vec{x}}, \vec{\xi}, \vec{\omega}) dt \quad (2.9.60)$$

$$\implies \delta S = \int_{t_0}^{t_f} \left(\frac{\partial \mathcal{L}}{\partial \vec{x}} \cdot \delta \vec{x} + \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \cdot \delta \dot{\vec{x}} + \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} \cdot \delta \vec{\xi}_a + \frac{\partial \mathcal{L}}{\partial \vec{\omega}} \cdot \delta \vec{\omega} \right) dt. \quad (2.9.61)$$

By equation (2.9.44), $\delta \vec{\xi}_a$ is given by:

$$\vec{\xi}_a = \hat{R} \vec{e}_a \implies \delta \vec{\xi}_a = \delta \hat{R} \vec{e}_a = (\hat{M} \delta \vec{\theta}) \times \hat{R} \vec{e}_a = \delta \vec{\Theta} \times \vec{\xi}_a \quad (2.9.62)$$

where we use the instantaneous angular variation $\delta \vec{\Theta}(t)$ defined as before in terms of the genuine angle coordinate variation $\delta \vec{\theta}$. The components of $\delta \vec{\Theta}$ are all linearly independent (because $\hat{M}$ is invertible and the $\delta \vec{\theta}$ are). We can actually cleanly solve for $\delta \vec{\Theta}$ in terms of $\delta \vec{\xi}_a$, which will turn out to be helpful:

$$\vec{\xi}_a \times \delta \vec{\xi}_a = (\vec{\xi}_a) \times (\delta \vec{\Theta} \times \vec{\xi}_a) = \delta \vec{\Theta} (\vec{\xi}_a \cdot \vec{\xi}_a) - \vec{\xi}_a (\vec{\xi}_a \cdot \delta \vec{\Theta}) \quad (2.9.63)$$

$$\implies \delta \vec{\Theta} = \frac{1}{2} \vec{\xi}_a \times \delta \vec{\xi}_a. \quad (2.9.64)$$

Here we have used that the $\vec{\xi}_a$ are orthonormal and complete. Following the same steps for $\vec{\omega}$ starting from (2.9.55) we have:

$$\vec{\omega} = \frac{1}{2} \vec{\xi}_a \times \frac{d \vec{\xi}_a}{dt}. \quad (2.9.65)$$

Then, the variation of $\vec{\omega}$ is given by:

$$\delta \vec{\omega} = \frac{1}{2} \delta \vec{\xi}_a \times \frac{d \vec{\xi}_a}{dt} + \frac{1}{2} \vec{\xi}_a \times \frac{d \delta \vec{\xi}_a}{dt} = \frac{1}{2} \delta \vec{\xi}_a \times \frac{d \vec{\xi}_a}{dt} + \frac{d}{dt} \left(\frac{1}{2} \vec{\xi}_a \times \delta \vec{\xi}_a \right) - \frac{1}{2} \frac{d \vec{\xi}_a}{dt} \times \delta \vec{\xi}_a \quad (2.9.66)$$

$$= \frac{d}{dt} \delta \vec{\Theta} + \delta \vec{\Theta} \times \vec{\omega}. \quad (2.9.67)$$

Returning all this to the variation of the action:

$$\delta S = \int_{t_0}^{t_f} \left(\frac{\partial \mathcal{L}}{\partial \vec{x}} \cdot \delta \vec{x} + \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \cdot \frac{d}{dt} \delta \vec{x} + \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} \cdot (\delta \vec{\Theta} \times \vec{\xi}_a) + \frac{\partial \mathcal{L}}{\partial \vec{\omega}} \cdot \left(\frac{d}{dt} \delta \vec{\Theta} + \delta \vec{\Theta} \times \vec{\omega} \right) \right) dt \quad (2.9.68)$$

$$= \int_{t_0}^{t_f} \left(\left(\frac{\partial \mathcal{L}}{\partial \vec{x}} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \right) \right) \cdot \delta \vec{x} + \left(\vec{\xi}_a \times \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \vec{\omega}} \right) + \vec{\omega} \times \frac{\partial \mathcal{L}}{\partial \vec{\omega}} \right) \cdot \delta \vec{\Theta} \right) dt \quad (2.9.69)$$

where we have used that the variations $\delta \vec{x}$ and $\delta \vec{\theta}$ (and so consequently $\delta \vec{\Theta}$) vanish at the time endpoints. Then, in the absence of any external forces we can see that the rigid body equations of motion given by this action are:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \quad (2.9.70)$$

$$\vec{\xi}_a \times \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} + \vec{\omega} \times \frac{\partial \mathcal{L}}{\partial \vec{\omega}} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \vec{\omega}}. \quad (2.9.71)$$

In the presence of external forces as usual we don’t require the variation of the free action to be 0 and

instead require its variation to match some external force terms as in equation (2.7.49). The external force on the position variables is called the linear force $\vec{F}_{\text{ext}}$ and the external force in the $\delta\vec{\Theta}$ is called the torque $\vec{\tau}_{\text{ext}}$. That is, we require:

$$\delta S = - \int_{t_0}^{t_f} \left(\vec{F}_{\text{ext}} \cdot \delta \vec{x} + \vec{\tau}_{\text{ext}} \cdot \delta \vec{\Theta} \right) dt. \quad (2.9.72)$$

Then, in the presence of external forces we see the equations of motion become:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{\partial \mathcal{L}}{\partial \vec{x}} + \vec{F}_{\text{ext}} \quad (2.9.73)$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{\omega}}} = \vec{\omega} \times \frac{\partial \mathcal{L}}{\partial \vec{\omega}} + \vec{\xi}_a \times \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} + \vec{\tau}_{\text{ext}}. \quad (2.9.74)$$

Now that we have our equations of motion for a general rigid body, let us finally return to our specific Lagrangian (2.9.47). In terms of our angular velocity and frame coordinates:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \vec{\omega}^T \tilde{I} \vec{\omega} + \int_{\text{M}} \left(\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha - \phi(t, \vec{x}_\alpha) \right) dq. \quad (2.9.75)$$

Then, from (2.9.70) for the position of the center of mass we have:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} = \int_{\text{M}} \left(\nabla (\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha) - \nabla \phi(t, \vec{x}_\alpha) \right) dq \quad (2.9.76)$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = m \dot{\vec{x}} + \int_{\text{M}} \vec{A}(t, \vec{x}_\alpha) dq \quad (2.9.77)$$

$$\implies m \ddot{\vec{x}} = \int_{\text{M}} \left(\vec{E}(t, \vec{x}_\alpha) + \dot{\vec{x}}_\alpha \times \vec{B}(t, \vec{x}_\alpha) \right) dq. \quad (2.9.78)$$

For the angular velocity we have:

$$\vec{\xi}_a \times \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} + \vec{\omega} \times \frac{\partial \mathcal{L}}{\partial \vec{\omega}} = \int_{\text{M}} \left(\alpha^a \vec{\xi}_a \times (\nabla (\dot{\vec{x}}_\alpha \cdot \vec{A}_\alpha) - \nabla \phi_\alpha) + \alpha^a \vec{A}_\alpha \times (\vec{\xi}_a \times \vec{\omega}) \right) dq \quad (2.9.79)$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{\omega}}} = \frac{d}{dt} (\tilde{I} \vec{\omega}) + \int_{\text{M}} \left(\alpha^a \vec{\xi}_a \times \left(\frac{\partial \vec{A}_\alpha}{\partial t} + (\dot{\vec{x}}_\alpha \cdot \nabla) \vec{A}_\alpha \right) + \alpha^a \vec{A}_\alpha \times (\vec{\xi}_a \times \vec{\omega}) \right) dq \quad (2.9.80)$$

Putting these results into (2.9.71):

$$\frac{d}{dt} (\tilde{I} \vec{\omega}) = \int_{\text{M}} (\vec{x}_\alpha - \vec{x}) \times \left(\vec{E}(t, \vec{x}_\alpha) + \dot{\vec{x}}_\alpha \times \vec{B}(t, \vec{x}_\alpha) \right) dq. \quad (2.9.81)$$

Hence (2.9.81) finally gives our equation of motion for the orientation of a Galilean rigid body.

2.9.4 Spin Angular Momentum and the Hamiltonian

Now that the object can change both position and orientation, there is a new kind of angular momentum present. By definition, angular momentum is the generator of rotations. So, we take $t' = t$ and $\mathcal{H}' = \mathcal{H}$ and from our formula for the generator of a transformation in (1.10.30), the total angular momentum $\vec{J}$ is given by:

$$\vec{J} = P_a \mathcal{D} Q^a = \vec{p} \cdot \vec{\mathcal{D}} \vec{x} + \vec{\pi} \cdot \vec{\mathcal{D}} \vec{\theta}. \quad (2.9.82)$$

where $\mathcal{D}$ indicates a derivative with respect to an applied rotation, $\vec{p}$ is the conjugate momentum to $\vec{x}$, and $\vec{\pi}$ is the conjugate momentum to $\vec{\theta}$ computed from the Lagrangian. The first term above we already calculated in equation (2.4.85). That term, called orbital angular momentum $\vec{L}$, is the angular momentum corresponding to rotations of the position of the center of mass:

$$\vec{L} = \vec{p} \cdot \vec{\mathcal{D}} \vec{x} = \vec{x} \times \vec{p}. \quad (2.9.83)$$

The second term is new. It is the angular momentum corresponding to rotations of the orientation of the body about its center of mass. It is called spin angular momentum $\vec{S}$. It is given using $\vec{\mathcal{D}} \vec{\theta}$ already calculated:

$$S_a = \pi_b \mathcal{D}_a \theta^b = \pi_b (\hat{M}^{-1})^b_a = (M^{-T} \vec{\pi})_a \implies \vec{S} = \hat{M}^{-T} \vec{\pi} \quad (2.9.84)$$

$$S_a = (\hat{M}^{-1})^b{}_a \pi_b = \left(\hat{M}^{-1} \right)^b{}_a \frac{\partial \mathcal{L}}{\partial \dot{\theta}^b} = \frac{\partial \dot{\theta}^b}{\partial \omega^a} \frac{\partial \mathcal{L}}{\partial \dot{\theta}^b} = \frac{\partial \mathcal{L}}{\partial \omega^a} \quad (2.9.85)$$

$$\implies \vec{S} = \frac{\partial \mathcal{L}}{\partial \vec{\omega}}. \quad (2.9.86)$$

Hence, the spin angular momentum is given quite nicely using the angular velocity. The total angular momentum is:

$$\vec{J} = \vec{L} + \vec{S}. \quad (2.9.87)$$

The Legendre transform is very nice using the spin angular momentum:

$$\mathcal{H}(t, \vec{x}, \vec{p}, \vec{\theta}, \vec{\pi}) = \vec{p} \cdot \dot{\vec{x}} + \vec{\pi} \cdot \dot{\vec{\theta}} - \mathcal{L} = \vec{p} \cdot \dot{\vec{x}} + \vec{S} \cdot \vec{\omega} - \mathcal{L}. \quad (2.9.88)$$

Hence, not only can $\vec{S}$ be computed directly from $\mathcal{L}$ using $\vec{\omega}$ but the Hamiltonian can be computed by doing the Legendre transformation in terms of $\vec{\omega}$ and $\vec{S}$ without specifically referencing $\vec{\theta}$, $\dot{\vec{\theta}}$, or $\vec{\pi}$. All of the emerging convenience of $\vec{S}$ is suggestive that it will be smart to leave the Hamiltonian in terms of it. That is, we will write $\mathcal{H}(t, \vec{x}, \vec{p}, \vec{\xi}, \vec{S})$ instead of in terms of $\vec{\theta}$, $\vec{\pi}$. Using the Legendre transformation with this parameterization:

$$d\mathcal{L} = \dot{\vec{x}} \cdot d\vec{p} + \vec{p} \cdot d\dot{\vec{x}} + \vec{\omega} \cdot d\vec{S} + \vec{S} \cdot d\vec{\omega} - d\mathcal{H}. \quad (2.9.89)$$

Now explicitly expanding out the derivatives:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial t} dt + \frac{\partial \mathcal{L}}{\partial \vec{x}} \cdot d\vec{x} + \frac{\partial \mathcal{L}}{\partial \vec{\xi}} \cdot d\vec{\xi} + \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} \cdot d\vec{\xi}_a + \frac{\partial \mathcal{L}}{\partial \vec{\omega}} \cdot d\vec{\omega} &= \dot{\vec{x}} \cdot d\vec{p} + \vec{p} \cdot d\dot{\vec{x}} + \vec{\omega} \cdot d\vec{S} + \vec{S} \cdot d\vec{\omega} \\ &\quad - \frac{\partial \mathcal{H}}{\partial t} dt - \frac{\partial \mathcal{H}}{\partial \vec{x}} \cdot d\vec{x} - \frac{\partial \mathcal{H}}{\partial \vec{p}} \cdot d\vec{p} - \frac{\partial \mathcal{H}}{\partial \vec{\xi}_a} \cdot d\vec{\xi}_a - \frac{\partial \mathcal{H}}{\partial \vec{S}} \cdot d\vec{S}. \end{aligned} \quad (2.9.90)$$

Matching for generic differentials gives:

$$\frac{\partial \mathcal{L}}{\partial t} = -\frac{\partial \mathcal{H}}{\partial t}, \quad \frac{\partial \mathcal{L}}{\partial \vec{x}} = -\frac{\partial \mathcal{H}}{\partial \vec{x}}, \quad \frac{\partial \mathcal{L}}{\partial \vec{\xi}} = \vec{p}, \quad \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} = -\frac{\partial \mathcal{H}}{\partial \vec{\xi}_a}, \quad (2.9.91)$$

$$\frac{\partial \mathcal{L}}{\partial \vec{\omega}} = \vec{S}, \quad \dot{\vec{x}} = \frac{\partial \mathcal{H}}{\partial \vec{p}}, \quad \omega = \frac{\partial \mathcal{H}}{\partial \vec{S}}. \quad (2.9.92)$$

Rewriting our equations of motion (2.9.73) and (2.9.74) in terms of the Hamiltonian then:

$$\boxed{\frac{d\vec{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{x}} + \vec{F}_{\text{ext}}, \quad \frac{d\vec{S}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{S}} \times \vec{S} + \frac{\partial \mathcal{H}}{\partial \vec{\xi}_a} \times \vec{\xi}_a + \vec{\tau}_{\text{ext}}.} \quad (2.9.93)$$

These are the equations of motion for a rigid body in terms of the linear momentum and spin angular momentum.

2.9.5 Angular Momentum Poisson Brackets

By definition spin angular momentum is the generator of rotations of the body about its center of mass. We found in 2.4 that the total angular momentum $\vec{J}$ satisfies the Poisson bracket (2.4.58). We also found that $\vec{J} = \vec{L} + \vec{S}$ and that $\vec{L}$, the orbital angular momentum, only depends on the center of mass position and its conjugate momentum $(\vec{x}, \vec{p})$ while $\vec{S}$, the spin angular momentum, only depends on the body orientation coordinates θ^a and its conjugate momenta π_a . So, automatically the Poisson bracket of $\vec{L}$ with $\vec{S}$ is 0, as they are functions of completely separate and independent variables from each other:

$$\{L_a, S_b\} = 0. \quad (2.9.94)$$

As well, from (2.9.83) and the Poisson bracket of $\vec{x}$ with $\vec{p}$:

$$\vec{L} = \vec{x} \times \vec{p} \implies \{L_a, L_b\} = \epsilon_{ab}{}^c L_c. \quad (2.9.95)$$

Then we can find the Poisson bracket of the components of spin with each other:

$$\{J_a, J_b\} = \epsilon_{ab}{}^c J_c \implies \{L_a + S_a, L_b + S_b\} = \epsilon_{ab}{}^c (L_c + S_c) \quad (2.9.96)$$

$$\implies \boxed{\{S_a, S_b\} = \epsilon_{ab}{}^c S_c.} \quad (2.9.97)$$

This derivation is insensitive to the fact that we are considering a rigid body and can apply unchanged in its reasoning to general bodies. One can arrive at this same result in particular for a rigid body by using the

explicit formula for the components of spin in terms of $\vec{\theta}$ and $\vec{\pi}$ and their canonical Poisson brackets with each other. Doing so is quite algebraically tedious.

The body frame vectors $\xi_a(t)$ are defined by (2.9.53) and so are functions of $\vec{\theta}$ but not $\vec{x}, \vec{p}, \vec{\pi}$. Consequently, they have vanishing Poisson brackets with all of $\vec{x}, \vec{p}$ as well as each other. Under a rotation we know they transform as vectors and so letting $(\vec{\xi}_a)^b$ indicate component b of the vector $\vec{\xi}_a$:

$$\mathcal{D}_b(\vec{\xi}_a)^c = \epsilon^c{}_{bd}(\vec{\xi}_a)^d \quad (2.9.98)$$

$$\mathcal{D}_b(\vec{\xi}_a)^c = \{(\vec{\xi}_a)^c, J_b\} = \{(\vec{\xi}_a)^c, L_b + S_b\} = \{(\vec{\xi}_a)^c, S_b\} \quad (2.9.99)$$

$$\implies \{(\vec{\xi}_a)^c, S_b\} = \epsilon^c{}_{bd}(\vec{\xi}_a)^d. \quad (2.9.100)$$

With this we now have enough information to compute the Poisson brackets of general functions $f(\vec{x}, \vec{p}, \vec{\xi}, \vec{S})$ and $g(\vec{x}, \vec{p}, \vec{\xi}, \vec{S})$ written in terms of these coordinates. Let α be the parameter corresponding to whatever transformation g generates. Then:

$$\{f, g\} = \frac{df}{d\alpha} = \frac{\partial f}{\partial x^a} \frac{dx^a}{d\alpha} + \frac{\partial f}{\partial p_a} \frac{dp_a}{d\alpha} + \frac{\partial f}{\partial (\vec{\xi}_a)^b} \frac{d(\vec{\xi}_a)^b}{d\alpha} + \frac{\partial f}{\partial S_a} \frac{dS_a}{d\alpha} \quad (2.9.101)$$

$$= \frac{\partial f}{\partial x^a} \{x^a, g\} + \frac{\partial f}{\partial p_a} \{p_a, g\} + \frac{\partial f}{\partial (\vec{\xi}_a)^b} \{(\vec{\xi}_a)^b, g\} + \frac{\partial f}{\partial S_a} \{S_a, g\}. \quad (2.9.102)$$

Taking $g = x^a$ we have:

$$\{f, x^a\} = -\frac{\partial f}{\partial p_a}. \quad (2.9.103)$$

Taking $g = p_a$ we have:

$$\{f, p_a\} = \frac{\partial f}{\partial x^a}. \quad (2.9.104)$$

Taking $g = (\vec{\xi}_a)^b$ we have:

$$\{f, (\vec{\xi}_a)^b\} = \left(\vec{\xi}_a \times \frac{\partial f}{\partial \vec{S}} \right)^b. \quad (2.9.105)$$

Finally taking $g = S_a$ we have:

$$\{f, S_a\} = \left(\vec{\xi}_b \times \frac{\partial f}{\partial \vec{\xi}_b} \right)_a + \left(\vec{S} \times \frac{\partial f}{\partial \vec{S}} \right)_a. \quad (2.9.106)$$

Returning this to (2.9.102) we have:

$$\boxed{\{f, g\} = \frac{\partial f}{\partial \vec{x}} \cdot \frac{\partial g}{\partial \vec{p}} - \frac{\partial f}{\partial \vec{p}} \cdot \frac{\partial g}{\partial \vec{x}} + \vec{\xi}_a \cdot \left(\frac{\partial f}{\partial \vec{\xi}_a} \times \frac{\partial g}{\partial \vec{S}} - \frac{\partial g}{\partial \vec{\xi}_a} \times \frac{\partial f}{\partial \vec{S}} \right) + \vec{S} \cdot \left(\frac{\partial f}{\partial \vec{S}} \times \frac{\partial g}{\partial \vec{S}} \right)}. \quad (2.9.107)$$

With this Poisson bracket we can reproduce all of the rigid body equations of motion in the usual way by using that the Hamiltonian is the generator of time evolution:

$$\frac{df}{dt} = \{f, \mathcal{H}\}. \quad (2.9.108)$$

This holds true in the absence of external forces. In the presence of external forces the equations of motion for $\vec{p}$ and $\vec{S}$ are modified by additional terms. In that case we have the equations of motion:

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{p}}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{x}} + \vec{F}_{\text{ext}} \quad (2.9.109)$$

$$\frac{d\vec{\xi}_a}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{S}} \times \vec{\xi}_a, \quad \frac{d\vec{S}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{S}} \times \vec{S} + \frac{\partial \mathcal{H}}{\partial \vec{\xi}_a} \times \vec{\xi}_a + \vec{\tau}_{\text{ext}}. \quad (2.9.110)$$

This formulation of rigid bodies is interesting because the variables $\vec{x}, \vec{p}, \vec{\xi}_a, \vec{S}$ are not all independent of each other and this is reflected in their structure in the Poisson bracket. In particular, $\vec{\xi}_a$ and $\vec{S}$ are not canonical coordinates, but it is still possible to compute equations of motion and the dynamics of the system in terms of them. As well, doing so is more physically transparent because the actual canonical variables θ^a, π_a carry huge amount of redundancy because they can be redefined by changing the definition of the default orientation of the body and the theory must have symmetry under that relabeling. Among the four vectors $\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3, \vec{S}$ there are only 6 variables defining them in θ^a and π_a and that is before applying relabeling symmetry. It

sometimes happens to be the case that it is useful to formulate the Hamiltonian in terms of coordinates which are not canonical conjugate pairs; we will encounter situations like this again. Within the Poisson bracket formalism as long as one uses the appropriate bracket implied by the underlying conjugate coordinates, this doesn't really cause us any issues, as explained in section 1.16. Altogether then, we have:

Theorem 2.17: Motion of Rigid Bodies

The configuration of a rigid body is given by the position of a point of the body $\vec{x}(t)$ and the orientation of the body relative to that point. That orientation can be represented by a rotating frame of coordinate axes $\vec{\xi}_a(t)$. The position of any mass element labeled by α within the body is given by:

$$\vec{x}_\alpha = \vec{x} + \alpha^a \vec{\xi}_a. \quad (2.9.111)$$

The Lagrangian equations of motion of the body are:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{\partial \mathcal{L}}{\partial \vec{x}} + \vec{F}_{\text{ext}} \quad (2.9.112)$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{\omega}}} = \vec{\xi}_a \times \frac{\partial \mathcal{L}}{\partial \vec{\xi}_a} + \vec{\omega} \times \frac{\partial \mathcal{L}}{\partial \vec{\omega}} + \vec{\tau}_{\text{ext}} \quad (2.9.113)$$

$$\frac{d\vec{\xi}_a}{dt} = \vec{\omega} \times \vec{\xi}_a. \quad (2.9.114)$$

The Hamiltonian is given through the Legendre transformation by:

$$\mathcal{H}(t, \vec{x}, \vec{p}, \vec{\xi}, \vec{S}) = \vec{p} \cdot \dot{\vec{x}} + \vec{S} \cdot \vec{\omega} - \mathcal{L}(t, \vec{x}, \dot{\vec{x}}, \vec{\xi}, \vec{\omega}). \quad (2.9.115)$$

The Hamiltonian produces the equations of motion:

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{p}} \quad (2.9.116)$$

$$\frac{d\vec{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{x}} + \vec{F}_{\text{ext}} \quad (2.9.117)$$

$$\frac{d\vec{\xi}_a}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{S}} \times \vec{\xi}_a \quad (2.9.118)$$

$$\frac{d\vec{S}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{S}} \times \vec{S} + \frac{\partial \mathcal{H}}{\partial \vec{\xi}_a} \times \vec{\xi}_a + \vec{\tau}_{\text{ext}}. \quad (2.9.119)$$

In the absence of external forces the dynamics can be recovered from the Hamiltonian by the Poisson bracket:

$$\frac{df}{dt} = \{f, \mathcal{H}\} \quad (2.9.120)$$

$$\{f, g\} = \frac{\partial f}{\partial \vec{x}} \cdot \frac{\partial g}{\partial \vec{p}} - \frac{\partial f}{\partial \vec{p}} \cdot \frac{\partial g}{\partial \vec{x}} + \vec{\xi}_a \cdot \left(\frac{\partial f}{\partial \vec{\xi}_a} \times \frac{\partial g}{\partial \vec{S}} - \frac{\partial g}{\partial \vec{\xi}_a} \times \frac{\partial f}{\partial \vec{S}} \right) + \vec{S} \cdot \left(\frac{\partial f}{\partial \vec{S}} \times \frac{\partial g}{\partial \vec{S}} \right). \quad (2.9.121)$$

When $\vec{x}$ is chosen to be the center of mass of the body, the Galilean Rigid Body Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} \vec{\omega}^T \tilde{I} \vec{\omega} + \int_{\text{M}} \left(\vec{A}(t, \vec{x}_\alpha) \cdot \dot{\vec{x}}_\alpha - \phi(t, \vec{x}_\alpha) \right) dq \quad (2.9.122)$$

which produces equations of motion:

$$m \ddot{\vec{x}} = \int_{\text{M}} \left(\vec{E}(t, \vec{x}_\alpha) + \dot{\vec{x}}_\alpha \times \vec{B}(t, \vec{x}_\alpha) \right) dq \quad (2.9.123)$$

$$\frac{d}{dt} (\tilde{I} \vec{\omega}) = \int_{\text{M}} (\vec{x}_\alpha - \vec{x}) \times \left(\vec{E}(t, \vec{x}_\alpha) + \dot{\vec{x}}_\alpha \times \vec{B}(t, \vec{x}_\alpha) \right) dq. \quad (2.9.124)$$

Exercises

Problem 2.47: Sliding vs. Rolling. Consider a uniformly massive solid cylinder of radius r , length l , and total mass m at the top of an incline plane which makes an angle θ with the ground and has a height h . Assume the cylinder starts from rest and that it only rolls along the cylinder axis. Compute the time it would take for the cylinder to reach the ground by sliding down the plane. As well, compute the time it

would take the cylinder to reach the ground by rolling down the plane without slipping. Which one takes longer?

Problem 2.48: ★ Measuring mass with a beam balance. Consider a flat light rod (treat as massless) of length l . The middle of the rod has a pin through it attaching it to a base so that the rod can tilt up or down freely. On one side of the rod is a mass M which can be moved along that side of the rod to any position. On the other side of the rod is a small platform at the rod's end. This apparatus is called a beam balance.

- Suppose a mass m is placed on the platform. How far should the mass M be moved away from the center of the rod so that the rod rests horizontally (the beam is balanced)?
- Suppose that the mass M is known and an unknown mass is placed on the platform. Explain how measuring where M should be placed so that the rod rests horizontally allows one to determine the unknown mass. Thus, this system, once one has defined a reference unit of mass like the kilogram, allows one to measure other masses in terms of the reference mass.

Problem 2.49: Catenary Problem. Consider a uniformly massive rope of fixed length l and mass m whose ends are fixed at $x = -w/2$ and $x = w/2$ which is hanging in equilibrium to form some curve $y(x)$.

- Show that the curve y must be a solution to the stationary variation of the functional:

$$\mathcal{L}[y] = -\frac{mg}{l} \int_{-w/2}^{w/2} y(x) \sqrt{1 + y'(x)^2} dx - \lambda \left(\int_{-w/2}^{w/2} \sqrt{1 + y'(x)^2} dx - l \right)$$

where λ is some Lagrange multiplier to enforce that the arclength of the rope is fixed.

- Take the variation of that action and show that the resulting differential equation is:

$$\frac{d}{ds} \left(\left(y + \frac{l\lambda}{mg} \right) \frac{dy}{ds} \right) = 1$$

where s refers to the arclength along the curve.

- Define s so that $s = 0$ at the minimum of the rope. Solve the above differential equation for y to get:

$$y = \sqrt{s^2 + a^2}$$

for some parameter a and for some choice of definition of how high to place the x -axis.

- Use the relationship between changes in x , y , and s to show that:

$$\frac{dx}{ds} = \frac{a}{\sqrt{s^2 + a^2}}$$

and integrate this to find $x(s)$.

- Invert $x(s)$ and substitute it into $y(s)$ to find y as a function of x and thus find the shape of a hanging rope (called a catenary).
- Relate the parameter a to the parameters of the rope through an implicit equation.

Problem 2.50: Euler's Law of Torque. Consider an otherwise free rigid body experiencing external force $\vec{F}$ on the translational variables and external force $\vec{\tau}$ on the rotational variables (a force on rotational variables is called a torque) with free Lagrangian $\mathcal{L}_0$.

- Show that if the free Lagrangian is translationally and rotationally invariant (meaning no surface term added) that this implies the equations of motion:

$$\frac{d\vec{p}_0}{dt} = \vec{F}, \quad \frac{d\vec{S}_0}{dt} = \vec{\tau}$$

where $\vec{p}_0$ is the linear momentum corresponding to the free Lagrangian and $\vec{S}_0$ is the spin angular momentum corresponding to the free Lagrangian.

- For our particular rigid body action which we derived, show that these become:

$$\vec{F} = m\ddot{\vec{x}}, \quad \vec{\tau} = \frac{d}{dt}(\tilde{I}\vec{\omega}).$$

The first of these is Newton's second law for a rigid body and the second is called Euler's law of Torque.

- Suppose that the external force and torque are provided locally to the body. That is, each mass element dm_α experiences some force $d\vec{F}_\alpha$ so that the equation of motion of this system will be given by requiring:

$$\delta S + \int_{t_0}^{t_f} \int_M d\vec{F}_\alpha \cdot \delta \vec{x}_\alpha dt = 0$$

where S here is the free action of the body and the variations of $\vec{x}_\alpha$ must satisfy the constraint $\vec{x}_\alpha = \vec{x} + \alpha^a \vec{\xi}_a$. Show that this implies the net force $\vec{F}$ and net torque $\vec{\tau}$ are given by:

$$\vec{F} = \int_M d\vec{F}_\alpha, \quad \vec{\tau} = \int_M (\vec{x}_\alpha - \vec{x}) \times d\vec{F}_\alpha.$$

Problem 2.51: Euler Top. An Euler top is a freely rotating rigid body experiencing no torque. Such a body is quite complicated but the solution can be written explicitly in principle. For convenience, define the vector $\vec{\Omega}$ by:

$$\vec{\Omega} = \hat{R}^T \vec{\omega}.$$

- (a) Show that the components of $\vec{\Omega}$ are the components of $\vec{\omega}$ along the principal axes of the body. That is: $\vec{e}_a \cdot \vec{\Omega} = \vec{\xi}_a \cdot \vec{\omega}$.
- (b) Show that the equation of motion for $\vec{\Omega}$ is:

$$\hat{I} \dot{\vec{\Omega}} + \vec{\Omega} \times (\hat{I} \vec{\Omega}) = 0.$$

- (c) Show that the above equation of motion in components becomes:

$$I_1 \dot{\omega}_1 = (I_2 - I_3) \omega_2 \omega_3, \quad I_2 \dot{\omega}_2 = (I_3 - I_1) \omega_3 \omega_1, \quad I_3 \dot{\omega}_3 = (I_2 - I_1) \omega_1 \omega_2.$$

- (d) Define the order of the axes so that $I_1 \geq I_2 \geq I_3$. Show using conservation of energy and conservation of the magnitude of the spin angular momentum that ω_1 and ω_3 can be algebraically eliminated and written in terms of ω_2 .
- (e) Use the equation of motion for ω_2 but written with ω_1 and ω_3 to arrive at a separable differential equation for ω_2 . Write the integral which one would integrate to get the solution but do not try to evaluate it. Once ω_2 is (in principle) known by this integral, ω_1 and ω_3 can be solved for as functions of time as well. This is possible because the Euler top is integrable.
- (f) Show that the Euler top is integrable in the sense of 1.14 by showing that $\mathcal{H}, |\vec{S}|^2, S_z$ form a set of conserved quantities satisfying the properties of the G conserved quantities in that section. Explain why having three independent conserved quantities is sufficient for this system to be integrable.
- (g) Assuming we now know the solution of $\omega_1(t)$, $\omega_2(t)$, and $\omega_3(t)$, show that the equations of motion for $\vec{\xi}_a(t)$ become:

$$\frac{d\vec{\xi}_1}{dt} = \omega_3 \vec{\xi}_2 - \omega_2 \vec{\xi}_3, \quad \frac{d\vec{\xi}_2}{dt} = \omega_1 \vec{\xi}_3 - \omega_3 \vec{\xi}_1, \quad \frac{d\vec{\xi}_3}{dt} = \omega_2 \vec{\xi}_1 - \omega_1 \vec{\xi}_2$$

and explain how one would solve them in principle.

- (h) Consider now the object to initially have its angular momentum directed along one of its principal axes. Show that its angular momentum will remain directed along that axis for all time.
- (i) Consider now the object to initially have its angular momentum nearly directed along one of its principal axes. That is, treat the deviation from being directed along that axis only to lowest order. Show that perturbations off of the largest and smallest principal axes (I_1 and I_3) are stable while perturbations off of the intermediate axis I_2 are unstable. This effect (known as the Dzhanibekov effect or tennis racket effect) causes objects to eventually flip whenever their rotation is imperfectly aligned with the medium axis.

Problem 2.52: Free Symmetric Top. Consider a special case of the Euler top in which $I_3 = I_2$ (here we do not need to assume we have ordered the axis numbering in any particular way).

- (a) Starting from the equations of motion found for $\omega_1, \omega_2, \omega_3$ for a general Euler top, apply this special case to simplify those equations. You should find:

$$\dot{\omega}_1 = 0, \quad \dot{\omega}_2 = \Omega \omega_3, \quad \dot{\omega}_3 = -\Omega \omega_2$$

where Ω is a parameter for which you should find an expression. Then, solve these equations of motion.

- (b) Let us turn to the axis vectors $\vec{\xi}_a$. Define $\vec{u}(t)$ and $\vec{v}(t)$ by:

$$\vec{u} = \omega_2 \vec{\xi}_2 + \omega_3 \vec{\xi}_3, \quad \vec{v} = \omega_3 \vec{\xi}_2 - \omega_2 \vec{\xi}_3$$

and show that the equations of motion of $\vec{\xi}_1, \vec{u}$ and $\vec{v}$ are:

$$\frac{d\vec{\xi}_1}{dt} = \vec{v}, \quad \frac{d\vec{u}}{dt} = (\Omega - \omega_1) \vec{v}, \quad \frac{d\vec{v}}{dt} = -(\Omega - \omega_1) \vec{u} - (\omega_2^2 + \omega_3^2) \vec{\xi}_1.$$

- (c) Differentiate the equation of motion for $\vec{v}$ to show that $\vec{v}$ satisfies:

$$\frac{d^2\vec{v}}{dt^2} + ((\Omega - \omega_1)^2 + \omega_2^2 + \omega_3^2)\vec{v}.$$

- (d) Find a simple expression for the coefficient appearing in front of $\vec{v}$ in the previous part, solve that equation of motion, and use that solution in the equations of motion for $\vec{u}$ and $\vec{\xi}_1$ to solve them as well.
 (e) Use the solutions for $\vec{u}$ and $\vec{v}$ to find the solutions for $\vec{\xi}_2$ and $\vec{\xi}_3$.
 (f) Thus, finally explain the geometric picture implied by our full solution $\omega_1, \omega_2, \omega_3, \vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3$. That is, answer the question: what does a free symmetric top *do*?

Problem 2.53: Spinning in a $\vec{B}$ Field. Consider a uniformly massive and uniformly charged ball to be experiencing a constant and uniform $\vec{B}$ field and no $\vec{E}$ field.

- (a) Using the potentials $\phi = 0$ and $\vec{A} = \frac{1}{2}\vec{B} \times \vec{x}$, show that the Lagrangian of the body becomes:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \frac{q}{2}\vec{B} \cdot (\vec{x} \times \dot{\vec{x}}) + \frac{1}{2}I|\vec{\omega}|^2 + \frac{qI}{2m}\vec{B} \cdot \vec{\omega}$$

where I is the moment of inertia of the ball about any axis.

- (b) Find the equations of motion of this system.
 (c) Solve the equations of motion and interpret the solution.

Problem 2.54: Top experiencing gravity. Consider a rigid body for which one point on the edge of the body is fixed to a table and the body is allowed to rotate about that point. As well, this body experiences gravity. Such a system is called a “torqued top”.

- (a) Although this object is not rotating about its center of mass, we can still use the formalism we have developed as the only time rotations were assumed to be about the center of mass was in simplifying the Lagrangian or equations of motion. By starting with the action all is well. Define the fixed point as the origin of our coordinate system so that $\vec{x}_\alpha = \hat{R}\vec{\alpha}$. Define the z direction as the direction in which gravity acts. In terms of the principle axes, the center of mass of the body when it is not rotated is $c_1\vec{l}_1 + c_2\vec{l}_2 + c_3\vec{l}_3$. Show that the potential term of the Action/Lagrangian becomes:

$$U = \int_M g z_\alpha dm = mgh\vec{l}_z \cdot (c_1\vec{\xi}_1 + c_2\vec{\xi}_2 + c_3\vec{\xi}_3).$$

For the rest of this question, let $n_a(t) \stackrel{\text{def}}{=} \vec{l}_z \cdot \vec{\xi}_a$.

- (b) Show that the full action now becomes:

$$S = \int_{t_0}^{t_f} \left(\frac{1}{2}\vec{\omega}^T \tilde{I} \vec{\omega} - mg(c_1 n_1 + c_2 n_2 + c_3 n_3) \right) dt$$

where $\tilde{I} = \hat{R}\hat{I}\hat{R}^T$ and $\hat{I}$ is the unrotated moment of inertia matrix defined relative to the point of rotation, not the center of mass.

- (c) Show that the variation of the action above becomes:

$$\delta S = \int_{t_0}^{t_f} \left(-\frac{d}{dt}(\tilde{I}\vec{\omega}) - mg\epsilon^{abc}c_a n_b \vec{\xi}_c \right) \cdot \delta\vec{\Theta} dt.$$

- (d) Show that the equations of motion for this system become:

$$\begin{aligned} I_1\dot{\omega}_1 + (I_3 - I_2)\omega_2\omega_3 &= mg(c_3 n_2 - c_2 n_3), & \dot{n}_1 &= n_2\omega_3 - n_3\omega_2, \\ I_2\dot{\omega}_2 + (I_1 - I_3)\omega_3\omega_1 &= mg(c_1 n_3 - c_3 n_1), & \dot{n}_2 &= n_3\omega_1 - n_1\omega_3, \\ I_3\dot{\omega}_3 + (I_2 - I_1)\omega_1\omega_2 &= mg(c_2 n_1 - c_1 n_2), & \dot{n}_3 &= n_1\omega_2 - n_2\omega_1. \end{aligned}$$

- (e) Show that the energy of this system is given by:

$$E = \frac{1}{2}I_1\omega_1^2 + \frac{1}{2}I_2\omega_2^2 + \frac{1}{2}I_3\omega_3^2 + mg(c_1 n_1 + c_2 n_2 + c_3 n_3)$$

and that it is conserved. As well, show that the spin angular momentum in the z direction is given by:

$$S_z = n_1 I_1 \omega_1 + n_2 I_2 \omega_2 + n_3 I_3 \omega_3$$

and that it is conserved. Finally, show that $n^2 = n_1^2 + n_2^2 + n_3^2$ is conserved and always equal to 1.

Problem 2.55: Lagrange Top. A Lagrange top is a top experiencing gravity which has its center of mass

directed along one of the principle axes in its displacement from the point of rotation and which has rotational symmetry about that axis. Let that axis be $\vec{l}_3$ so that $(c_1, c_2, c_3) = (0, 0, h)$. Then, symmetry about this axis requires $I_2 = I_1$. Such is the case for a conventional uniform conical top.

- Show that the spin angular momentum along the axis of symmetry, S_3 , is conserved.
- By reducing the equations of motion, count the conserved quantities to show that the Lagrange top system is reducible to only two differential equations. (In fact, it is integrable.)
- Show that this top is integrable in the sense of section 1.14 by showing that $\mathcal{H}, S_3, S_z$ form a set of conserved quantities satisfying the properties of the G conserved quantities in that section.

Problem 2.56: Kovalevskaya Top. A Kovelevskaya top is a top experiencing gravity which again has its center of mass directed along one of the principle axes in its displacement from the point of rotation but with symmetry under rotations about an axis perpendicular to that axis and for which the moment of inertia in the third orthogonal direction is half that of that first two. That is, we will take $(c_1, c_2, c_3) = (h, 0, 0)$ $I_1 = I_2 = 2I_3 = I$. For analyzing this top, define:

$$\psi = I(\omega_1 + i\omega_2)^2 - 2mgh(n_1 + in_2).$$

- Find the equation of motion for ψ and show that $K = \psi^* \psi$ is conserved (ψ^* is the complex conjugate of ψ).
- By reducing the equations of motion, count the conserved quantities to show that the Kovalevskaya top system is reducible to only two differential equations. Show that this top is integrable in the sense of section 1.14 by showing that $\mathcal{H}, K, S_z$ form a set of conserved quantities satisfying the properties of the G conserved quantities in that section. Sofia Kovalevskaya (1850-1891, Russian), the first woman to receive a PhD in mathematics, proved that this top of hers and the previous top of Lagrange are the only integrable cases of the torqued top.

Problem 2.57: Ball in a Valley. Consider a small uniformly massive ball of radius r and mass m rolling on the ground. Let the set of the points allowed by the shape of ground for the center of the ball to be at be given by the points $\vec{x}$ for which $f(\vec{x}) = 0$ for some smooth function f . Assume the ball is small enough compared to the curvature of the ground to only ever make contact with 1 point on the ground at any given time and that the ball rolls without slipping or leaving the ground. Suppose f is defined so that $f > 0$ above the ground.

- Show that the unit vector pointing from the point of contact to the center of the ball is given by:

$$\vec{n} = \frac{\nabla f}{|\nabla f|}.$$

- Show that the condition that the ball rolls without slipping is given by the non-holonomic constraint:

$$\vec{\omega} = \frac{1}{r} \vec{n} \times \dot{\vec{x}}.$$

- Show that the unconstrained action for the ball is:

$$S = \int_{t_0}^{t_f} \left(\frac{1}{2} m |\dot{\vec{x}}|^2 + \frac{1}{2} I |\vec{\omega}|^2 - mgz \right) dt$$

where I is simply a constant (and find its expression in terms of the given parameters of the problem).

- Take the unconstrained variation of the above action to show:

$$\delta S = \int_{t_0}^{t_f} \left(-m\ddot{\vec{x}} \cdot \delta\vec{x} - \frac{2}{5} mr^2 \dot{\vec{\omega}} \cdot \delta\vec{\omega} - mg\delta z \right) dt.$$

- Using only constrained variations, show:

$$\delta\vec{x} \cdot (\dot{\vec{\omega}} \times \vec{n}) = \frac{1}{r} \ddot{\vec{x}} \cdot \delta\vec{x}$$

and use this to show that among variations which satisfy the constraints:

$$\delta S = \int_{t_0}^{t_f} \left(-\frac{7}{5} m\ddot{\vec{x}} \cdot \delta\vec{x} - mg\delta z \right) dt.$$

- (f) Show that the same variational expression is given by the following action:

$$S_{\text{eff}} = \int_{t_0}^{t_f} \left(\frac{7}{10} m |\dot{\vec{x}}|^2 - mgz \right) dt$$

thus this problem has an effective action in which the non-holonomic constraint has been removed. This is possible specifically because we used a sphere and so there is no angle dependence to appear in our action. It is possible to apply the constraints to the action for a non-holonomic system if all of the variables that have anything non-holonomic about them can just be removed!

- (g) Now that we have a nice effective action, we only have the holonomic constraint that $f(\vec{x}) = 0$ left. Take the derivative of this constraint and assume that $\frac{\partial f}{\partial z}$ is never 0. Use this to show that you can write a differential equation which implicitly defines z as a function of x and y . Thus, we can in principle consider $z = z(x, y)$ as a holonomic constraint.
- (h) Using the effective action and the holonomic constraint $z = z(x, y)$, show that the Lagrangian of the system becomes:

$$\mathcal{L} = \frac{7}{10} m \left(\dot{x}^2 + \dot{y}^2 + \left(\frac{\partial z}{\partial x} \dot{x} + \frac{\partial z}{\partial y} \dot{y} \right)^2 \right) - mgz(x, y).$$

- (i) Consider the system to be near stable equilibrium at $(x, y) = (0, 0)$. Show that a stable equilibrium corresponds to a local minimum of $z(x, y)$ and show that near the equilibrium the Lagrangian becomes (to quadratic order):

$$\mathcal{L} = \frac{7}{10} m (\dot{x}^2 + \dot{y}^2) - \frac{mg}{2} \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} \frac{\partial^2 z}{\partial x^2}(0, 0) & \frac{\partial^2 z}{\partial x \partial y}(0, 0) \\ \frac{\partial^2 z}{\partial x \partial y}(0, 0) & \frac{\partial^2 z}{\partial y^2}(0, 0) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

- (j) The 2x2 matrix of partial derivatives of $z(x, y)$ appearing above is called the Hessian matrix of the function $z(x, y)$. Using that the matrix is by definition real-symmetric and that $(x, y) = (0, 0)$ is a local minimum of the function $z(x, y)$, justify the following statements: (i) the Hessian matrix above is diagonalizable with an orthonormal eigenbasis and real eigenvalues. (ii) those eigenvalues are positive and (iii) geometrically each eigenvalue is the reciprocal of the radius of curvature of the curve gotten by following along the function z in the direction of the corresponding eigenvector to that eigenvalue.
- (k) Using the results of the previous part, let $\vec{l}_1$ and $\vec{l}_2$ be the orthonormal eigenvectors of the Hessian matrix. Let $u(t)$ and $v(t)$ be variables related to $x(t)$ and $y(t)$ by: $(x, y) = u\vec{l}_1 + v\vec{l}_2$ and let R_1 and R_2 be the radii of curvature corresponding to $\vec{l}_1$ and $\vec{l}_2$ respectively. Show that the quadratic order Lagrangian in terms of these coordinates is:

$$\mathcal{L} = \frac{7}{10} m \dot{u}^2 - \frac{mg}{2R_1} u^2 + \frac{7}{10} m \dot{v}^2 - \frac{mg}{2R_2} v^2.$$

- (l) Show that the above Lagrangian implies the ball's motion near the bottom of the valley can be decomposed into two independent, non-interacting, and orthogonal simple harmonic motions with angular frequencies:

$$\omega_1 = \sqrt{\frac{5g}{7R_1}} \quad \text{and} \quad \omega_2 = \sqrt{\frac{5g}{7R_2}}.$$

- (m) In each of the $\vec{l}_1$ and $\vec{l}_2$ directions the motion of the ball is periodic. What condition must be satisfied for the overall motion of the ball to be periodic when it is perturbed from equilibrium by a small amount in an arbitrary direction?

Problem 2.58: Drag Force. Let us consider a rigid body of mass M to be moving through a region of space filled with many much smaller equal masses m (air particles) without rotating¹⁴. As the mass M moves through space, it will collide many times with these smaller masses.

- (a) Let $\vec{l}(\vec{x})$ be the outward pointing normal vector of the surface of our rigid body at the point $\vec{x}$ on its surface. Assume that each collision between M and one of the air particles is elastic. Show using the results of the 2.30 question that the change in M 's momentum in a single collision with an air particle of velocity $\vec{v}$ at location $\vec{x}$ is:

$$\Delta \vec{p}(\vec{x}, \vec{v}) = -2 \frac{m}{1 + \frac{m}{M}} \vec{l} \cdot (\vec{v} - \vec{u})$$

¹⁴This whole analysis can be done analogously for the torque due to drag if one includes rotations and the appropriate kinematics corresponding to angular momentum as we do here for linear momentum.

where $\vec{v}$ is the velocity of M before the collision.

- (b) Let $f(\vec{x}, \vec{u})$ be the number of air particles per unit volume at $\vec{x}$ per unit velocity at velocity $\vec{u}$. Show that the force per unit area experienced by M at $\vec{x}$ on its surface would be:

$$\frac{d\vec{F}(\vec{x})}{d\mathbb{A}} = \int_{\mathbb{R}^3} \Delta \vec{p}(\vec{x}, \vec{u}) f(\vec{x}, \vec{u}) \vec{u} \cdot (\vec{v} - \vec{u}) \vartheta(\vec{u} \cdot (\vec{v} - \vec{u})) d^3 \vec{u}$$

where the integral is taken over all possible velocities $\vec{u}$ of the air particles. (Hint: consider the number of collisions which occur per unit time.)

- (c) Assume that M is much larger than m so that we can approximate $m/M \approx 0$ in the expression for $\Delta \vec{p}$. As well, assume that the distribution of velocities in the air is independent of location. That is, $f(\vec{x}, \vec{u}) = n(\vec{x}) \varphi(\vec{u})$ where $n(\vec{x})$ is the number of air particles per unit volume at $\vec{x}$ and $\varphi(\vec{u})$ is the probability density that an air particle has velocity $\vec{u}$. Show that then the force per unit area simplifies to:

$$\frac{d\vec{F}(\vec{x})}{d\mathbb{A}} = -2mn(\vec{x}) \int_{\mathbb{R}^3} (\vec{u} \cdot (\vec{v} - \vec{u}))^2 \vartheta(\vec{u} \cdot (\vec{v} - \vec{u})) \varphi(\vec{u}) d^3 \vec{u}$$

- (d) Let $\rho(\vec{x})$ be the mass density of air. Show that if $\vec{v} = 0$ and the distribution $\varphi(\vec{u})$ is spherically symmetric then:

$$\frac{d\vec{F}}{d\mathbb{A}} = -\mu^2 \rho(\vec{x}) \vec{v}$$

where

$$\mu^2 \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} u_z^2 \varphi_z(u_z) du_z$$

and $\varphi_z(u_z)$ is the distribution for the z component of u_z only. Thus, show that if also $\rho(\vec{x})$ is uniform and the body is closed then the net force on the body at $\vec{v} = 0$ is 0.

- (e) Retain the previous assumptions and consider taking the speed $v = |\vec{v}|$ to 0 while keeping the direction $\hat{v} = \vec{v}/v$ fixed. Show that:

$$\lim_{v \rightarrow 0^+} \frac{1}{v} \left(\frac{d\vec{F}}{d\mathbb{A}} + \rho \mu^2 \vec{v} \right) = -\eta \rho \vec{v} \cdot \hat{v}$$

where

$$\eta \stackrel{\text{def}}{=} 4 \int_0^{\infty} u_z \varphi(u_z) du_z.$$

Thus, show that the force per unit area on the body for slow speeds is:

$$\frac{d\vec{F}}{d\mathbb{A}} = -\rho \mu^2 \vec{v} - \eta \rho \vec{v} \cdot \vec{v} + \mathcal{O}(v^2)$$

and that the net force on the body is:

$$\vec{F} = -\eta \rho \int_{\partial M} \vec{u} d\mathbb{A} \cdot \vec{v} + \mathcal{O}(v^2).$$

Thus, for small velocities the force of drag due to the air is proportional to velocity. It is useful then to define a slow drag tensor $\hat{C}_s$ by:

$$\hat{C}_s = \frac{1}{\mathbb{A}_s} \int_{\partial M} \vec{u} d\mathbb{A}$$

where $\mathbb{A}_s$ is the surface area of the body. Manifestly then, $\hat{C}_s$ depends only on the shape of the body and not on its size. Then, conclude:

$$\vec{F} = -\eta \rho \mathbb{A}_s \hat{C}_s \cdot \vec{v} + \mathcal{O}(v^2).$$

- (f) Now consider taking the speed to infinity while keeping the direction fixed. Show that:

$$\lim_{v \rightarrow \infty} \frac{1}{v^2} \frac{d\vec{F}}{d\mathbb{A}} = -2\rho \vec{v} (\vec{v} \cdot \hat{v})^2 \vartheta(\vec{v} \cdot \hat{v}).$$

Thus, show that the force per unit area on the body for high speeds is:

$$\frac{d\vec{F}}{d\mathbb{A}} = -2\rho \vec{v} (\vec{v} \cdot \vec{v})^2 \vartheta(\vec{v} \cdot \vec{v}) + \mathcal{O}(v)$$

and that the net force on the body is:

$$\vec{F} = -2\rho \int_{\partial M} \vec{\iota}(\vec{\iota} \cdot \vec{v})^2 \vartheta(\vec{\iota} \cdot \vec{v}) d\mathbb{A} + \mathcal{O}(\vec{v})$$

Thus, for large velocities the force of drag due to the air is proportional to v^2 . It is similarly useful to define a fast drag tensor by:

$$C_f^{abc} = \frac{2}{\mathbb{A}_{cs}} \int_{\partial M} \iota^a \iota^b \iota^c \vartheta(\vec{\iota} \cdot \hat{v}) d\mathbb{A}$$

where $\mathbb{A}_{cs}$ is the cross sectional area of the body in the direction of the velocity. $\hat{C}_f$ does not depend on the size of the body but it does depend on the direction of the velocity. Thus conclude that for large velocities, the drag due to the air is given by:

$$F^a = -\rho \mathbb{A}_{cs} C_f^{abc} v_b v_c + \mathcal{O}(v)$$

- (g) For a sphere, compute the drag tensors to show that for slow and fast velocities respectively:

$$\vec{F}_{\text{slow}} \approx -\frac{4}{3}\pi R^2 \eta \rho \vec{v}, \quad \vec{F}_{\text{fast}} \approx -\frac{\pi}{2} R^2 \rho v^2 \hat{v}.$$

- (h) Explain that the following approximation for the drag force:

$$F^a \approx -\eta \rho \mathbb{A}_s \hat{C}_s^{ab} v_b - \rho \mathbb{A}_{cs} C_f^{abc} v_b v_c$$

should be an okay approximation for both large and small velocities and so is reasonable to use as a simple replacement for the more precise expression gotten from integrating part (c).

Problem 2.59: Damped Harmonic Oscillator. Consider a mass m on a spring of spring constant k which moves in 1 dimension at a slow speed experiencing air resistance so that it experiences linear drag.

- (a) Show that its equation of motion is:

$$m\ddot{x} + m\gamma\dot{x} + kx = 0$$

where $\gamma > 0$ is some constant which characterizes the air resistance.

- (b) Let $\omega_0^2 = \frac{k}{m}$. Show that the variable $y(t) = e^{\frac{\gamma t}{2}} x(t)$ satisfies the familiar equation:

$$\ddot{y} + \left(\omega_0^2 - \frac{\gamma^2}{4} \right) y = 0.$$

- (c) Assume $\gamma < 2\omega_0$. Solve the equation of motion for y and then use it to find the solution for $x(t)$. The result should be an exponentially decaying harmonic oscillator. Identify the new angular frequency of this oscillator and the rate at which the amplitude decays. Because oscillations still occur, this scenario is called “underdamped”.
- (d) Assume $\gamma > 2\omega_0$. Solve the equation of motion for y and then use it to find the solution for $x(t)$. The result should be an exponential decay with no oscillation. Find the two rates of decay. Why does the slowest one characterize the rate at which the overall solution decays? Because oscillations no longer occur, this scenario is called “overdamped”.
- (e) Assume $\gamma = 2\omega_0$. Solve the equation of motion for y and then use it to find the solution for $x(t)$. Show that the resulting solutions decay faster than any overdamped solution. This scenario is called “critically damped”.

Problem 2.60: Driven Damped Harmonic Oscillator. Consider again the damped harmonic oscillator and assume $\gamma < 2\omega_0$. However, now allow the oscillator to experience an external force $F(t)$ provided in addition to the air resistance and effect of the spring so that the equation of motion of the position of the mass is:

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = \frac{F(t)}{m}.$$

- (a) Again make the change of variables $y(t) = e^{\frac{\gamma t}{2}} x(t)$ and show that:

$$\ddot{y} + \left(\omega_0^2 - \frac{\gamma^2}{4} \right) y = e^{\frac{\gamma t}{2}} \frac{F(t)}{m}.$$

Thus, we can transform this system into a driven but not damped harmonic oscillator.

- (b) Use the solution of problem 2.29 to show that $y(t)$ is given by:

$$y(t) = \int_{-\infty}^t \frac{F_{\text{eff}}(t')}{\omega_{\text{eff}} m} \sin(\omega_{\text{eff}}(t - t')) dt'$$

for some constant ω_{eff} and function $F_{\text{eff}}(t)$ (both of which you should determine from given information).

- (c) Reexpress everything in terms of $x(t)$ to show that it is given by:

$$x(t) = \int_{-\infty}^t \frac{F(t')}{m\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}} e^{-\frac{\gamma}{2}(t-t')} \sin\left(\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}(t - t')\right) dt'$$

and thus also show that the delayed Green's function for a driven damped harmonic oscillator is:

$$G(t) = \frac{e^{-\frac{\gamma}{2}t}}{m\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}} \sin\left(t\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}\right) \vartheta(t).$$

- (d) Take the Fourier transform of the equation of motion to show that:

$$(-\omega^2 - i\gamma\omega + \omega_0^2) \tilde{x}(\omega) = \frac{\tilde{F}(\omega)}{m}$$

and thus also show that the transfer function for a driven damped harmonic oscillator is:

$$\tilde{G}(\omega) = \frac{1}{m(\omega_0^2 - i\gamma\omega - \omega^2)}.$$

- (e) Verify by direct calculation that $G(t)$ and $\tilde{G}(\omega)$ for our damped oscillator are related as described by problem 2.29.
- (f) It was discussed in problem 2.29 that the amplification $A(\omega) = |\tilde{G}(\omega)|$ gives how much the input at a given frequency is amplified in the output. Explain how the phase $\varphi(\omega)$ so that $\tilde{G}(\omega) = Ae^{i\varphi}$ gives what portion of a cycle (in radians) the output lags behind the input. As well, determine and plot $A(\omega)$ and $\varphi(\omega)$ for our damped harmonic oscillator.
- (g) The interval of values of ω on either side of a resonance for which the amplification is at least half of its resonance value is called the transmission band or just band of the resonance. The width of this interval is called the full width at half maximum (FWHM) or bandwidth of the resonance. Conceptually, the band approximates the range of frequencies around a resonance for which the system has a “strong” response¹⁵. Find the resonant frequency, band, and bandwidth of our damped oscillator. Show that they reduce to the undamped results as $\gamma \rightarrow 0$.
- (h) Explain how by definition the energy transferred/work done by a driving force on an object over all time is given by:

$$W = \int_{-\infty}^{\infty} F(t)\dot{x}(t)dt$$

and use this to show that by going to the Fourier domain, the work can be rewritten as:

$$W = \int_0^{\infty} \mathcal{P}(\omega) |\tilde{F}(\omega)|^2 d\omega$$

where $\mathcal{P}(\omega)$ is a real valued function called the power transfer function given by:

$$\mathcal{P}(\omega) = 2\omega \text{Im}(\tilde{G}(\omega)).$$

As well, explain conceptually what the power transfer function of the system means.

- (i) Find the resonance, band, and bandwidth of the power transfer function of our damped harmonic oscillator and plot them together on a plot of the power transfer function. What do these values tell you?

Problem 2.61: Falling due to gravity with drag. Let us return to the issue of an object falling straight down due to gravity. Now though, include the effect of drag on the object and assume it is in the quadratic drag regime so that its equation of motion is given by:

$$m\ddot{y} - k\dot{y}^2 + mg = 0$$

for some constant k which characterizes the drag.

¹⁵Based on application, one may require a different threshold than half the resonant value for the range they consider “strong”, but one may relate the width at any threshold to the FWHM by a simple numerical proportionality

- (a) Show that the speed of the falling object limits to a finite value as it is falling. That value is called the terminal speed. Find an expression for it.
- (b) Find the velocity of the object as a function of time assuming it starts at $\dot{y}(0) = 0$.
- (c) Find the position of the object as a function of time assuming it starts at $y(0) = h$. How long does it take to hit the ground at $y = 0$?

Problem 2.62: Coulomb Friction. The surfaces of everyday objects are not perfectly smooth. Because of this, two surfaces will microscopically get caught on each other when one is moved while pressed against the other (the protrusions of one surface will dig into the grooves of the other and can get stuck or bent). The effective external force due to this catching is called friction. Here we will justify the basic elements of the most common basic model of friction, called Coulomb friction. Consider two surfaces which are pressed against each other so that they make contact at some points. Each surface we will assume has some small bumps and dips so that we can locally assign an averaged plane of the surface and think of the bumps and dips as deviations from the average. (For this to be meaningful the scale on which the average plane is defined needs to be large enough that the bumps and dips average each other out but small enough that the surface doesn't appreciably curve.) When two surfaces are pressed against each other then their macroscopic average planes are approximately parallel locally. Let $\mathcal{N}$ be the magnitude of the constraint force exerted by such average planes on each other to prevent them from crossing each other (the constraint force due to not allowing the objects to pass through each other).

- (a) When the surfaces are not moving macroscopically relative to each other the points of contact between them will relax to local minima due to being pressed together by gravity (these are the stable equilibria when the surfaces are pressed together). Let θ be the angle of the bottom surface locally above horizontal at a specific point of contact. Show that in order to accelerate the second surface out of the local minima an external horizontal force F_{ext} of at least $\mathcal{N} \tan \theta$ is necessary if this is taken to be the only point of contact. Thus conclude that if one object is not moving relative to another then there is a critical force (whose value is proportional to the normal force between the two objects) which is necessary to induce relative motion. This is called static friction and the proportionality constant is called the coefficient of static friction.
- (b) When the surfaces are moving macroscopically relative to each other and we again assume one point of contact, show that the net force parallel to the macroscopic surfaces due to the constraint forces between the surfaces is $-\mathcal{N} \sin \theta \cos \theta$ in terms of the previously defined θ where $\mathcal{N}$ is the macroscopic normal force between the average surface planes. Thus conclude that while in motion the frictional force (now called kinetic friction) is proportional again to the normal force, opposes the motion, is otherwise velocity independent, and has proportionality constant (coefficient of kinetic friction) less than the coefficient of static friction.
- (c) Suppose that there are multiple points of contact with varying angles θ_n at the different points and vertical normal force $\mathcal{N}_n$ at each point. Show that the resulting horizontal forces result from summing the contributions at each point of contact and that because $\mathcal{N} = \sum_n \mathcal{N}_n$ is fixed, the total frictional force does not scale at all with the area of contact. Thus, conclude that static friction between two surfaces can be modeled as an external force F_{fr} which opposes the potential start of motion, acts parallel to the surface of contact, and is limited in strength to $\mu_s \mathcal{N}$ where μ_s is some nonnegative dimensionless coefficient determined by the microscopic shapes of the surfaces and $\mathcal{N}$ is the macroscopic normal force between the surfaces. This μ_s is called the coefficient of static friction. Show similarly that the kinetic friction between two surfaces can be modeled as an external force which opposes the ongoing motion, acts parallel to the surface of contact, and has strength given by $\mu_k \mathcal{N}$ where μ_k is some nonnegative dimensionless coefficient determined by the microscopic shapes of the surfaces. This μ_k is called the coefficient of kinetic friction.

Problem 2.63: Rolling revisited. Let us return to problem 2.47 and the issue of a uniform cylinder rolling down an incline plane.

- (a) Without assuming rolling without slipping, show that if the cylinder experiences an external force F and torque τ then its equations of motion are given by:

$$F = -mg \sin \theta + m\ddot{s}, \quad \tau = \frac{mr^2}{2} \ddot{\varphi}.$$

- (b) Showing that if the cylinder experiences friction with the incline plane at the point of contact:

$$F = -F_{\text{fr}}, \quad \tau = rF_{\text{fr}}.$$

- (c) Now show that the condition of rolling without slipping requires:

$$F_{\text{fr}} = \frac{1}{3}mg \sin \theta.$$

Furthermore, use that the static friction is limited in strength to show that the cylinder can only roll without slipping if the inclination angle is such that:

$$\theta \leq \arctan(3\mu_s).$$

- (d) Now assume that the inclination is as needed for rolling without slipping but that the cylinder enters the top of the ramp going a speed v and not rolling. As well, assume $\tan \theta < 3\mu_k$. Show that the cylinder will begin rolling as it goes down the ramp and that after a time T it will reach the condition of rolling without slipping with that time given by:

$$T = \frac{v}{g} \frac{1}{3\mu_k \cos \theta - \sin \theta}.$$

Problem 2.64: Sliding blocks on a table. Consider a block of mass m sliding on a table. Suppose the block starts with initial velocity v and experiences coefficient of kinetic friction μ . How far will the block slide before coming to a stop due to the friction between it and the table?

Problem 2.65: Sliding harmonic oscillator. Consider a block of mass m sliding on a frictionful table of coefficient of kinetic friction μ and connected to a spring of spring constant k . Suppose the system starts from rest with an amplitude A . What is the total distance the block slides on the table before coming to a stop?

2.10 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 2.5: Newton's First Law** and
- **Problem 2.18: Newton's Second Law** and
- **Problem 2.20: Newton's Third Law** derive Newton's laws of motion from the Galilean Lagrangian, showing that they are a particular special case of analytical mechanics.
- **Problem 2.6: Cross Product Identities** and
- **Problem 2.7: Rotation Identities** prove important identities related to rotations which we will use going forward.
- **Problem 2.16: Aristotle's Force** gives another perspective on establishing that the Galilean Lagrangian is the correct form for the symmetries it requires.
- **Problem 2.19: Lorentz Force Law** derives the force on a charged particle due to electric and magnetic fields.
- **Problem 2.25: Hooke's Law and the Harmonic Oscillator** derives the most important system in physics.
- **Problem 2.27: Fundamental Fourier Integral** and
- **Problem 2.28: Fourier Transform Primer** introduce the Fourier transform which we will use often going forward.
- **Problem 2.29: Driven Harmonic Oscillator** exactly solves the most important system in physics.
- **Problem 2.42: Huygens' Pendulum** develops how to accurately measure time in terms of a reference unit of time with a basic mechanical system.
- **Problem 2.48: Measuring mass with a beam balance** develops how to measure mass in terms of a reference unit of mass with a basic mechanical system.

In this chapter we developed the theory of Galilean matter and how it is affected by external factors. This theory of Galilean Classical Mechanics (GCM) is defined by two sets of assumptions (the division between which we have not yet noticed), one set of assumptions which are generically taken in physics and one set of assumptions which are specific to GCM.

Assumptions generally made in Physics:

- PHSXI: Smoothness of Time and Time Evolution.**
- PHSXII: Smoothness of 3-dimensional Space.**
- PHSXIII: Time Translational Symmetry.**
- PHSXIV: Space Translational Symmetry.**
- PHSXV: Rotational Symmetry.**

Assumptions specific to Galilean Classical Mechanics:

- GCM I: Matter consists of moving points.**
- GCM II: Galilean Boost Symmetry.**
- GCM III: Space is static and Euclidean.**

In section 2.1, we developed the generic Lagrangian for an object in a system consistent with these assumptions. In 2.2, we explored that time translation symmetry implies the conservation of Energy and found how this reduces the Lagrangian from 2.1. In 2.3, we explored that space translation symmetry implies the conservation of linear momentum and found how this reduces the Lagrangian found in 2.2. In 2.4, we studied rotations and rotation matrices and explored that rotational symmetry implies the conservation of angular momentum and found how this reduces the Lagrangian found in 2.3. In 2.5, we developed interpretations for all of the terms in our particle Lagrangian and discovered that a particle in our theory is characterized by its mass m , which is a property measuring how hard it is to change the object's motion, and the charges q_s which give the strength with which the object interacts with the potentials appearing in the Lagrangian. As well, we found that those potentials are not quite uniquely defined due to the fact that the Lagrangian is not quite uniquely defined (from gauge symmetry). In 2.6, we found the equation of motion for our Galilean object and identified that the gauge invariants of the potentials are given by the functions $\vec{E}$ and $\vec{B}$ which appear in the equations of motion, called the electric and magnetic fields. In 2.7, we found how to consider compositions of systems as well as how to consider subsystems of larger systems. Both of these are useful for theoretical and

practical applications, as explored in the corresponding homework and applied in the subsequent sections. In 2.8, we found how to consider the motion of systems in which the variables are constrained to move only in certain allowed ways and explored several models in which such constraints can be used for real systems. In 2.9, we finally found how to write the motion of a macroscopic (non-point) rigid object and found that it is quite complicated. Through all of this, we have arrived at a theory of how matter moves but not ultimately how to determine the potentials appearing in the Lagrangian for that matter. That part of the story has not yet been told.

In addition to the development of theory in this chapter, we also established key techniques for measuring a basic set of physical quantities. In particular, we found how to measure lengths with a stick (which defines a reference unit of length such as the meter), how to measure times with Huygens' pendulum (which defines a reference unit of time such as the second), and how to measure masses using a spring (which defines a reference unit of mass such as the kilogram). Thus, we can perform any measurement which can be reduced to comparing the quantities to be measured directly to those given reference values using those experimental techniques.

This chapter is by no means a complete treatment of essential topics in (Galilean) Classical Mechanics. For completeness sake, here is a list of some important topics we have not covered (in no particular order) with places to read about them:

- Classical Mechanics in Non-Inertial Reference Frames. Just a nasty coordinate transformation away from what we have done so far. But, real life is often done in nasty coordinates (you might think you are at rest on Earth, but it is rotating underneath you – the coordinates of you are nasty and have effects) [117].
- Simple machines [117], [56].
- Chaotic classical systems (the swinging Atwood machine, the double pendulum) [117], [2].
- Countless classic problems and scenarios (GCM was the dominant theory of physics for over 200 years, it has a lot to its name) [117], [56].

Chapter 3

Nonrelativistic Interactions

There are things done today in electrical science which would have been deemed unholy by the very men who discovered electricity, who would themselves not so long before been burned as wizards.
 – John Seward [114]

We have our theory now for particles experiencing potentials. But, we do not have the theory for what those potentials should be. The Lagrangian in equation (2.5.5) is only half the story. It tells how the particles are affected by the background. Here we will find how the background is affected by the particles.

3.1 The Potentials as Variables

While making a theory for our particle, we had variables for the particle ($\vec{x}(t)$) and found they moved according to some given background functions ($\phi(t, \vec{x})$, $\vec{A}(t, \vec{x})$). Now that we know what a particle does in the presence of given backgrounds (the potentials), we would like to figure out what happens to the potentials due to those particles. This is precisely the situation outlined in Theorem 2.11: we know how the $Q_1 = \vec{x}(t)$ are affected by the $Q_2 = (\phi, \vec{A})$ but not how the Q_2 are affected by the Q_1 . By using Theorem 2.11, we can identify that our Lagrangian in Theorem 2.7 is the Lagrangian of 1|2 ($\vec{x}$ given the potentials). Now we simply need to find the free Lagrangian for the potentials to complete the Lagrangian for the whole theory. To do this, it will be useful to identify the interaction term of the Lagrangian from Theorem 2.11 contained within our Lagrangian of 1|2. From equation (2.5.5), the Lagrangian for a GCM particle with background potentials $\phi, \vec{A}$ is:

$$\mathcal{L}_{1|2} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \sum_s q_s \left(\vec{A}_s(t, \vec{x}) \cdot \dot{\vec{x}} - \phi_s(t, \vec{x}) \right) \quad (3.1.1)$$

$$\implies \mathcal{L}_1 = \frac{1}{2}m|\dot{\vec{x}}|^2, \quad \mathcal{L}_{\text{int}} = \sum_s q_s \left(\vec{A}_s(t, \vec{x}) \cdot \dot{\vec{x}} - \phi_s(t, \vec{x}) \right) \quad (3.1.2)$$

Because the potentials for different values of s represent different backgrounds, they are independent variables and so we can study one at a time and then add their non-interacting Lagrangians together just as we have done here. So, for now consider only one kind of charge and so only one pair of potentials ϕ and $\vec{A}$. Moreover, if instead of just one particle we had N particles, the Lagrangian for the N of them would simply be gotten by adding together the Lagrangians for each by this same argument:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2}m_n|\dot{\vec{x}}_n|^2 + q_n\vec{A}(t, \vec{x}_n) \cdot \dot{\vec{x}}_n - q_n\phi(t, \vec{x}_n) \right) + \mathcal{L}_{\phi, \vec{A}}. \quad (3.1.3)$$

Here $\mathcal{L}_{\phi, \vec{A}}$ is the free Lagrangian for the potentials which we currently don't know. Then, the interaction term between the particles and the potentials is:

$$\mathcal{L}_{\text{int}} = \sum_{n=1}^N q_n \left(\vec{A}(t, \vec{x}_n) \cdot \dot{\vec{x}}_n - \phi(t, \vec{x}_n) \right). \quad (3.1.4)$$

3.1.1 The Continuity Equation

It is convenient to define the **charge density** $\rho(t, \vec{x})$ as the charge per unit volume. Then, the charge $q[\mathbb{V}]$ contained in any region $\mathbb{V}$ is given (by definition of ρ) by the integral of ρ over that region:

$$q[\mathbb{V}] = \int_{\mathbb{V}} \rho d\mathbb{S}. \quad (3.1.5)$$

(Throughout this book $d\mathbb{S}$ will be used for the differential volume element: $d\mathbb{S} = d^3\vec{x} = dx dy dz$. Similarly $d\vec{\mathbb{A}}$ will be used for the differential area element in surface integrals and $d\vec{\mathbb{A}}$ will be used for the directed area element where the direction is taken to be the outward pointing normal of the surface. The notation $\partial\mathbb{V}$ will be used to mean the boundary of the region $\mathbb{V}$.) By definition, the charge contained in the region $\mathbb{V}$ is the sum over all charges whose positions are in $\mathbb{V}$. Let $\vartheta(x)$ be the indicator function, that is the function which is 1 when its argument is true and 0 when its argument is false. For example, $\vartheta(\vec{x} \in \mathbb{V})$ is 1 when the position $\vec{x}$ is in the volume $\mathbb{V}$ and 0 when it is not. Then, the sum over all charges whose positions are in $\mathbb{V}$ is given by:

$$q[\mathbb{V}] = \sum_{n=1}^N q_n \vartheta(\vec{x}_n \in \mathbb{V}). \quad (3.1.6)$$

Any function $f(\vec{x})$ can be written as:

$$f(\vec{x}) = \int_{\mathbb{S}} f(\vec{x}') \delta(\vec{x} - \vec{x}') d\mathbb{S}' \quad (3.1.7)$$

by definition of the multidimensional Dirac delta (explored in the homework). Applying this to the indicator function and using that the indicator vanishes outside of the volume $\mathbb{V}$ and is 1 inside:

$$\vartheta(\vec{x} \in \mathbb{V}) = \int_{\mathbb{S}} \vartheta(\vec{x}' \in \mathbb{V}) \delta(\vec{x} - \vec{x}') d\mathbb{S}' = \int_{\mathbb{V}} \delta(\vec{x} - \vec{x}') d\mathbb{S}'. \quad (3.1.8)$$

Thus, we can rewrite (3.1.6) as:

$$q[\mathbb{V}] = \sum_{n=1}^N q_n \vartheta(\vec{x}_n \in \mathbb{V}) = \sum_{n=1}^N q_n \int_{\mathbb{V}} \delta(\vec{x}_n - \vec{x}) d\mathbb{S} = \int_{\mathbb{V}} \sum_{n=1}^N q_n \delta(\vec{x} - \vec{x}_n) d\mathbb{S}. \quad (3.1.9)$$

As such, observing that (3.1.5) and (3.1.9) must match by definition for all regions $\mathbb{V}$, the integrands must match giving that for N point charges the charge density is:

$$\rho(t, \vec{x}) = \sum_{n=1}^N q_n \delta(\vec{x} - \vec{x}_n(t)). \quad (3.1.10)$$

Now consider the rate at which charge flows out of the region $\mathbb{V}$. That is, take the time derivative:

$$\frac{dq}{dt}[\mathbb{V}] = \frac{d}{dt} \int_{\mathbb{V}} \sum_{n=1}^N q_n \delta(\vec{x} - \vec{x}_n(t)) d\mathbb{S} = \int_{\mathbb{V}} \sum_{n=1}^N q_n \left(-\dot{\vec{x}}_n \cdot \nabla \right) \delta(\vec{x} - \vec{x}_n(t)) d\mathbb{S} \quad (3.1.11)$$

$$= - \int_{\mathbb{V}} \nabla \cdot \left(\sum_{n=1}^N q_n \dot{\vec{x}}_n \delta(\vec{x} - \vec{x}_n(t)) \right) d\mathbb{S} = - \int_{\partial\mathbb{V}} \sum_{n=1}^N q_n \dot{\vec{x}}_n \delta(\vec{x} - \vec{x}_n) \cdot d\vec{\mathbb{A}}. \quad (3.1.12)$$

Hence the rate at which charge flows out of the region is given by an integral over the boundary of the region. The integrand is called the **current density** $\vec{J}(t, \vec{x})$:

$$\vec{J}(t, \vec{x}) = \sum_{n=1}^N q_n \dot{\vec{x}}_n(t) \delta(\vec{x} - \vec{x}_n(t)) \quad (3.1.13)$$

$$\Rightarrow \boxed{\frac{dq}{dt}[\mathbb{V}] = - \int_{\partial\mathbb{V}} \vec{J} \cdot d\vec{\mathbb{A}}.} \quad (3.1.14)$$

Then we can rewrite the interaction term of the Lagrangian as an integral over space with these definitions:

$$\int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho \phi \right) d\mathbb{S} = \int_{\mathbb{S}} \sum_{n=1}^N q_n \left(\dot{\vec{x}}_n \delta(\vec{x} - \vec{x}_n(t)) \vec{A}(t, \vec{x}) - \delta(\vec{x} - \vec{x}_n(t)) \phi(t, \vec{x}) \right) d\mathbb{S} \quad (3.1.15)$$

$$= \sum_{n=1}^N q_n \left(\dot{\vec{x}}_n \cdot \vec{A}(t, \vec{x}_n) - \phi(t, \vec{x}_n) \right) \quad (3.1.16)$$

$$\implies \boxed{\mathcal{L}_{\text{int}} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho \phi \right) d\mathbb{S}} \quad (3.1.17)$$

We should note that (3.1.14) has a nice interpretation. As we found, the rate of change of the amount of charge in the region $\mathbb{V}$ is given by an integral over the boundary of that region. Thus, the integrand $\vec{J}$ in (3.1.14) is the rate at which charge flows across the boundary of $\mathbb{V}$ per unit area of the boundary (and the direction of $\vec{J}$ is the direction of the charge flow). In particular, by using (3.1.5) together with (3.1.14):

$$\frac{dq}{dt}[\mathbb{V}] = \int_{\mathbb{V}} \frac{\partial \rho}{\partial t} d\mathbb{S} = - \int_{\partial \mathbb{V}} \vec{J} \cdot d\vec{\mathbb{A}} = - \int_{\mathbb{V}} \nabla \cdot \vec{J} \cdot d\mathbb{S} \quad (3.1.18)$$

$$\implies \int_{\mathbb{V}} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} \right) d\mathbb{S} = 0. \quad (3.1.19)$$

Because this integral vanishes for all regions $\mathbb{V}$, the integrand must vanish and so we are left with:

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0.} \quad (3.1.20)$$

Equation (3.1.20) is called the **Continuity Equation**. As derived, it is equivalent to the statement that the amount of charge in a region changes only by the amount that flows in or out of that region. By taking the region to be all of space, there is by definition no flow out of space and so the total charge is conserved. So, the continuity equation gives the conservation law of charge: charge is neither created nor destroyed. However, because we could consider any region it goes even further by giving the *local conservation law* of charge: charge is neither created nor destroyed, it only flows from place to neighboring place. The continuity equation is much more general than the point-particle way of thinking about charge; it would hold for any continuous model of charge in which it is locally conserved. We will see the continuity equation many more times (and the quantity in it will not always be charge).

3.1.2 Charge Conservation Causes Gauge Symmetry

The local conservation of charge means that for any function $f(t, \vec{x})$ we can always add to the Lagrangian the term:

$$\mathcal{L}'_{\text{int}} = \mathcal{L}_{\text{int}} - \int_{\mathbb{S}} f(t, \vec{x}) \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} \right) d\mathbb{S}. \quad (3.1.21)$$

The reason we can add this term is that we haven't actually added anything; this term is always 0 by the continuity equation! Therefore, while $\mathcal{L}_{\text{int}}$ and $\mathcal{L}'_{\text{int}}$ might look different, they are exactly the same. Adding this f term can be rewritten as:

$$\mathcal{L}'_{\text{int}} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho \phi - f(t, \vec{x}) \frac{\partial \rho}{\partial t} - f(t, \vec{x}) \nabla \cdot \vec{J} \right) d\mathbb{S} \quad (3.1.22)$$

$$= \int_{\mathbb{S}} \left(\vec{J} \cdot (\vec{A} + \nabla f) - \rho \left(\phi - \frac{\partial f}{\partial t} \right) \right) d\mathbb{S} - \frac{d}{dt} \int_{\mathbb{S}} \rho f d\mathbb{S} - \int_{\mathbb{S}} \nabla \cdot (f \vec{A}) d\mathbb{S} \quad (3.1.23)$$

$$\simeq \int_{\mathbb{S}} \left(\vec{J} \cdot (\vec{A} + \nabla f) - \rho \left(\phi - \frac{\partial f}{\partial t} \right) \right) d\mathbb{S} - \int_{\partial \mathbb{S}} f \vec{A} \cdot d\vec{\mathbb{A}}. \quad (3.1.24)$$

For all functions f which are 0 at sufficient large distances, the surface integral above will go to 0 (because it is an integral over the spatial boundary very far away and we consider f which are 0 sufficiently far away). Then, (3.1.24) is in exactly the same form as (3.1.17) but with new potentials. Therefore, for such f , adding a term equal to 0 (proportional to the continuity equation) to the integrand of the Lagrangian is equivalent (because Lagrangians which differ by a total time derivative are equivalent) to modifying the potentials according to:

$$\vec{A}' = \vec{A} + \nabla f, \quad \phi' = \phi - \frac{\partial f}{\partial t} \quad (3.1.25)$$

$$\implies \mathcal{L}'_{\text{int}} \simeq \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A}' - \rho \phi' \right) d\mathbb{S}. \quad (3.1.26)$$

This is precisely the gauge transformation! That is, **the potentials are only defined up to a gauge transformation because of the local conservation of charge**. The continuity equation provides a term equal to 0 we can add to the integrand of the Lagrangian and doing so is equivalent to performing a gauge transformation on the potentials. The gauge freedom in defining the potentials is a symmetry of how they are formulated and the conserved quantity due to that symmetry is the local conservation of charge. We will study later in chapter 6 how this is literally just an application of Noether's theorem. If f decays sufficiently quickly at large distances that the surface integral $f\vec{A}$ goes to 0, f is said to produce a **small gauge transformation**. If instead f decays slowly enough or not at all that the surface integral $f\vec{A}$ is finite, f is said to produce a **large gauge transformation**. Both large and small gauge transformations leave the equations of motion on the inside of the region of interest unchanged and so will not affect the physics of Part I. However, in some theories we will discuss in Part II, large gauge transformations do have some important subtleties.

Because of translational symmetry, you can pick any point in space you want as the origin of your coordinates and physics will be the same. Consequently, linear momentum is conserved from Noether's theorem. Conversely, because of momentum conservation, the transformation generated by linear momentum (translations) is a symmetry of our world, and there is a symmetry (a redundancy/ambiguity) to pick whatever origin you want. Angular momentum is conserved and the transformation generated by angular momentum (rotations) is a symmetry of our world, and there is a symmetry to pick whatever coordinate axes you want. Charge is conserved and the transformation generated by charge (gauge transformations) is a symmetry of our world, and there is a symmetry to pick whatever gauge you want for the potentials. We will see in chapter 4 how this is not just a persuasive analogy but literally mathematically true.

The gauge transformation of the potentials is a continuous transformation (because f can be made arbitrarily small, consider for example $\varepsilon f(t, \vec{x})$ for ε a real number we can make arbitrarily close to 0). A composition of gauge transformations is itself a gauge transformation with the total gauge function being the sum of the individual gauge functions:

$$\vec{A}' = (\vec{A} + \nabla f_1) + \nabla f_2 = \vec{A} + \nabla(f_1 + f_2) = \vec{A} + \nabla f \quad (3.1.27)$$

$$\phi' = \left(\phi - \frac{\partial f_1}{\partial t} \right) - \frac{\partial f_2}{\partial t} = \phi - \frac{\partial}{\partial t} (f_1 + f_2) = \phi - \frac{\partial f}{\partial t} \implies f(t, \vec{x}) = f_1(t, \vec{x}) + f_2(t, \vec{x}). \quad (3.1.28)$$

One can quickly see that addition of real numbers satisfies the definition of a Lie group (where real addition is the group "multiplication" and 0 is the identity). Of course, addition of real numbers is commutative and so the gauge group of the potentials is Abelian (Abelian is another word for commutative when discussing groups). So, the potentials are an **Abelian gauge theory**.

We tend to name Lie groups by how they relate to a matrix representation. So, let us try to find a way to represent real number addition as a form of matrix multiplication. We know how to turn addition into multiplication: the exponential. Immediately, for real numbers θ_1 and θ_2 :

$$e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1 + \theta_2)}. \quad (3.1.29)$$

Let $u(\theta) = e^{i\theta}$ be a 1x1 complex matrix (in other words, a complex number). Then:

$$u(\theta_1)u(\theta_2) = u(\theta_1 + \theta_2) \quad (3.1.30)$$

and:

$$|u|^2 = |e^{i\theta}|^2 = |\cos \theta + i \sin \theta|^2 = \cos^2 \theta + \sin^2 \theta = 1. \quad (3.1.31)$$

Conversely, by simple algebra any complex number of magnitude 1 can be written in the form $e^{i\theta}$. When u multiplies another complex number, it does not change the magnitude of that number:

$$|uz| = |u||z| = |z|. \quad (3.1.32)$$

The set of $N \times N$ complex matrices which preserve the magnitude of all N dimensional complex vectors is called the set of **unitary** $N \times N$ matrices and it is written as $U(N)$. One can check quickly against the definition of a group that $U(N)$ is in fact a group. The set of $u(\theta)$ is then the group of 1x1 unitary matrices $U(1)$. Because $f(t, \vec{x})$ is a function and not just a single real number, we have the complex exponential of f is a function of $(t, \vec{x})$ and so we say that the theory of the potentials has **$U(1)$ gauge symmetry**.

Exercises

Problem 3.1: The Interaction Hamiltonian. Instead of the Lagrangian for a charge experiencing the

potentials, consider the corresponding Hamiltonian:

$$\mathcal{H} = \frac{|\vec{p} - q\vec{A}|^2}{2m} + q\phi.$$

- Find the corresponding expression for the interaction term of the Hamiltonian and note that it is **NOT** simply the negative of the interaction term of the Lagrangian (a common and mistaken claim).
- Show that the Hamiltonian is exactly conserved under the equations of motion (assume for this part that ϕ and $\vec{A}$ do not depend on time explicitly).
- Keep the Hamiltonian only to order q (that is, approximate terms q^2 or higher as 0). Find the corresponding equations of motion of that Hamiltonian and show that the order q Hamiltonian is exactly conserved under its equations of motion.
- Show that if one approximates the exact Hamiltonian only to order q and the exact equations of motion only to order q , then the approximate Hamiltonian is **NOT** conserved by the approximate equations of motion. This is a common issue one may overlook when making approximations. It is often important to keep conservation laws exact in order for an approximation to be a qualitatively accurate description of the exact solution. As illustrated here, just directly approximating the Hamiltonian and the equations of motion does not protect conservation laws. To protect the energy conservation law, if one approximates the Hamiltonian then one must use the corresponding equations of motion one would get by treating that Hamiltonian as exact.

Problem 3.2: ★ Change of Variables in the Dirac Delta. Sometimes it will come up that we will need to evaluate expressions like:

$$I = \int_{-\infty}^{\infty} g(x)\delta(f(x))dx$$

where $f(x)$ is a differentiable function.

- Divide the real line up into a list of intervals $M_1, \dots, M_N$ so that on each interval $f(x)$ is monotone. Explain how then on each interval one can define a unique inverse function $f_n^{-1}(y)$ so that for all x in the interval M_n , $f_n^{-1}(f(x)) = x$.
- Show that I can be rewritten as:

$$I = \sum_{n=1}^N \int_{M_n} g(x)\delta(f(x))dx.$$

- On each interval above, make the u-substitution: $y = f(x)$ and show that the resulting integral is:

$$I = \sum_{n=1}^N \int_{f(M_n)} g(f_n^{-1}(y)) \frac{\delta(y)}{|f'(f_n^{-1}(y))|} dy$$

- Simplify the above integral to show that it becomes:

$$I = \sum_k \frac{g(x_k)}{|f'(x_k)|}$$

where x_k are the zeros of the function $f(x)$.

- Rewrite that simplification using the Dirac delta and compare with the original definition of I to conclude that:

$$\delta(f(x)) = \sum_k \frac{\delta(x - x_k)}{|f'(x_k)|}.$$

This is known as the Dirac Delta Change of Variables formula.

- Show that in the special case $f(x) = ax$ the change of variables formula becomes:

$$\delta(ax) = \frac{1}{|a|} \delta(x).$$

Problem 3.3: ★ Multidimensional Dirac Delta. In this section we introduced the multi-dimensional Dirac Delta. In Cartesian coordinates, it is defined as:

$$\delta(\vec{x}) = \delta(x)\delta(y)\delta(z).$$

As with the single variable Dirac delta, it will be useful to compute expressions of the form:

$$I = \int_{\mathbb{S}} g(\vec{x}) \delta(\vec{F}(\vec{x})) d^d \vec{x}$$

where d indicates the number of spatial dimensions.

- (a) Assume that the function $\vec{F}(\vec{x})$ is invertible. (From vector calculus, this is equivalent to the condition that the Jacobi determinant $\det \left(\frac{\partial \vec{F}}{\partial \vec{x}} \right)$ is never 0.) Make the u-substitution $\vec{y} = \vec{F}(\vec{x})$ to show that:

$$I = \int_{\vec{F}(\mathbb{S})} g(\vec{F}^{-1}(\vec{y})) \delta(\vec{y}) \frac{d^d \vec{y}}{\left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} (\vec{F}^{-1}(\vec{y})) \right) \right|}.$$

- (b) Simplify the above integral to show that:

$$I = \frac{g(\vec{x}_0)}{\left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} (\vec{x}_0) \right) \right|}$$

where $\vec{x}_0$ is the value of $\vec{x}$ for which $\vec{F}(\vec{x}) = 0$.

- (c) Use the above result and the original definition of I to conclude that:

$$\delta(\vec{F}(\vec{x})) = \frac{\delta(\vec{x} - \vec{x}_0)}{\left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} (\vec{x}_0) \right) \right|}.$$

- (d) Show that in the special case $\vec{F}(\vec{x}) = \hat{M}\vec{x}$ for a matrix $\hat{M}$:

$$\delta(\hat{M}\vec{x}) = \frac{\delta(\vec{x})}{|\det \hat{M}|}.$$

Problem 3.4: ★ Derivatives of the Dirac Delta. For many calculations, it will be useful to define a “derivative” of the Dirac delta. We can do this through intelligent integration by parts.

- (a) By definition of the Dirac delta, for a function $f(x)$,

$$\int_{-\infty}^{\infty} f'(x) \delta(x) dx = f'(0).$$

Then, use integration by parts to show formally that:

$$\int_{-\infty}^{\infty} f'(x) \delta(x) dx = f'(x) \delta(x) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(x) \delta'(x) dx.$$

- (b) Then, use that the Dirac delta is defined through the limit of the box function to justify that the boundary terms should vanish.
 (c) Thus, conclude that:

$$\int_{-\infty}^{\infty} f(x) \delta'(x) dx = -f'(0).$$

- (d) Repeat the above line of argumentation to justify that:

$$\int_{-\infty}^{\infty} f(x) \delta^{(n)}(x) dx = (-1)^n f^{(n)}(0).$$

Thus, the Dirac Delta is “infinitely differentiable” in the sense that the behavior of its derivatives is well-defined whenever it is integrated against a function for which that corresponding number exists. More properly, the Dirac Delta can be treated as “as smooth” as the function it is integrated against.

3.2 Classical Field Theory

Now that we have the interaction term, we know that the action for the potentials ϕ and $\vec{A}$ given fixed charge and current densities must be of the form (by Theorem 2.11):

$$S[\phi, \vec{A}] = S_0[\phi, \vec{A}] + \int_0^t \int_{\mathbb{S}} (\vec{J} \cdot \vec{A} - \rho\phi) dS dt. \quad (3.2.1)$$

Notice that trying to study the potentials ϕ and $\vec{A}$ through a Lagrangian is a little different than anything we have done so far. So far, we varied the action with respect to $Q^a(t)$ where a was a discrete index. However, the potentials are functions of space as well as time. We can still use the same formalism though if we think about the spatial dependence as a “continuous index” just as we did when we defined functional differentiation in section 1.5. That is, if we consider $\phi(t, \vec{x})$ to be a function of t at fixed $\vec{x}$ and that $\vec{x}$ just indexes which function of t we are looking at. A theory in which the variables are continuously indexed is called a **classical field theory**.

3.2.1 The Action in Classical Field Theory

Consider a list of fields $\phi^a(t, \vec{x})$ with action $S[\phi]$. We can understand exactly what is going on with field theory by thinking about it as the limit of a discretely indexed theory. Let Δx be the length at which we discretize and let $\vec{n}$ be a vector of integers. Then, we define $\phi_{\vec{n}}(t) = \phi(t, \vec{x}_{\vec{n}})$ where $\vec{x}_{\vec{n}} = \Delta x \vec{n}$. That is, we have essentially divided space up into a d -dimensional lattice of lattice spacing Δx (we will take the lattice to be d dimensional because sometimes it is useful to consider field theories on a line so $d = 1$ or in the plane so $d = 2$ in addition to in space where $d = 3$). In the end, we will take this spacing to 0 to recover our continuous theory. Let $S_{\Delta x}$ be a discretization of the action S . Then we have from section 1.5:

$$S[\phi] = \lim_{\Delta x \rightarrow 0} S_{\Delta x} \quad (3.2.2)$$

$$\frac{\delta S}{\delta \phi(t, \vec{x})} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}(t)}. \quad (3.2.3)$$

The reason we have Δx^d is because we discretize in d dimensions and each discretization picks up a factor of Δx . For the discretized theory, the equations of motion would be exactly as we have done so far (because it isn't yet a field theory):

$$\frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}^a(t)} = \frac{\partial \mathcal{L}_{\Delta x}}{\partial \phi_{\vec{n}}^a(t)} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}_{\Delta x}}{\partial \dot{\phi}_{\vec{n}}^a(t)} \right) \stackrel{!}{=} 0. \quad (3.2.4)$$

Now we can rewrite this in a way which after taking $\Delta x \rightarrow 0$ and using Theorem 1.3 gives the equation of motion of our field theory:

$$\frac{1}{\Delta x^d} \frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}^a(t)} = \frac{1}{\Delta x^d} \frac{\partial \mathcal{L}_{\Delta x}}{\partial \phi_{\vec{n}}^a(t)} - \frac{d}{dt} \left(\frac{1}{\Delta x^d} \frac{\partial \mathcal{L}_{\Delta x}}{\partial \dot{\phi}_{\vec{n}}^a(t)} \right) \stackrel{!}{=} 0 \quad (3.2.5)$$

$$\Rightarrow \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}^a(t)} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\partial \mathcal{L}_{\Delta x}}{\partial \phi_{\vec{n}}^a(t)} - \frac{d}{dt} \left(\lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\partial \mathcal{L}_{\Delta x}}{\partial \dot{\phi}_{\vec{n}}^a(t)} \right) \stackrel{!}{=} 0 \quad (3.2.6)$$

$$\Rightarrow \frac{\delta S}{\delta \phi^a(t, \vec{x})} = \frac{\delta \mathcal{L}}{\delta \phi^a} - \frac{d}{dt} \left(\frac{\delta \mathcal{L}}{\delta \dot{\phi}^a} \right) \stackrel{!}{=} 0. \quad (3.2.7)$$

Equation (3.2.7) gives the equation of motion for field theory but because ϕ is now also a function of $\vec{x}$ it is conventional to write the $\frac{d}{dt}$ using a partial derivative:

$$\frac{\delta S}{\delta \phi^a} = \frac{\delta \mathcal{L}}{\delta \phi^a} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\phi}^a} \stackrel{!}{=} 0. \quad (3.2.8)$$

This is the general equation of motion for a field theory which contains only first time derivatives in the fields in the Lagrangian (if one is interested, the generalization to higher time derivatives is gotten just as before using the method of Theorem 1.12). As well, the variation formula in (1.5.40) still holds:

$$\delta S = \lim_{\Delta x \rightarrow 0} \delta S_{\Delta x} = \lim_{\Delta x \rightarrow 0} \int_0^t \sum_{\vec{n} \in \mathbb{Z}^d} \frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}^a(t)} \delta \phi_{\vec{n}}^a dt = \lim_{\Delta x \rightarrow 0} \int_0^t \sum_{\vec{n} \in \mathbb{Z}^d} \frac{1}{\Delta x^d} \frac{\delta S_{\Delta x}}{\delta \phi_{\vec{n}}^a(t)} \delta \phi_{\vec{n}}^a \Delta x^d dt \quad (3.2.9)$$

$$= \int_0^t \int_{\mathcal{S}} \frac{\delta S}{\delta \phi^a(t, \vec{x})} \delta \phi^a(t, \vec{x}) d^d \vec{x} dt. \quad (3.2.10)$$

3.2.2 The Hamiltonian in Classical Field Theory

We can also formulate a Hamiltonian for our field theory by the same kind of discretization process by starting with the Hamiltonian for the discretized theory. For lattice spacing Δx , define the conjugate momentum to $\phi_{\vec{n}}(t)$:

$$P_a^{\vec{n}} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_{\vec{n}}^a}. \quad (3.2.11)$$

Taking the Euler-Lagrange equation for $\phi_{\vec{n}}$ (3.2.4) and Hamilton's second equation:

$$\frac{dP_a^{\vec{n}}}{dt} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_{\vec{n}}^a} = \frac{\partial \mathcal{L}}{\partial \phi_{\vec{n}}^a} = -\frac{\partial \mathcal{H}}{\partial \phi_{\vec{n}}^a}. \quad (3.2.12)$$

Based on the equation of motion (3.2.7), we expect the functional derivatives of $\mathcal{L}$ with respect to ϕ^a and $\dot{\phi}^a$ to have finite $\Delta x \rightarrow 0$ limits. Accordingly, it is helpful to rescale these last two equations as:

$$\frac{1}{\Delta x^d} P_a^{\vec{n}} = \frac{1}{\Delta x^d} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_{\vec{n}}^a}, \quad \frac{d}{dt} \left(\frac{1}{\Delta x^d} \frac{dP_a^{\vec{n}}}{dt} \right) = \frac{1}{\Delta x^d} \frac{\partial \mathcal{L}}{\partial \phi_{\vec{n}}^a} = -\frac{1}{\Delta x^d} \frac{\partial \mathcal{H}}{\partial \phi_{\vec{n}}^a}. \quad (3.2.13)$$

Along these lines, define the variables $\varphi_a^{\vec{n}}(t)$ by:

$$\varphi_a^{\vec{n}}(t) \stackrel{\text{def}}{=} \frac{1}{\Delta x^d} P_a^{\vec{n}}. \quad (3.2.14)$$

Then, in the $\Delta x \rightarrow 0$ limit we have:

$$\lim_{\Delta x \rightarrow 0} \varphi_a^{\vec{n}}(t) = \frac{\delta \mathcal{L}}{\delta \dot{\phi}^a}, \quad \frac{d}{dt} \left(\lim_{\Delta x \rightarrow 0} \varphi_a^{\vec{n}} \right) = \frac{\delta \mathcal{L}}{\delta \phi^a} = -\frac{\delta \mathcal{H}}{\delta \phi^a}. \quad (3.2.15)$$

So, we see that these rescaled momentum variables have finite $\Delta x \rightarrow 0$ limit for their value and equations of motion. As such, we define the conjugate momentum field $\varphi_a(t, \vec{x})$ to the field $\phi^a(t, \vec{x})$ by:

$$\varphi_a(t, \vec{x}) \stackrel{\text{def}}{=} \lim_{\Delta x \rightarrow 0} \varphi_a^{\vec{n}}(t) = \frac{\delta \mathcal{L}}{\delta \dot{\phi}^a}. \quad (3.2.16)$$

Then, (3.2.15) gives the field theory equivalent of Hamilton's second equation:

$$\frac{\partial \varphi_a(t, \vec{x})}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi^a}. \quad (3.2.17)$$

To get Hamilton's first equation for field theory, the following will be useful:

$$\frac{\delta f}{\delta \varphi_a} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\partial f}{\partial \varphi_a^{\vec{n}}} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\partial f}{\partial P_a^{\vec{n}}} \frac{\partial P_a^{\vec{n}}}{\partial \varphi_a^{\vec{n}}} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^d} \frac{\partial f}{\partial P_a^{\vec{n}}} \Delta x^d = \lim_{\Delta x \rightarrow 0} \frac{\partial f}{\partial P_a^{\vec{n}}}. \quad (3.2.18)$$

We have by Hamilton's first equation for the discretized variables:

$$\frac{\partial \phi^a(t, \vec{x})}{\partial t} = \lim_{\Delta x \rightarrow 0} \frac{d\phi_{\vec{n}}^a}{dt} = \lim_{\Delta x \rightarrow 0} \frac{\partial \mathcal{H}}{\partial P_a^{\vec{n}}} = \frac{\delta \mathcal{H}}{\delta \varphi_a}. \quad (3.2.19)$$

Equations (3.2.19) and (3.2.15) give Hamilton's equations for fields $\phi^a(t, \vec{x})$ and their conjugate momenta $\varphi_a(t, \vec{x})$. The Legendre transformation also retains a familiar form in field theory. Again, take the $\Delta x \rightarrow 0$ limit of the usual Legendre transform:

$$\mathcal{L} = \lim_{\Delta x \rightarrow 0} \sum_{\vec{n}} P_a^{\vec{n}} \dot{\phi}_{\vec{n}}^a - \mathcal{H} \quad (3.2.20)$$

$$= \lim_{\Delta x \rightarrow 0} \sum_{\vec{n}} \Delta x^d \varphi_a^{\vec{n}} \dot{\phi}_{\vec{n}}^a - \mathcal{H}. \quad (3.2.21)$$

As $\Delta x \rightarrow 0$, the sum over all $\vec{n}$ with a factor of Δx^d is exactly a Riemann sum for an integral over all $\vec{x}$. Thus, this becomes:

$$\mathcal{L}[\phi, \dot{\phi}] = \int_{\mathcal{S}} \varphi_a(t, \vec{x}) \dot{\phi}^a(t, \vec{x}) d^d \vec{x} - \mathcal{H}[\phi, \varphi]. \quad (3.2.22)$$

Finally, it will be useful to develop the Poisson bracket for field theory. Again taking the $\Delta x \rightarrow 0$ limit

of the standard Poisson bracket formula and recognizing the appearing Riemann sum:

$$\{f, g\} = \lim_{\Delta x \rightarrow 0} \sum_{\vec{n}} \left(\frac{\partial f}{\partial \phi_{\vec{n}}^a} \frac{\partial g}{\partial P_a^{\vec{n}}} - \frac{\partial g}{\partial \phi_{\vec{n}}^a} \frac{\partial f}{\partial P_a^{\vec{n}}} \right) \quad (3.2.23)$$

$$= \lim_{\Delta x \rightarrow 0} \sum_{\vec{n}} \left(\frac{1}{\Delta x^d} \frac{\partial f}{\partial \phi_{\vec{n}}^a} \frac{\partial g}{\partial P_a^{\vec{n}}} - \frac{1}{\Delta x^d} \frac{\partial g}{\partial \phi_{\vec{n}}^a} \frac{\partial f}{\partial P_a^{\vec{n}}} \right) \Delta x^d \quad (3.2.24)$$

$$= \int_{\mathbb{S}} \left(\frac{\delta f}{\delta \phi^a(\vec{x})} \frac{\delta g}{\delta \varphi_a(\vec{x})} - \frac{\delta g}{\delta \phi^a(\vec{x})} \frac{\delta f}{\delta \varphi_a(\vec{x})} \right) d^d \vec{x}. \quad (3.2.25)$$

We can use this to compute the canonical brackets for the fields and conjugate momenta. To do so, we will use the multidimensional Dirac delta and apply to it (1.5.40):

$$f(\vec{x}) = \int_{\mathbb{S}} f(\vec{x}') \delta(\vec{x} - \vec{x}') d^d \vec{x}' \implies \delta f(\vec{x}) = \int_{\mathbb{S}} \delta f(\vec{x}') \delta(\vec{x} - \vec{x}') d^d \vec{x}' \quad (3.2.26)$$

$$\implies \frac{\delta f(\vec{x})}{\delta f(\vec{x}')} = \delta(\vec{x} - \vec{x}'). \quad (3.2.27)$$

This gives the canonical brackets:

$$\{\phi^a(\vec{x}), \phi^b(\vec{x}')\} = 0, \quad \{\phi^a(\vec{x}), \varphi_b(\vec{x}')\} = \delta_b^a \delta(\vec{x} - \vec{x}'), \quad \{\varphi_a(\vec{x}), \varphi_b(\vec{x}')\} = 0. \quad (3.2.28)$$

3.2.3 Locality

So far we have worked with field theory in general; however, the overwhelming majority of the time in physics we study a much smaller special class of field theories which are called **local** field theories. A local field theory is a field theory whose equations of motion only depend on fields and their derivatives (to finite order of differentiation¹) at only a single point. In general, the equation of motion for fields could contain interactions between fields at different points in space. This behavior is called non-local because the behavior of the field at one point is affected by the state of the field at other locations than that point. Because we believe by the prejudice of our day to day experiences that what happens at a location in the universe only depends on the neighborhood of that location, we assume that the physics of our universe is local and so we usually only consider non-local theories as effective theories of a fundamental local theory. Thus, we have:

Assumption :: PHSXVI: Locality

The time evolution of the Universe is given by local equations of motion.

To see what locality implies, let $F_a(t, \vec{x}, \phi, \partial\phi, \partial^2\phi, \dots)$ (where $\partial^n\phi$ is shorthand for dependence on the n^{th} derivative of ϕ) be the equations of motion gotten from differentiating the action:

$$\frac{\delta S}{\delta \phi^a(t, \vec{x})} = F_a(t, \vec{x}, \phi, \partial\phi, \partial^2\phi, \dots). \quad (3.2.29)$$

Because the equation of motion is local, the ... terminates at some finite order of differentiation and F only depends on ϕ and its derivatives at the points $(t, \vec{x})$ specified on the left hand side of the equation. Then, using the action recovery theorem, we can write the action:

$$S[\phi] = \int_{t_0}^{t_f} \int_{\mathbb{S}} \phi^a \int_0^1 F_a(t, \vec{x}, \lambda\phi, \lambda\partial\phi, \lambda\partial^2\phi, \dots) d\lambda d^d \vec{x} dt \quad (3.2.30)$$

$$\implies \mathcal{L} = \frac{dS}{dt} = \int_{\mathbb{S}} \phi^a \int_0^1 F_a(t, \vec{x}, \lambda\phi, \lambda\partial\phi, \lambda\partial^2\phi, \dots) d\lambda d^d \vec{x}. \quad (3.2.31)$$

The integral taken over space is the “continuous sum” over the continuous “index” $\vec{x}$ which would appear in the action recovery theorem (the skeptical reader can try a discretization argument to see this explicitly). Field theory can be done over a region of space (just by setting the appropriate region of integration) but is often done over all space. In (3.2.31), the Lagrangian is written as an integral of a function of the fields and

¹It is important that the order of differentiation be finite. A field evaluated at a shifted location can be written using a Taylor series as a series in the derivatives of the field at the unshifted location but with infinitely high order of differentiation. Thus, allowing infinitely many derivatives allows one to shift the point of evaluation to a different point in space, which is precisely what locality intends to avoid.

their derivatives to finite order at that point over all space. That function is called the **Lagrangian density** $\mathfrak{L}$:

$$\mathcal{L} = \int_{\mathbb{S}} \mathfrak{L}(\phi, \partial\phi, \partial^2\phi, \dots, \partial^N\phi) d^d\vec{x}. \quad (3.2.32)$$

As we see, the existence of the Lagrangian density is implied by locality. In principle, the Lagrangian density could also explicitly depend on t and $\vec{x}$ but because we generally assume time and space translational symmetry, they by definition do not appear explicitly in the equation of motion function. Then, they automatically do not appear in the Lagrangian density as constructed in (3.2.31). Thus, because of space and time translational symmetry, we take the Lagrangian density to not depend explicitly on t or $\vec{x}$.

In principle, the Lagrangian density can depend up to any order of differentiation on the fields. However, we will typically only have dependence on first derivatives. It can be understood why this is often a good approximation by looking at the Fourier transform of the fields with respect to their spatial variables:

$$\phi^a(t, \vec{x}) = \int_{\mathbb{K}} \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{d/2}} \tilde{\phi}^a(t, \vec{k}) d^d\vec{k} \quad (3.2.33)$$

where $\mathbb{K}$ is the $\mathbb{R}^d$ space of all values of $\vec{k}$. A spatial derivative of the field then pulls down a power of $\vec{k}$:

$$\nabla\phi^a(t, \vec{x}) = \int_{\mathbb{K}} \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{d/2}} i\vec{k}\tilde{\phi}^a(t, \vec{k}) d^d\vec{k}. \quad (3.2.34)$$

As well, each further spatial derivative pulls down another power:

$$\nabla^n\phi^a(t, \vec{x}) = \int_{\mathbb{K}} \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{d/2}} (i\vec{k})^n \tilde{\phi}^a(t, \vec{k}) d^d\vec{k}. \quad (3.2.35)$$

So, considering terms in the Lagrangian up to differentiation of order n is equivalent to a Taylor expansion in the wavenumber $\vec{k}$ to power n . It would then be a valid approximation to truncate our series and only consider a few orders of differentiation if the magnitude of the integrand is small except for small wavenumbers as for small values of k , k^n gets smaller with increasing n . Because the inverse Fourier transform of a function expresses that function as a linear combination of sines and cosines, we can see that the distance λ one must travel to complete one period of the basis sine or cosine (called the wavelength) would be the amount necessary to change the exponential argument by 2π . Thus, $|\vec{k}|\lambda = 2\pi$. The Fourier transform gives the coefficient of each basis sine/cosine in the inverse Fourier transform. Therefore, when the Fourier transform of a function has small magnitude for a particular value of $\vec{k}$, it means the original function hardly had any component which oscillated with that wavenumber. As such, the magnitude of the integrand being small except for small wavenumber is equivalent to the fields we consider only having significant contributions from small wavenumbers and correspondingly long wavelengths (because they are inversely related). Thus, keeping to a certain order of differentiation is essentially approximating our fields by their long distance/large scale behavior and may miss effects on short length scales. It is possible that we would need to include higher order derivative terms to account for these effects if they are found. The generalization of the equations in this section to include higher derivatives is straightforward using the techniques we have developed so far with 1.12, so we will not dwell on it. For now, we will assume we have made this approximation and only kept first derivatives in the Lagrangian density.

Note that the Lagrangian density is not uniquely defined, just as the original Lagrangian was not. As always, we can add an arbitrary total time derivative of a function which only depends on the initial and final values of the coordinates (which here would be the initial and final values of ϕ) to the Lagrangian. If we choose that time derivative to be an integral over all space of some function of the fields, then we see that:

$$\mathcal{L}' = \mathcal{L} + \frac{df}{dt}[\phi], \quad f = \int_{\mathbb{S}} F(\phi) d^d\vec{x} \implies \frac{df}{dt} = \int_{\mathbb{S}} \frac{dF}{dt} d^d\vec{x} \quad (3.2.36)$$

$$\implies \mathcal{L}' = \int_{\mathbb{S}} \left(\mathfrak{L} + \frac{dF}{dt} \right) d^d\vec{x} \implies \mathfrak{L}' = \mathfrak{L} + \frac{dF}{dt}. \quad (3.2.37)$$

Hence we can also add a time derivative at fixed position to the Lagrangian density arbitrarily. The reason this function F here was written only to depend on ϕ and not its derivatives is so that the terms it adds to the Lagrangian are only up to first derivative in ϕ . If one wanted to consider more derivatives on ϕ , one could correspondingly include derivatives of ϕ dependence in F . Regardless of what F depends on, it will not affect the equations of motion. There is one other way in which the Lagrangian density is not unique. Because it is defined as the volume integrand of the Lagrangian, we can add a term on the boundary of the

region of integration without affecting the variations on the interior. That is, we can define:

$$\mathcal{L}' = \mathcal{L} + \int_{\partial\mathbb{S}} \vec{F} \cdot d\vec{\mathbb{A}} \quad (3.2.38)$$

for an arbitrary vector field $\vec{F}$ on the boundary of the integration region. Because the surface term only depends on the fields on the boundary of the region of integration, it will not affect variations on the interior and thus will not affect the equations of motion on the interior. By the divergence theorem, the integral of a vector field on the boundary of a volume is given by the divergence of that vector field over the interior:

$$\int_{\partial\mathbb{V}} \vec{F} \cdot d\vec{\mathbb{A}} = \int_{\mathbb{V}} \nabla \cdot \vec{F} d\mathbb{S} \quad (3.2.39)$$

$$\implies \mathcal{L}' = \int_{\mathbb{S}} \mathfrak{L} d\mathbb{S} + \int_{\mathbb{S}} \nabla \cdot \vec{F} d\mathbb{S} = \int_{\mathbb{S}} (\mathfrak{L} + \nabla \cdot \vec{F}) d\mathbb{S} \quad (3.2.40)$$

$$\implies \mathfrak{L}' = \mathfrak{L} + \nabla \cdot \vec{F}. \quad (3.2.41)$$

Therefore, adding such a divergence term to our Lagrangian density will not affect the equations of motion. If one wants the terms added to the Lagrangian density to only have up to first derivatives with respect to space or time, then $\vec{F}$ should be chosen to depend on ϕ but not its derivatives (because it gets differentiated through the divergence). The Lagrangian is the integral of the Lagrangian density, just as the action is the integral of the Lagrangian. This divergence term is the analog of the $\frac{df}{dt}$ term; they both just result from the fundamental theorem of calculus. Adding a derivative to an integral only has an effect at the boundary (the end-points) which thus has no effect on variations of the interior (and so drops out of the equations of motion). Thus, overall we have the freedom to modify the Lagrangian density by:

$$\mathfrak{L} \simeq \mathfrak{L} + \nabla \cdot \vec{F} + \frac{df}{dt}. \quad (3.2.42)$$

Using (3.2.32), we can rewrite our equation of motion in (3.2.8).

$$\mathcal{L} = \int_{\mathbb{S}} \mathfrak{L}(\phi, \nabla\phi, \dot{\phi}) d\mathbb{S} \quad (3.2.43)$$

$$\implies \delta\mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial\mathfrak{L}}{\partial\phi^a} \delta\phi^a + \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \cdot \delta\nabla\phi^a + \frac{\partial\mathfrak{L}}{\partial\dot{\phi}^a} \delta\dot{\phi}^a \right) d\mathbb{S} \quad (3.2.44)$$

$$= \int_{\mathbb{S}} \left(\frac{\partial\mathfrak{L}}{\partial\phi^a} \delta\phi^a + \nabla \cdot \left(\frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \delta\phi^a \right) - \nabla \cdot \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \delta\phi^a + \frac{\partial\mathfrak{L}}{\partial\dot{\phi}^a} \delta\dot{\phi}^a \right) d\mathbb{S} \quad (3.2.45)$$

$$= \int_{\mathbb{S}} \left(\left(\frac{\partial\mathfrak{L}}{\partial\phi^a} - \nabla \cdot \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \right) \delta\phi^a + \frac{\partial\mathfrak{L}}{\partial\dot{\phi}^a} \delta\dot{\phi}^a \right) d\mathbb{S} + \int_{\partial\mathbb{S}} \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \delta\phi^a \cdot d\vec{\mathbb{A}}. \quad (3.2.46)$$

As always, we choose our variations $\delta\phi$ to be 0 at the boundary in a functional derivative and so we have (using (3.2.8)):

$$\frac{\delta\mathcal{L}}{\delta\phi^a} = \frac{\partial\mathfrak{L}}{\partial\phi^a} - \nabla \cdot \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} \quad (3.2.47)$$

$$\frac{\delta\mathcal{L}}{\delta\dot{\phi}^a} = \frac{\partial\mathfrak{L}}{\partial\dot{\phi}^a} \quad (3.2.48)$$

$$\implies \partial_t \frac{\partial\mathfrak{L}}{\partial\dot{\phi}^a} + \nabla \cdot \frac{\partial\mathfrak{L}}{\partial\nabla\phi^a} = \frac{\partial\mathfrak{L}}{\partial\phi^a}. \quad (3.2.49)$$

It is useful to point out that the calculation which led to (3.2.47) would apply to any functional $\mathcal{L}$ and its corresponding density $\mathfrak{L}$ which depends only on a field and its first derivative. If the theory is local, we also find that the Hamiltonian can be written as the integral of a Hamiltonian density:

$$\mathcal{H} = \int_{\mathbb{S}} \varphi_a \dot{\phi}^a d\mathbb{S} - \mathcal{L} = \int_{\mathbb{S}} (\varphi_a \dot{\phi}^a - \mathfrak{L}) d\mathbb{S} = \int_{\mathbb{S}} H d\mathbb{S} \implies H = \varphi_a \dot{\phi}^a - \mathfrak{L}. \quad (3.2.50)$$

Then, if the Hamiltonian density only depends up to first derivatives on the fields and conjugate momenta, the functional derivatives in Hamilton's equations become by recycling (3.2.47):

$$\frac{\delta\mathcal{H}}{\delta\phi^a} = \frac{\partial H}{\partial\phi^a} - \nabla \cdot \frac{\partial H}{\partial\nabla\phi^a} \quad (3.2.51)$$

$$\frac{\delta\mathcal{H}}{\delta\varphi_a} = \frac{\partial H}{\partial\varphi_a} - \nabla \cdot \frac{\partial H}{\partial\nabla\varphi_a} \quad (3.2.52)$$

This gives us:

Theorem 3.1: Equations of motion for Classical Field Theory

For a classical field theory with configuration $Q = \phi^a(t, \vec{x})$, the equations of motion are given in terms of the Action by:

$$\frac{\delta S}{\delta \phi^a(t, \vec{x})} = 0 \quad (3.2.53)$$

or in terms of the Lagrangian by:

$$\mathcal{L} = \frac{dS}{dt} \implies \frac{\delta \mathcal{L}}{\delta \phi^a} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\phi}^a} = 0 \quad (3.2.54)$$

or in terms of the Hamiltonian by:

$$\varphi_a = \frac{\delta \mathcal{L}}{\delta \dot{\phi}^a}, \quad \mathcal{H} = \int_{\mathbb{S}} \varphi_a \dot{\phi}^a d\mathbb{S} - \mathcal{L} \quad (3.2.55)$$

$$\implies \frac{\partial \phi^a}{\partial t} = \frac{\delta \mathcal{H}}{\delta \varphi_a} \quad (3.2.56)$$

$$\implies \frac{\partial \varphi_a}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi^a} \quad (3.2.57)$$

with Poisson bracket:

$$\{f, g\} = \int_{\mathbb{S}} \left(\frac{\delta f}{\delta \phi^a(\vec{x})} \frac{\delta g}{\delta \varphi_a(\vec{x})} - \frac{\delta g}{\delta \phi^a(\vec{x})} \frac{\delta f}{\delta \varphi_a(\vec{x})} \right) d\mathbb{S}. \quad (3.2.58)$$

If the theory is local, meaning the equations of motion depend on the fields and their derivatives to finite order of differentiation at a single point, then the Lagrangian can be written as the integral over all space of a Lagrangian density $\mathfrak{L}$ which depends on the fields and their derivatives at finite order of differentiation at a single point:

$$\mathcal{L} = \int_{\mathbb{S}} \mathfrak{L}(\phi, \partial \phi, \partial^2 \phi, \dots) d\mathbb{S}. \quad (3.2.59)$$

If the system has space and time translational symmetry then $\mathfrak{L}$ can be written so that it does not explicitly depend on $(t, \vec{x})$. Correspondingly, the Hamiltonian can be written as the integral over all space of a Hamiltonian density H through the Legendre transform:

$$H = \varphi_a \dot{\phi}^a - \mathfrak{L} \quad (3.2.60)$$

$$\mathcal{H} = \int_{\mathbb{S}} H d\mathbb{S}. \quad (3.2.61)$$

The Lagrangian density is only defined up to adding surface terms:

$$\mathfrak{L}' = \mathfrak{L} + \frac{df}{dt} + \nabla \cdot \vec{F}. \quad (3.2.62)$$

If the Lagrangian density only depends on the fields to first derivatives, then the equations of motion simplify to:

$$\partial_t \frac{\partial \mathfrak{L}}{\partial \dot{\phi}^a} + \nabla \cdot \frac{\partial \mathfrak{L}}{\partial \nabla \phi^a} = \frac{\partial \mathfrak{L}}{\partial \phi^a} \quad (3.2.63)$$

or, in terms of the Hamiltonian density, if it only depends on the fields up to first derivatives, to:

$$\frac{\partial \phi^a}{\partial t} = \frac{\partial H}{\partial \varphi_a} - \nabla \cdot \frac{\partial H}{\partial \nabla \varphi_a} \quad (3.2.64)$$

$$\frac{\partial \varphi_a}{\partial t} = -\frac{\partial H}{\partial \phi^a} + \nabla \cdot \frac{\partial H}{\partial \nabla \phi^a}. \quad (3.2.65)$$

We should be careful to note that the Lagrangian density only depending on the fields up to first order in differentiation and the Hamiltonian density only depending on the fields up to first order in differentiation are not the same condition. Due to the space derivatives that appear in the Legendre transformation relating $\dot{\phi}$ and φ , the number of spatial derivatives appearing the Hamiltonian or Lagrangian may not coincide.

Exercises

Problem 3.5: Verifying the Gauge Transformation of the Lagrangian Density. Verify by direction calculation, using the Euler-Lagrange equations of motion, that if the Lagrangian density is modified as $\mathfrak{L}' = \mathfrak{L} + \frac{df}{dt} + \nabla \cdot \vec{F}$ for functions $f(\phi, \nabla\phi)$ and $\vec{F}(\phi, \dot{\phi})$ then the equations motion given are entirely unchanged. Notice that the functions chosen here will actually introduce second derivative terms into the Lagrangian density. Be careful about how the presence of these second derivative terms affect the equations of motion.

Problem 3.6: The Wave Equation. Consider a field $\phi(t, x)$ in 1 spatial dimension with the following “classic” Lagrangian:

$$\mathcal{L} = \int_{-\infty}^{\infty} \left(\frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{v^2}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 \right) dx$$

where $v > 0$ is a constant.

- (a) Show that the corresponding equation of motion to this Lagrangian gives:

$$\frac{\partial^2 \phi}{\partial t^2} = v^2 \frac{\partial^2 \phi}{\partial x^2}.$$

This is called the (d'Alembert) wave equation.

- (b) Find the energy corresponding to this Lagrangian and show that it is conserved by the equations of motion.
 (c) Perform the Legendre transform to show that the Hamiltonian is given by:

$$\mathcal{H} = \int_{-\infty}^{\infty} \left(\frac{1}{2} \dot{\phi}^2 + \frac{v^2}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 \right) dx$$

and verify that Hamilton's equations reproduce the wave equation.

- (d) Make the change of variables $x_+ = x + vt$ and $x_- = x - vt$ with the chain rule to show that in these new coordinates the wave equation becomes:

$$\frac{\partial^2 \phi}{\partial x_+ \partial x_-} = 0.$$

- (e) Use the previous simplification to show that the solution to the wave equation is:

$$\phi(t, x) = f(x + vt) + g(x - vt)$$

where f and g are arbitrary functions determined by initial conditions. Thus, explain how the wave equation has left-moving solutions and right-moving solutions and that both solutions move exactly with speed v .

- (f) Evaluate ϕ and its time derivative at $t = 0$ to show that the initial conditions are related to f and g by:

$$\phi_0(x) = f(x) + g(x), \quad \dot{\phi}_0(x) = v f'(x) - v g'(x)$$

and solve these equations for $f(x)$ and $g(x)$ to find:

$$\begin{aligned} f(x) &= \frac{f(0) - g(0)}{2} + \frac{\phi_0(x)}{2} + \frac{1}{2v} \int_0^x \dot{\phi}_0(x') dx' \\ g(x) &= -\frac{f(0) - g(0)}{2} + \frac{\phi_0(x)}{2} - \frac{1}{2v} \int_0^x \dot{\phi}_0(x') dx'. \end{aligned}$$

Finally, use these to arrive at d'Alembert's formula:

$$\phi(t, x) = \frac{\phi_0(x + vt) + \phi_0(x - vt)}{2} + \frac{1}{2v} \int_{x-vt}^{x+vt} \dot{\phi}_0(x') dx.$$

Problem 3.7: ★ The Diffusion Equation. Consider a field $\phi(t, x)$ in 1 spatial dimension with the following “classic” Hamiltonian:

$$\mathcal{H} = \int_{-\infty}^{\infty} \kappa \varphi \frac{\partial^2 \phi}{\partial x^2} dx$$

where $\kappa > 0$ is called the diffusivity.

- (a) Show that the corresponding equation of motion to this Hamiltonian gives:

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2}.$$

This is called the diffusion equation. Show that this can be interpreted as a continuity equation with ϕ as the “charge density” and the current density given by:

$$J = -\kappa \frac{\partial \phi}{\partial x}.$$

Explain how this formula for the current density implies that for the diffusion equation the quantity ϕ “flows” from regions of high ϕ to regions of lower ϕ .

- (b) The partial derivative with respect to position measures the slope of a function in space. Thus, a crude summary measure of the total steepness of a function throughout space is:

$$S = \int_{-\infty}^{\infty} \left(\frac{\partial \phi}{\partial x} \right)^2 dx.$$

Show that this S is a strictly decreasing quantity in time under the diffusion equation for all ϕ which are not simply a spatial uniform constant and that it is exactly 0 if and only if ϕ is a spatially uniform constant. So, the diffusion equation “levels out” a function in time. Explain how this is consistent with the identification made about the current density made in the previous part.

- (c) Suppose $u(t, x)$ and $v(t, x)$ are both solutions to the diffusion equation with the same initial conditions $u(0, x) = v(0, x)$. Show that $w(t, x) = u(t, x) - v(t, x)$ is a solution to the diffusion equation with initial condition $w(0, x) = 0$ and use the result of the previous part to show in fact that $w(t, x) = 0$ for all time. From this conclude that $u(t, x) = v(t, x)$ and thus conclude the diffusion equation has unique solutions for given initial conditions.
- (d) Show that the quantity:

$$Q = \int_{-\infty}^{\infty} \phi(t, x) dx$$

is conserved by the diffusion equation. Explain how this is not surprising given the continuity equation identification made earlier.

- (e) Suppose that $\phi(t, x)$ solves the diffusion equation. Identify that if we want the function $\phi'(t, x) = \phi(\beta t, \alpha x)$ for positive constants α and β to solve the same diffusion equation then $\beta = \alpha^2$. Thus, from one solution $\phi(t, x)$ we can make a whole family of solutions to the diffusion equation which are related by scaling.
- (f) Suppose that we had a function $G(t, x)$ which solved the diffusion equation:

$$\frac{\partial G}{\partial t} = \kappa \frac{\partial^2 G}{\partial x^2}$$

with initial condition $G(0, x) = \delta(x)$. Such a function G is called the Green’s function or fundamental solution to the diffusion equation. Show then that the function:

$$\phi(t, x) = \int_{-\infty}^{\infty} \phi_0(x') G(t, x - x') dx'$$

solves the diffusion equation with initial condition $\phi(0, x) = \phi_0(x)$. Thus, (using uniqueness of solutions) if we know the Green’s function, we can automatically write down the solution to the diffusion equation for any initial conditions.

- (g) For our Green’s function above, define:

$$g(t, x) \stackrel{\text{def}}{=} \int_{-\infty}^x G(t, x') dx'.$$

Show that $g(t, x)$ satisfies the same diffusion equation but with the initial condition $g(0, x) = \vartheta(x)$.

- (h) Show that under the scaling transformation defined in (e) that $g(\alpha^2 t, \alpha x)$ satisfies the same diffusion equation with the same initial condition as g . Thus, explain why $g(\alpha^2 t, \alpha x) = g(t, x)$ for all $\alpha > 0$ using the uniqueness of solutions to the diffusion equation. Then, differentiate this conclusion with respect to α and evaluate at $\alpha = 1$ to derive:

$$2t \frac{\partial g}{\partial t}(t, x) + x \frac{\partial g}{\partial x}(t, x) = 0.$$

- (i) Reexpress the differential equation found in the previous part using the diffusion equation for g and replacing g by its expression in terms of G to show that G satisfies:

$$2t\kappa \frac{\partial G}{\partial x} + xG = 0.$$

Solve this differential equation to show that:

$$G(t, x) = N(t)e^{-\frac{x^2}{4\kappa t}}$$

for some to-be-determined coefficient $N(t)$.

- (j) Use the conservation law in (d) and the original definition of G to show that the coefficient $N(t)$ is:

$$N(t) = \frac{1}{I\sqrt{4\kappa t}}$$

where I is the number given by the Gaussian integral:

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx.$$

- (k) Consider the above integral I and square it, write the square as a double integral over $\mathbb{R}^2$ Cartesian coordinates, and then convert that double integral into polar coordinates. Show that the integral can be completed in polar coordinates to give:

$$I^2 = \pi.$$

- (l) Thus, finally show that the solution to the diffusion equation is:

$$\phi(t, x) = \int_{-\infty}^{\infty} \phi_0(x') \frac{e^{-\frac{(x-x')^2}{4\kappa t}}}{\sqrt{4\pi\kappa t}} dx'.$$

This solution has the very nice property that (1) for small t , $\phi(t, x)$ can be made arbitrarily close to the initial condition $\phi_0(0, x)$ and (2) for all $t > 0$, $\phi(t, x)$ is smooth and even real-analytic. Thus, diffusion is an excellent way to take extremely noisy and discontinuous data and make a completely smooth signal out of it without changing much of anything.

3.3 Accounting for Symmetries

Now that we know how to compute equations of motion for a field theory and believe that our field theory is local (and so it is defined by the Lagrangian density), it is time to find the possible Lagrangian densities for our theory. As we have discussed, the potentials are not uniquely defined because of the gauge transformation. This “gauge symmetry” just simply reflects that they are not uniquely defined as a set of variables because the Lagrangian itself is not uniquely defined. By the nature of the Lagrangian, the potentials automatically inherit gauge symmetry. As such, now that we are finding the Lagrangian density for the potentials, we must make sure it has this same symmetry. By equation (3.1.3) and (3.1.17), the total Lagrangian of the interacting theory is:

$$\mathcal{L} = \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + \mathcal{L}_{\text{int}} + \mathcal{L}_{\phi, \vec{A}}. \quad (3.3.1)$$

where the interaction term is given by:

$$\mathcal{L}_{\text{int}} = \int_{\mathbb{S}} \mathfrak{L}_{\text{int}} d\mathbb{S}, \quad \mathfrak{L}_{\text{int}} = \vec{J} \cdot \vec{A} - \rho \phi \quad (3.3.2)$$

and the currently undetermined $\mathcal{L}_{\phi, \vec{A}}$ takes the form:

$$\mathcal{L}_{\phi, \vec{A}} = \int_{\mathbb{S}} \mathfrak{L}_0(\phi, \vec{A}, \dot{\phi}, \nabla \phi, \dot{\vec{A}}, \nabla \vec{A}) d\mathbb{S} \quad (3.3.3)$$

for some undetermined function $\mathfrak{L}_0$. We do not take $\mathfrak{L}_0$ to have explicit t or $\vec{x}$ dependence due to time and space translational symmetries. In principle, $\mathfrak{L}_0$ could depend on higher derivatives of the potential as well as well but at the lowest order of approximation on long distances, these terms will not be present by the argument made in the previous section. Before trying to determine $\mathfrak{L}_0$ from symmetries, we first should study how the potentials transform under our various transformations of interest (translations, rotations, boosts).

3.3.1 Transformation Properties of the Potentials

When we transform the interaction term under some transformation under which the theory should have symmetry, we know we must have that for some surface terms:

$$\mathfrak{L}'_{\text{int}} = \mathfrak{L}_{\text{int}} + \frac{dF_0}{dt} + \nabla \cdot \vec{F} \implies \vec{J}' \cdot \vec{A}' - \rho' \phi' = \vec{J} \cdot \vec{A} - \rho \phi + \frac{dF_0}{dt} + \nabla \cdot \vec{F}. \quad (3.3.4)$$

All of the transformations we will use will happen to act linearly on $\rho, \vec{J}$ so that $\rho', \vec{J}'$ are made of linear combinations of $\rho, \vec{J}$. Thus, the left hand side above will be linear in ρ and $\vec{J}$. To match then, $\frac{dF_0}{dt} + \nabla \cdot \vec{F}$ must be linear in $\rho, \vec{J}$ as well (and not depend on the derivatives of $\rho, \vec{J}$). Because of this, $F_0, \vec{F}$ must depend on $\rho, \vec{J}$. However, if $F_0, \vec{F}$ do depend on $\rho, \vec{J}$ then generically their derivatives $\frac{dF_0}{dt}$ and $\nabla \cdot \vec{F}$ will depend on derivatives of $\rho, \vec{J}$. So, the contribution $\frac{dF_0}{dt} + \nabla \cdot \vec{F}$ will generically depend on derivatives of ρ and $\vec{J}$ unless the derivative dependence happens to cancel between these two terms. F_0 is only differentiated in time while $\vec{F}$ is only differentiated in space and so the only way they may cancel each other's derivative dependence is if a time derivative of $\rho, \vec{J}$ can be related to a spatial derivative of $\rho, \vec{J}$. There is precisely one such relation, the continuity equation. Thus, because F_0 is the piece that gets differentiated with respect to t and the t derivative must hit ρ and not $\vec{J}$ to get the continuity equation, F_0 must be proportional to ρ . Similarly, $\vec{F}$ must be proportional to $\vec{J}$ and the proportionalities must be such that the derivatives on $\rho, \vec{J}$ cancel when the continuity equation is applied. This is only possible if for some function λ :

$$F_0 = \lambda(t, \vec{x}) \rho, \quad \vec{F} = \lambda(t, \vec{x}) \vec{J} \quad (3.3.5)$$

$$\implies \vec{J}' \cdot \vec{A}' - \rho' \phi' = \vec{J} \cdot (\vec{A} + \nabla \lambda) - \rho \left(\phi - \frac{\partial \lambda}{\partial t} \right). \quad (3.3.6)$$

Hence, under any symmetry transformation which acts linearly on $\rho, \vec{J}$ the interaction term can only transform by applying a gauge transformation to the potentials. Let T be whatever symmetry transformation was applied above and which had the effect of performing this gauge transformation by λ . Because we always demand gauge symmetry, we can define a new transformation T^* which is T followed by a gauge transformation by $-\lambda$ so that it cancels the gauge transformation of the potentials above. Then, under this T^* transformation the theory must also have symmetry because the theory has symmetry under both T and gauge transformations.

So, we can treat T^* as the transformation of interest and under that transformation we always have:

$$\vec{J}' \cdot \vec{A}' - \rho' \phi' = \vec{J} \cdot \vec{A} - \rho \phi \implies \mathfrak{L}'_{\text{int}} = \mathfrak{L}_{\text{int}} \quad (3.3.7)$$

with no surfaces terms added. Thus, for the rest of our symmetry transformations of the potentials **we can take the interaction term to be invariant under that transformation by definition.**

From our expression for the interaction term in the Lagrangian density, observe that:

$$\phi = -\frac{\partial \mathfrak{L}_{\text{int}}}{\partial \rho} \quad A_a = \frac{\partial \mathfrak{L}_{\text{int}}}{\partial J^a}. \quad (3.3.8)$$

This allows us to fruitfully apply the chain rule to see how ϕ and $\vec{A}$ transform when ρ and $\vec{J}$ are transformed by using that $\mathfrak{L}_{\text{int}}$ is invariant under the symmetry transformation:

$$\phi' = -\frac{\partial \mathfrak{L}'_{\text{int}}}{\partial \rho'} = -\frac{\partial \rho}{\partial \rho'} \frac{\partial \mathfrak{L}_{\text{int}}}{\partial \rho} - \frac{\partial J^a}{\partial \rho'} \frac{\partial \mathfrak{L}_{\text{int}}}{\partial J^a} = \frac{\partial \rho}{\partial \rho'} \phi - \frac{\partial \vec{J}}{\partial \rho'} \cdot \vec{A} \quad (3.3.9)$$

$$A'_a = \frac{\partial \mathfrak{L}'_{\text{int}}}{\partial J'^a} = \frac{\partial \rho}{\partial J'^a} \frac{\partial \mathfrak{L}_{\text{int}}}{\partial \rho} + \frac{\partial J^b}{\partial J'^a} \frac{\partial \mathfrak{L}_{\text{int}}}{\partial J^b} = -\frac{\partial \rho}{\partial J'^a} \phi + \frac{\partial J^b}{\partial J'^a} A_b. \quad (3.3.10)$$

Hence we only need how the charge and current densities change to compute how the potentials change. Then, because $\vec{E}$ and $\vec{B}$ are given by definition as:

$$\vec{E} = -\nabla \phi - \frac{\partial \vec{A}}{\partial t}, \quad \vec{B} = \nabla \times \vec{A} \quad (3.3.11)$$

we only need how the potentials and differential operators change to compute how $\vec{E}$ and $\vec{B}$ change. The transformation laws of the differential operators are just given by the chain rule. Under a coordinate change $\vec{x}' = \vec{x}'(t, \vec{x})$ and $t' = t'(t, \vec{x})$:

$$\frac{\partial}{\partial t'} = \frac{\partial t}{\partial t'} \frac{\partial}{\partial t} + \frac{\partial \vec{x}}{\partial t'} \cdot \nabla = \frac{\partial t}{\partial t'} \frac{\partial}{\partial t} + \frac{\partial \vec{x}}{\partial t'} \cdot \nabla \quad (3.3.12)$$

$$\nabla'_a = \frac{\partial}{\partial x'^a} = \frac{\partial t}{\partial x'^a} \frac{\partial}{\partial t} + \frac{\partial x^b}{\partial x'^a} \frac{\partial}{\partial x^b} = (\nabla'_a t) \frac{\partial}{\partial t} + \frac{\partial x^b}{\partial x'^a} \nabla_b. \quad (3.3.13)$$

Then, the transformation properties of $\vec{E}$ and $\vec{B}$ will always by definition be given by:

$$\vec{E}' = -\nabla' \phi' - \frac{\partial \vec{A}'}{\partial t'}, \quad \vec{B}' = \nabla' \times \vec{A}'. \quad (3.3.14)$$

3.3.2 Gauge Symmetry

First of course we need to ensure that our theory has symmetry under the gauge transformation inherent in the formulation of the potentials:

$$\phi' = \phi - \frac{\partial \chi}{\partial t}, \quad \vec{A}' = \vec{A} + \nabla \chi \quad (3.3.15)$$

where $\chi(t, \vec{x})$ is an arbitrary differentiable function. Because the equations of motion must have gauge symmetry and a symmetry of the equations of motion must leave them unchanged, the equation of motion functions for the potentials must be gauge invariant. The full list of gauge invariants are the $\vec{E}$ and $\vec{B}$ fields. If we consider a Lagrangian density which is up through first derivatives in the potentials, the equations of motion will have up through second derivatives on the potentials. The $\vec{E}$ and $\vec{B}$ fields are already first derivatives of the potentials, and so the equations of motion will have up through first derivatives of $\vec{E}$ and $\vec{B}$. So, let F_ϕ and F_A^a be the equation of motion functions of ϕ and $\vec{A}$ according to $\mathfrak{L}_0$:

$$F_\phi(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}) = \frac{\partial \mathfrak{L}_0}{\partial \phi} - \partial_a \frac{\partial \mathfrak{L}_0}{\partial \partial_a \phi} - \partial_t \frac{\partial \mathfrak{L}_0}{\partial \dot{\phi}} \quad (3.3.16)$$

$$F_A^a(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}) = \frac{\partial \mathfrak{L}_0}{\partial A_a} - \partial_b \frac{\partial \mathfrak{L}_0}{\partial \partial_b A_a} - \partial_t \frac{\partial \mathfrak{L}_0}{\partial \dot{A}_a} \quad (3.3.17)$$

where we have started using the notation:

$$\partial_t = \frac{\partial}{\partial t}, \quad \partial_a = \frac{\partial}{\partial x^a}. \quad (3.3.18)$$

The equation of motion functions do not depend on $t, \vec{x}$ directly due to time translational symmetry and space translational symmetry. By equation (3.2.31), from the equation of motion functions we can take the

Lagrangian density:

$$\mathfrak{L}_0 = \phi G_\phi(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}) + A_a G_A^a(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}). \quad (3.3.19)$$

where we have defined the functions G_ϕ and G_A^a by:

$$G_\phi(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}) = \int_0^1 F_\phi(\lambda \vec{E}, \lambda \vec{B}, \lambda \dot{\vec{E}}, \lambda \dot{\vec{B}}, \lambda \nabla \vec{E}, \lambda \nabla \vec{B}) d\lambda \quad (3.3.20)$$

$$G_A^a(\vec{E}, \vec{B}, \dot{\vec{E}}, \dot{\vec{B}}, \nabla \vec{E}, \nabla \vec{B}) = \int_0^1 F_A^a(\lambda \vec{E}, \lambda \vec{B}, \lambda \dot{\vec{E}}, \lambda \dot{\vec{B}}, \lambda \nabla \vec{E}, \lambda \nabla \vec{B}) d\lambda. \quad (3.3.21)$$

The integral structure over λ from (3.4.18) only goes through so nicely from the potentials to the fields because the fields depend linearly on the potentials. The form (3.3.19) now has a very mild apparent gauge dependence. Under gauge transformation we see:

$$\mathfrak{L}'_0 \simeq \mathfrak{L}_0 + \chi(t, \vec{x}) \left(\frac{\partial G_\phi}{\partial t} - \partial_a G_A^a \right). \quad (3.3.22)$$

Because χ is an arbitrary function, in order for this additional pieces to be a surface term, we must have:

$$\frac{\partial G_\phi}{\partial t} = \frac{\partial G_A^a}{\partial x^a}. \quad (3.3.23)$$

This identity must hold without applying the equations of motion for the Lagrangian density to have gauge symmetry.

In addition to expanding $\mathfrak{L}_0$ in numbers of derivatives acting on the potentials, we will also series expand in powers of the fields, which is typical the approach in field theory for practicality's sake. Naturally, such a Taylor expansion we would expect to be valid for “weak fields” meaning that the fields and their derivatives are not too large. The larger they are, the more terms are necessary to get a good approximation. Applying this, we Taylor expand G_ϕ and G_A^a through linear order and take that expansion as their form:

$$G_\phi = a + \vec{\mathfrak{t}} \cdot \vec{E} + \vec{\mathfrak{c}} \cdot \vec{B} + \vec{\mathfrak{d}} \cdot \dot{\vec{E}} + \vec{\mathfrak{e}} \cdot \dot{\vec{B}} + \mathfrak{f}^{ab} \partial_a E_b + \mathfrak{g}^{ab} \partial_a B_b, \quad (3.3.24)$$

$$G_A^a = \mathfrak{h}^a + \mathfrak{i}^{ab} E_b + \mathfrak{j}^{ab} B_b + \mathfrak{k}^{ab} \dot{E}_b + \mathfrak{l}^{ab} \dot{B}_b + \mathfrak{m}^{abc} \partial_b E_c + \mathfrak{n}^{abc} \partial_b B_c \quad (3.3.25)$$

where $a, \dots, n$ (with appropriate indices) are some constants. We can now put these into (3.3.23) and reexpress $\vec{E}$ and $\vec{B}$ in terms of the potentials. Doing so gives:

$$\begin{aligned} & -\mathfrak{t}^a \partial_a \phi - \mathfrak{t}^a \dot{A}_a + (\epsilon^{abc} \mathfrak{c}_c + \mathfrak{i}^{ab}) \partial_a \dot{A}_b + \mathfrak{i}^{ab} \partial_{ab}^2 \phi - \mathfrak{j}^{ab} \epsilon_b{}^{cd} \partial_{ac}^2 A_d - \mathfrak{d}^a \partial_a \ddot{\phi} - \mathfrak{d}^a \ddot{A}_a + (\epsilon^{abc} \mathfrak{e}_c - \mathfrak{f}^{ab} + \mathfrak{k}^{ab}) \partial_a \ddot{A}_b \\ & + (\mathfrak{k}^{ab} - \mathfrak{f}^{ab}) \partial_{ab}^2 \dot{\phi} + (\mathfrak{m}^{abc} + (\mathfrak{g}^{ad} - \mathfrak{l}^{ad}) \epsilon_d{}^{bc}) \partial_{ab}^2 \dot{A}_c + \mathfrak{m}^{abc} \partial_{abc}^3 \phi - \mathfrak{n}^{abc} \epsilon_c{}^{de} \partial_{abd}^3 A_e = 0. \end{aligned} \quad (3.3.26)$$

Because this must hold for all field configurations, we can simplify this enormously by considering particular potentials which isolated singular terms. Consider:

$$\phi = x^a, \quad \vec{A} = 0 \quad \implies \mathfrak{t}^a = 0 \quad (3.3.27)$$

$$\phi = 0, \quad \vec{A} = tx^a \vec{t}_b \quad \implies \mathfrak{i}^{ab} = -\epsilon^{abc} \mathfrak{c}_c \quad (3.3.28)$$

$$\phi = 0, \quad \vec{A} = tx^a x^b \vec{t}_c \quad \implies \mathfrak{j}^{ad} \epsilon_d{}^{bc} + \mathfrak{j}^{bd} \epsilon_d{}^{ac} = 0 \quad (3.3.29)$$

$$\phi = t^2 x^a, \quad \vec{A} = 0 \quad \implies \mathfrak{d}^a = 0 \quad (3.3.30)$$

$$\phi = 0, \quad \vec{A} = t^2 x^a \vec{t}_b \quad \implies \mathfrak{k}^{ab} = \mathfrak{f}^{ab} - \epsilon^{abc} \mathfrak{e}_c \quad (3.3.31)$$

$$\phi = 0, \quad \vec{A} = tx^a x^b \vec{t}_c \quad \implies \mathfrak{m}^{abc} + \mathfrak{m}^{bac} + (\mathfrak{g}^{ad} - \mathfrak{l}^{ad}) \epsilon_d{}^{bc} + (\mathfrak{g}^{bd} - \mathfrak{l}^{bd}) \epsilon_d{}^{ac} = 0 \quad (3.3.32)$$

$$\begin{aligned} \phi = 0, \quad \vec{A} = x^a x^b x^c \vec{t}_d \quad \implies & \mathfrak{n}^{abe} \epsilon_e{}^{cd} + \mathfrak{n}^{bae} \epsilon_e{}^{cd} + \mathfrak{n}^{bce} \epsilon_e{}^{ad} \\ & + \mathfrak{n}^{cbe} \epsilon_e{}^{ad} + \mathfrak{n}^{cae} \epsilon_e{}^{bd} + \mathfrak{n}^{ace} \epsilon_e{}^{bd} = 0. \end{aligned} \quad (3.3.33)$$

If these conditions vanish then automatically the rest of (3.3.26) is satisfied. We can simplify a few a these conditions further. Contract the condition on $\mathfrak{j}^{ab}$ with ϵ_{bce} and use the double Levi-Civita identity. After simplifying, we find:

$$\mathfrak{j}^{ab} = \frac{1}{3} \mathfrak{j}^c{}_c \delta^{ab} = \kappa \delta^{ab} \quad (3.3.34)$$

where we defined the constant κ . Define the coefficients $\mathfrak{o}^{ab}$ by:

$$\mathfrak{o}^{ab} = \frac{1}{2} \mathfrak{m}^{cda} \epsilon^b{}_{cd}. \quad (3.3.35)$$

Then, using the double Levi-Civita identity:

$$\mathbf{m}^{abc} - \mathbf{m}^{bac} = 2\mathfrak{o}^{cd}\epsilon_d^{ab}. \quad (3.3.36)$$

With this and the condition on $\mathbf{m}^{abc}$, we have:

$$\mathbf{m}^{abc} = \mathfrak{o}^{cd}\epsilon_d^{ab} - \frac{1}{2}(\mathfrak{g}^{ad} - \ell^{ad})\epsilon_d^{bc} - \frac{1}{2}(\mathfrak{g}^{bd} - \ell^{bd})\epsilon_d^{ac} \quad (3.3.37)$$

Contract the condition on $\mathbf{n}^{abc}$ with ϵ_{cde} and use the double Levi-Civita identity. After simplifying, we find:

$$\mathbf{n}^{abc} + \mathbf{n}^{bac} = \frac{1}{4}(\mathbf{n}^{ad} + \mathbf{n}^{da})\delta^{bc} + \frac{1}{4}(\mathbf{n}^{bd} + \mathbf{n}^{db})\delta^{ac}. \quad (3.3.38)$$

Define the coefficients $\mathbf{p}^a$:

$$\mathbf{p}^a = \frac{1}{8}(\mathbf{n}^{ab}{}_b + \mathbf{n}^{ba}{}_b) \quad (3.3.39)$$

and the coefficients $\mathbf{q}^{ab}$:

$$\mathbf{q}^{ab} = \frac{1}{2}\mathbf{n}^{cda}\epsilon_{cd}^b. \quad (3.3.40)$$

With these, we can rewrite $\mathbf{n}^{abc}$ as:

$$\mathbf{n}^{abc} = \mathbf{q}^{cd}\epsilon_d^{ab} + \mathbf{p}^a\delta^{bc} + \mathbf{p}^b\delta^{ac}. \quad (3.3.41)$$

With our simplifications on the coefficients together, the G_ϕ and G_A^a simplify to:

$$G_\phi = \alpha + \vec{\mathfrak{c}} \cdot \vec{B} + \vec{\mathfrak{e}} \cdot \dot{\vec{B}} + \mathfrak{f}^{ab}\partial_a E_b + \mathfrak{g}^{ab}\partial_a B_b \quad (3.3.42)$$

$$\begin{aligned} G_A^a &= \mathfrak{h}^a + (\vec{\mathfrak{c}} \times \vec{E})^a + \kappa B^a + \mathfrak{f}^{ab}\dot{E}_b + (\vec{\mathfrak{e}} \times \dot{\vec{E}})^a + \ell^{ab}\dot{B}_b + \mathfrak{o}^{cd}\epsilon_d^{ab}\partial_b E_c \\ &\quad - \frac{1}{2}(\mathfrak{g}^{ad} - \ell^{ad})(\nabla \times \vec{E})_d - \frac{1}{2}(\mathfrak{g}^{bd} - \ell^{bd})\epsilon_d^{ac}\partial_b E_c + \mathbf{q}^{cd}\epsilon_d^{ab}\partial_b B_c + \mathbf{p}^b\partial_b B^a. \end{aligned} \quad (3.3.43)$$

Now we take these and return them to the Lagrangian density. Again simplifying, we find:

$$\mathfrak{L}_0 = \alpha\phi + \vec{\mathfrak{h}} \cdot \vec{A} + \phi\vec{\mathfrak{c}} \cdot \vec{B} + \vec{\mathfrak{c}} \cdot (\vec{E} \times \vec{A}) + \kappa\vec{A} \cdot \vec{B} + \mathfrak{f}^{ab}E_a E_b + \left(\mathfrak{o}^{ab} + \frac{1}{2}(\mathfrak{g}^{ab} + \ell^{ab}) \right) E_a B_b + \mathbf{q}^{ab}B_a B_b. \quad (3.3.44)$$

There is nothing special about the parameter names we have used so far, and so to avoid having our parameters be random letters from throughout the alphabet, let us rename them. Through quadratic order in the potentials, gauge invariance requires that the Lagrangian density of the potentials takes the form:

$$\mathfrak{L}_0 = \alpha\phi + \vec{\mathfrak{b}} \cdot \vec{A} + \phi\vec{\mathfrak{c}} \cdot \vec{B} + \vec{\mathfrak{c}} \cdot (\vec{E} \times \vec{A}) + \mathfrak{d}\vec{A} \cdot \vec{B} + \mathfrak{e}^{ab}E_a E_b + \mathfrak{f}^{ab}E_a B_b + \mathfrak{g}^{ab}B_a B_b \quad (3.3.45)$$

for some arbitrary constants $\alpha, \mathfrak{b}^a, \mathfrak{c}^a, \mathfrak{d}, \mathfrak{e}^{ab}, \mathfrak{f}^{ab}, \mathfrak{g}^{ab}$. This is the form we will use going forward.

3.3.3 Rotational Symmetry

Now we will enforce rotational symmetry on the theory of the potentials. We found in (3.3.9) and (3.3.10) how the potentials transform under a linear transformation of the charge and current densities. So, let us now specialize that result to rotations. Under a rotation by rotation matrix $\hat{R}$:

$$t' = t, \quad \vec{x}'_n = \hat{R}\vec{x}_n \implies \dot{\vec{x}}'_n = \hat{R}\dot{\vec{x}}_n. \quad (3.3.46)$$

Recall the expressions for the charge and current densities in terms of the charges and positions of point particles:

$$\rho = \sum_{n=1}^N q_n \delta(\vec{x} - \vec{x}_n), \quad \vec{J} = \sum_{n=1}^N q_n \dot{\vec{x}}_n \delta(\vec{x} - \vec{x}_n). \quad (3.3.47)$$

Then, the charge density changes by:

$$\rho'(t', \vec{x}') = \sum_{n=1}^N q_n \delta(\vec{x}' - \vec{x}'_n) = \sum_{n=1}^N q_n \delta(\hat{R}\vec{x} - \hat{R}\vec{x}_n). \quad (3.3.48)$$

Using the scaling property of the Dirac delta:

$$\delta(\hat{R}\vec{x} - \hat{R}\vec{x}_n) = \delta(\hat{R}(\vec{x} - \vec{x}_n)) = \frac{\delta(\vec{x} - \vec{x}_n)}{|\det \hat{R}|} = \delta(\vec{x} - \vec{x}_n) \quad (3.3.49)$$

where in the last step we have used that the determinant of any rotation matrix is 1. Thus:

$$\rho'(t', \vec{x}') = \rho(t, \vec{x}). \quad (3.3.50)$$

Similarly calculating for the current density:

$$\vec{J}'(t', \vec{x}') = \hat{R}\vec{J}(t, \vec{x}). \quad (3.3.51)$$

Now applying this to the potentials:

$$\phi'(t', \vec{x}') = \phi(t, \vec{x}), \quad \vec{A}'(t', \vec{x}') = \hat{R}\vec{A}(t, \vec{x}). \quad (3.3.52)$$

So, ϕ is unchanged by a rotation (which is why it is called a scalar) and $\vec{A}$ rotates like a displacement (which is why it is called a vector). By the chain rule, the differential operators change as:

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t}, \quad \nabla' = \hat{R}\nabla. \quad (3.3.53)$$

Thus, under a rotation $\vec{E}$ and $\vec{B}$ transform as:

$$\vec{E}' = \hat{R}\vec{E}, \quad \vec{B}' = \hat{R}\vec{B}. \quad (3.3.54)$$

Hence, both $\vec{E}$ and $\vec{B}$ are genuine vector fields in that they rotate like displacements under a rotation. Rotating everything in the Lagrangian density then, we find:

$$\begin{aligned} \mathcal{L}'_0 = \mathcal{L}_0 &+ (\hat{R}^{-1}\vec{\mathfrak{e}} - \vec{\mathfrak{e}}) \cdot \vec{A} + (\hat{R}^{-1}\vec{\mathfrak{c}} - \vec{\mathfrak{c}}) \cdot (\phi\vec{B} + \vec{E} \times \vec{A}) + (\epsilon^{cd}R_c^a R_d^b - e^{ab})E_a E_b \\ &+ (\mathfrak{f}^{cd}R_c^a R_d^b - \mathfrak{f}^{ab})E_a B_b + (\mathfrak{g}^{cd}R_c^a R_d^b - \mathfrak{g}^{ab})B_a B_b. \end{aligned} \quad (3.3.55)$$

Demanding this to be a symmetry will then require that for some functions $f_0(\phi, \vec{A})$ and $\vec{f}(\phi, \vec{A})$ the above matches the original Lagrangian density up to boundary terms:

$$\mathcal{L}'_0 \stackrel{!}{=} \mathcal{L}_0 + \frac{df_0}{dt} + \nabla \cdot \vec{f} = \mathcal{L}_0 + \frac{\partial f_0}{\partial t} + \frac{\partial f_0}{\partial \phi} \dot{\phi} + \frac{\partial f_0}{\partial \vec{A}} \cdot \dot{\vec{A}} + \frac{\partial f^a}{\partial x^a} + \frac{\partial \vec{f}}{\partial \phi} \cdot \nabla \phi + \frac{\partial f^a}{\partial A_b} \partial_a A_b. \quad (3.3.56)$$

The given variable dependencies for f_0 and $\vec{f}$ were chosen so that they would produce no second derivative terms in the Lagrangian (because those terms are not already present to cancel on either side). Altogether then, putting all the terms on the same side of the equals sign, we have:

$$\begin{aligned} 0 = &(\hat{R}^{-1}\vec{\mathfrak{e}} - \vec{\mathfrak{e}}) \cdot \vec{A} + (\hat{R}^{-1}\vec{\mathfrak{c}} - \vec{\mathfrak{c}}) \cdot (\phi\vec{B} + \vec{E} \times \vec{A}) + (\epsilon^{cd}R_c^a R_d^b - e^{ab})E_a E_b \\ &+ (\mathfrak{f}^{cd}R_c^a R_d^b - \mathfrak{f}^{ab})E_a B_b + (\mathfrak{g}^{cd}R_c^a R_d^b - \mathfrak{g}^{ab})B_a B_b - \frac{\partial f_0}{\partial \phi} \dot{\phi} - \frac{\partial f_0}{\partial \vec{A}} \cdot \dot{\vec{A}} - \frac{\partial \vec{f}}{\partial \phi} \cdot \nabla \phi - \frac{\partial f^a}{\partial A_b} \partial_a A_b. \end{aligned} \quad (3.3.57)$$

This must hold for all field configurations. Thus, the terms of each type (meaning each particular combination of fields and derivatives) must cancel and must do so for any field value. Matching the terms without any field derivatives:

$$\vec{\mathfrak{e}} = \hat{R}\vec{\mathfrak{e}}. \quad (3.3.58)$$

Therefore, $\vec{\mathfrak{e}}$ must be a vector which is unchanged by all rotations. The only such vector is the 0 vector:

$$\vec{\mathfrak{e}} = 0. \quad (3.3.59)$$

Matching the $\partial_a \phi \partial_b \phi$ terms (which happen to only appear in the form of $E_a E_b$):

$$e^{ab} = R^a_c R^b_d e^{cd}. \quad (3.3.60)$$

So, e^{ab} viewed as the components of a matrix must form a matrix which is unchanged by all rotations. As proven in problem 2.7, this means it must be proportional to the identity matrix. So, for some coefficient ϵ :

$$e^{ab} = \frac{\epsilon}{2} \delta^{ab}. \quad (3.3.61)$$

Matching the $\partial_a \phi \partial_b A_c$ terms (which happen to only appear in the form of $E_a B_b$):

$$\mathfrak{f}^{ab} = R^a_c R^b_d \mathfrak{f}^{cd}. \quad (3.3.62)$$

Again, $\mathfrak{f}^{ab}$ are the components of a rotationally invariant matrix, meaning that for some coefficient θ :

$$\mathfrak{f}^{ab} = \theta \delta^{ab}. \quad (3.3.63)$$

Matching the $\partial_a A_b \partial_c A_d$ terms (which happen to only appear in the form of $B_a B_b$):

$$\mathfrak{g}^{ab} = R^a_c R^b_d \mathfrak{g}^{cd}. \quad (3.3.64)$$

We have yet another rotationally invariant matrix, and so for some coefficient μ :

$$g^{ab} = -\frac{\mu}{2}\delta^{ab}. \quad (3.3.65)$$

Matching the remaining $\dot{\vec{A}}$ terms:

$$\frac{\partial f_0}{\partial A_a} = \epsilon^{abc}(\hat{R}^{-1}\vec{c} - \vec{c})_b A_c. \quad (3.3.66)$$

Differentiating this with respect to A_b , we have:

$$\frac{\partial^2 f_0}{\partial A_a \partial A_b} = -\epsilon^{abc}(\hat{R}^{-1}\vec{c} - \vec{c})_c. \quad (3.3.67)$$

The left hand side is symmetric under exchanging a and b while the right hand side is antisymmetric under the same exchange. This is only possible if both sides are 0. Thus:

$$\vec{c} = \hat{R}\vec{c}. \quad (3.3.68)$$

So, $\vec{c}$ has to be a rotationally invariant vector, forcing it to be 0:

$$\vec{c} = 0. \quad (3.3.69)$$

This leaves no term more to match and we can just take $\vec{f} = 0$.

After all of this matching and renaming $\alpha = \rho_0$ and $d = \frac{\kappa}{2}$, we have that rotational symmetry puts our Lagrangian density into the form:

$$\mathcal{L}_0 = \rho_0\phi + \frac{\kappa}{2}\vec{A} \cdot \vec{B} + \frac{\epsilon}{2}|\vec{E}|^2 + \theta\vec{E} \cdot \vec{B} - \frac{\mu}{2}|\vec{B}|^2. \quad (3.3.70)$$

It looks like we have 5 independent terms, but it turns out that the θ term is a total derivative. By a bit of pushing derivatives around:

$$2\vec{E} \cdot \vec{B} = -\frac{\partial}{\partial t}(\vec{A} \cdot \vec{B}) - \nabla \cdot (\phi\vec{B} + \vec{E} \times \vec{A}). \quad (3.3.71)$$

Because this term is a total derivative, it doesn't contribute to the equations of motion. Thus, after totally requiring gauge invariance and rotationally symmetry, our lowest order Lagrangian density becomes:

$$\mathcal{L}_0 = \rho_0\phi + \frac{\kappa}{2}\vec{A} \cdot \vec{B} + \frac{\epsilon}{2}|\vec{E}|^2 - \frac{1}{2\mu}|\vec{B}|^2 \quad (3.3.72)$$

where ρ_0 , κ , ϵ , and μ are currently undetermined constants. The names chosen for these coefficients may be suggestive to readers familiar with electromagnetism.

3.3.4 Galilean Boost Symmetry

We can repeat all the same steps for Galilean boosts and it will be much simpler now that our Lagrangian density is so reduced. Under a Galilean boost:

$$t' = t, \quad \vec{x}'_n = \vec{x}_n + \vec{v}t \implies \dot{\vec{x}}'_n = \dot{\vec{x}}_n + \vec{v}. \quad (3.3.73)$$

Thus, the charge and current densities change as:

$$\rho'(t', \vec{x}') = \rho(t, \vec{x}), \quad \vec{J}'(t', \vec{x}') = \vec{J}(t, \vec{x}) + \rho(t, \vec{x})\vec{v}. \quad (3.3.74)$$

We can now use this to compute that the potentials transform as:

$$\phi' = \phi + \vec{v} \cdot \vec{A}, \quad \vec{A}' = \vec{A}. \quad (3.3.75)$$

The chain rule gives the transformation of the differential operators:

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t} - \vec{v} \cdot \nabla, \quad \nabla' = \nabla. \quad (3.3.76)$$

Finally computing the transformations of the fields:

$$\vec{E}' = \vec{E} - \vec{v} \times \vec{B}, \quad \vec{B}' = \vec{B} \quad (3.3.77)$$

Then, under the boost, the Lagrangian density changes as:

$$\mathcal{L}'_0 = \mathcal{L}_0 + \rho_0\vec{v} \cdot \vec{A} + \epsilon\vec{v} \cdot (\vec{E} \times \vec{B}) + \mathcal{O}(v^2). \quad (3.3.78)$$

In order for this to be a symmetry, the added terms must be removable by surface terms (at each order in $\vec{v}$):

$$\rho_0\vec{v} \cdot \vec{A} + \epsilon\vec{v} \cdot (\vec{E} \times \vec{B}) = \frac{df_0}{dt} + \nabla \cdot \vec{f}. \quad (3.3.79)$$

However, $\vec{E} \times \vec{B} = -\nabla\phi \times (\nabla \times \vec{A}) - \dot{\vec{A}} \times (\nabla \times \vec{A})$ and so the left hand side here contains $\partial_a\phi\partial_b A_c$ terms. The general surface terms which get added cannot produce a $\partial_a\phi\partial_b A_c$ term without adding other higher derivative terms which are not present. Therefore, the only way the $\vec{E} \times \vec{B}$ term can be a surface term for all field configurations is if its coefficient is 0:

$$\epsilon = 0. \quad (3.3.80)$$

Similarly, there is no way to produce the ρ_0 term without also including $\vec{A}$ dependence in the surface term. However, doing so would then produce $\dot{\vec{A}}$ or $\partial_b A_c$ terms which are not present. Hence, ρ_0 must vanish as well:

$$\rho_0 = 0. \quad (3.3.81)$$

Then, we have that the lowest order Lagrangian density for this theory must be:

$$\mathfrak{L}_0 = \frac{\kappa}{2} \vec{A} \cdot \vec{B} - \frac{1}{2\mu} |\vec{B}|^2. \quad (3.3.82)$$

However, there is one tricky other possibility. The above reasoning is true if it is required to hold for all field configurations. However, if $\vec{B}$ is identically 0, then $\vec{A}$ is actually a gradient:

$$\vec{B} = \nabla \times \vec{A} = 0 \implies \exists \chi : \vec{A} = \nabla \chi. \quad (3.3.83)$$

Under such a condition, the added terms under the transformation become:

$$\rho_0 \vec{v} \cdot \nabla \chi + 0 = \nabla \cdot (\rho_0 \vec{v} \chi). \quad (3.3.84)$$

Thus, the ρ_0 and ϵ terms are actually allowed in the special case that $\vec{B}$ is required to be 0. Consequently, we have a second possible Lagrangian density, valid for a theory in which $\vec{B} = 0$:

$$\boxed{\mathfrak{L}_0 = \rho_0 \phi + \frac{\epsilon}{2} |\vec{E}|^2.} \quad (3.3.85)$$

We are left with two distinct theories to study the predictions of, (3.3.82) and (3.3.85).

3.3.5 Parity Symmetry

There is one final symmetry which we haven't yet discussed but which is observed in Galilean mechanics: parity symmetry. Parity, or spatial inversion, is the transformation of sending all positions $\vec{x}$ to $-\vec{x}$. In three dimensions, rotating by 180° about a fixed axis inverts both axes perpendicular to the fixed axis. Mirroring or reflecting about a single axis inverts that axis only. Therefore, in three dimensions, mirroring about a fixed axis and then rotating by 180° about that axis is equivalent to a parity transformation. Because we have already assumed rotational symmetry, parity symmetry then is equivalent to additionally requiring mirror/reflection symmetry. So, assuming parity symmetry for us is the same as assuming that any experiment which you could do directly would also give the same apparent result in a mirror (if the appropriate mirrored setup was made in the experiment). That is, parity symmetry assumes that for any physical process which is possible, its mirrored image is also possible (meaning consistent with the equations of motion for appropriately mirrored initial conditions). At a pedestrian level, "left and right obey exactly the same rules". Again, by the prejudice of day to day experience we believe this to be true and so we will take parity symmetry as an assumption for our Galilean theory.

Assumption :: GCMIV: Parity Symmetry

Isolated systems have parity symmetry.

Under parity transformation the charge and current densities change as:

$$\rho'(t', \vec{x}') = \sum_{n=1}^N q_n \delta(\vec{x}' - \vec{x}'_n) = \sum_{n=1}^N q_n \delta(-\vec{x} + \vec{x}_n) = \rho(t, \vec{x}) \quad (3.3.86)$$

$$\vec{J}'(t', \vec{x}') = \sum_{n=1}^N q_n \dot{\vec{x}}'_n \delta(\vec{x}' - \vec{x}'_n) = \sum_{n=1}^N q_n (-\dot{\vec{x}}_n) \delta(\vec{x} - \vec{x}_n) = -\vec{J}(t, \vec{x}). \quad (3.3.87)$$

Then the potentials become:

$$\phi' = \phi, \quad \vec{A}' = -\vec{A} \quad (3.3.88)$$

As well, the derivative operators become:

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t}, \quad \nabla' = -\nabla. \quad (3.3.89)$$

Then, the electric and magnetic fields become:

$$\vec{E}' = -\vec{E}, \quad \vec{B}' = \vec{B}. \quad (3.3.90)$$

Applying the parity transformation to the Lagrangian density in (3.3.85):

$$\mathcal{L}'_0 = \mathcal{L}_0 \quad (3.3.91)$$

automatically and so this Lagrangian density already has parity symmetry. Now let us apply the parity transformation to (3.3.82):

$$\mathcal{L}'_0 = \mathcal{L}_0 - \kappa \vec{A} \cdot \vec{B}. \quad (3.3.92)$$

In order for parity to be a symmetry of (3.3.82), $\kappa \vec{A} \cdot \vec{B} = \kappa \vec{A} \cdot (\nabla \times \vec{A})$ must be a surface term. We have already found that in general it is not a surface term (otherwise it would have already been removed). It only becomes a surface term if $\kappa = 0$, and so it must be to have parity symmetry. Enforcing parity symmetry on (3.3.82) we have:

$$\boxed{\mathcal{L}_0 = -\frac{|\vec{B}|^2}{2\mu}}. \quad (3.3.93)$$

This will be the final form of our Galilean theory² in the context in which $\vec{B} \neq 0$.

Exercises

Problem 3.8: Equations of Motion

- (a) Find the equations of motion corresponding to (3.3.85) with consideration of the interaction term:

$$\mathcal{L} = (\rho_0 - \rho)\phi + \vec{J} \cdot \vec{A} + \frac{\epsilon}{2} |\vec{E}|^2.$$

- (b) Find the equation of motion corresponding to (3.3.82) with consideration of the interaction term:

$$\mathcal{L} = \frac{\kappa}{2} \vec{A} \cdot \vec{B} - \frac{|\vec{B}|^2}{2\mu} + \vec{J} \cdot \vec{A} - \rho\phi.$$

- (c) Show by explicit calculation that the equation of motion from the previous part does not have parity symmetry unless $\kappa = 0$.
 (d) Show, by explicitly computing its contribution to the equations of motion, that if a Lagrangian density is modified by:

$$\mathcal{L}' = \mathcal{L} + \theta \vec{E} \cdot \vec{B}$$

then its equations of motion are unchanged for constant θ .

²There are circumstances where it is interesting to not believe in parity symmetry and to include the κ term. That term, called the Chern-Simons term, does have some specialized applications in modern physics. It (and some terms like it in theories we will consider later) can arise naturally in effective theories. However, experiments indicate that when viewing the full theory Lagrangian for the potentials, the appropriate value of κ is $\kappa = 0$.

3.4 Gauss' Law

Of our two possible lowest order theories, let us first study equation (3.3.85), which is called the scalar theory. Then, the Lagrangian for the potentials experiencing charge and current densities is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\vec{E}|^2 + \vec{J} \cdot \vec{A} + (\rho_0 - \rho)\phi \right) d\mathbb{S} \quad (3.4.1)$$

Let us find the Euler-Lagrange equation of motion for the scalar potential ϕ :

$$\frac{\delta \mathcal{L}}{\delta \phi} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\phi}} = 0. \quad (3.4.2)$$

For the moment let us work without referring to our specific Lagrangian density so that we can have a general result for use later. In principle, the Lagrangian density can depend on ϕ directly or through $\vec{E}$ (which by definition is an expression depending of ϕ). So, under a variation of ϕ :

$$\delta \mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}}{\partial \vec{E}} \cdot \delta \vec{E} \right) d\mathbb{S}. \quad (3.4.3)$$

By the definition of $\vec{E}$, under a variation of ϕ :

$$\vec{E} = -\nabla \phi - \dot{\vec{A}} \implies \delta \vec{E} = -\nabla \delta \phi. \quad (3.4.4)$$

Then, the variation of the Lagrangian becomes:

$$\delta \mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \phi} + \left(\nabla \cdot \frac{\partial \mathcal{L}}{\partial \vec{E}} \right) \right) \delta \phi d\mathbb{S} - \int_{\partial \mathbb{S}} \frac{\partial \mathcal{L}}{\partial \vec{E}} \delta \phi \cdot d\vec{\mathbb{A}}. \quad (3.4.5)$$

By taking the variation $\delta \phi$ only on the interior of the integration region (meaning we consider variations that are 0 on the boundary) we can drop the boundary term. If we considering variations on all space, what we mean by “variations on the interior” is really just variations which go to 0 sufficiently quickly so that the surface term is 0. That is, for a ball $\mathbb{B}$ of radius R centered at $\vec{x}$, we require our variations $\delta \phi$ to satisfy:

$$\lim_{R \rightarrow \infty} \int_{\partial \mathbb{B}(\vec{x}, R)} \frac{\partial \mathcal{L}}{\partial \vec{E}} \delta \phi \cdot d\vec{\mathbb{A}} = 0. \quad (3.4.6)$$

We then have:

$$\frac{\delta \mathcal{L}}{\delta \phi} = \frac{\partial \mathcal{L}}{\partial \phi} + \nabla \cdot \frac{\partial \mathcal{L}}{\partial \vec{E}}, \quad \frac{\delta \mathcal{L}}{\delta \dot{\phi}} = 0. \quad (3.4.7)$$

With this, the Euler-Lagrange equation becomes:

$$\frac{\partial \mathcal{L}}{\partial \phi} + \nabla \cdot \frac{\partial \mathcal{L}}{\partial \vec{E}} = 0. \quad (3.4.8)$$

For our specific Lagrangian (3.4.1), this gives:

$$\nabla \cdot \vec{E}(t, \vec{x}) = \frac{\rho(t, \vec{x}) - \rho_0}{\epsilon}. \quad (3.4.9)$$

One can now see why I have named the constant parameter ρ_0 as such as it is the value of the charge density at which this differential equation just becomes the homogeneous equation $\nabla \cdot \vec{E} = 0$. However, there is a subtle issue in this equation. Consider the case in which there is no charge density anywhere in space and the potentials are left completely on their own. Then, $\rho = 0$ and this equation becomes:

$$\nabla \cdot \vec{E} = -\frac{\rho_0}{\epsilon}. \quad (3.4.10)$$

The absence of charge density or anything else means we are just considering empty space and thus by our belief in rotational symmetry and translational symmetry, this solution, call it $\vec{E}_0$ should share those symmetries. Under a rotation we found $\vec{E}$ transforms as a vector:

$$\vec{E}'_0 = \hat{R} \vec{E}_0. \quad (3.4.11)$$

Requiring rotational symmetry then demands:

$$\vec{E}'_0 \stackrel{!}{=} \vec{E}_0 \implies \hat{R} \vec{E}_0 = \vec{E}_0. \quad (3.4.12)$$

However, the only rotationally invariant vector is the zero vector. Thus, requiring empty space to have rotational symmetry gives:

$$\vec{E}_0 = 0 \implies \nabla \cdot \vec{E}_0 = 0 \implies \rho_0 = 0. \quad (3.4.13)$$

We must take $\rho_0 = 0$ in order to preserve the rotational symmetry of empty space. One can alternatively find that ρ_0 must be 0 in order to preserve the translational symmetry of empty space. Because of translational symmetry, $\vec{E}_0$ must not depend on position. Consequently, its spatial derivatives are 0 and again we find $\rho_0 = 0$ ³. Then, our theory actually reduces to:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\vec{E}|^2 + \vec{J} \cdot \vec{A} - \rho\phi \right) d\mathbb{S} \quad (3.4.14)$$

$$\implies \boxed{\nabla \cdot \vec{E} = \frac{\rho}{\epsilon}} \quad (3.4.15)$$

Equation (3.4.15) is called **Gauss' Law** and as we see it is the lowest order possible equation of motion in the scalar theory. We could go on to find the equation of motion for $\vec{A}$. However, recall that we can only use this theory when $\vec{B} = 0$ as only then is it consistent with our boost symmetry. This restriction allows us to write the vector potential as a gradient:

$$\vec{B} = \nabla \times \vec{A} = 0 \implies \exists f : \vec{A} = \nabla f. \quad (3.4.16)$$

Then, by gauge transformation, we can transform $\vec{A}$ to be 0 everywhere (choose $-f$ as your gauge function to do it). Then, in this gauge:

$$\vec{E} = -\nabla\phi \quad (3.4.17)$$

and the only dynamical variable left is ϕ , which is why this is called the Galilean *scalar* theory. This gauge condition is a holonomic constraint on $\vec{A}$, so we can substitute it directly into the Lagrangian:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla\phi|^2 - \rho\phi \right) d\mathbb{S}. \quad (3.4.18)$$

This gauge fixing is called the **electrostatic gauge** and importantly it only exists (can be done) when $\nabla \times \vec{A} = 0$. As well, the gauge condition $\vec{A} = 0$ does not completely eliminate the gauge freedom. In principle, ϕ is still undefined up to a gauge function which depends on t only (as then $\nabla f(t) = 0$ and so $\vec{A}$ remains 0 under such a transformation). By theorem 2.14, (3.4.18) should give the same equation of motion for ϕ as (3.4.14). A short calculation gives:

$$-\nabla^2\phi = \frac{\rho}{\epsilon}. \quad (3.4.19)$$

This is precisely Gauss' law by using that in electrostatic gauge. Equation (3.4.19) written in terms of the potential is a classic differential equation known as the **Poisson equation** and as we see it is the equation of motion for the lowest order of Galilean scalar theory. It turns out that because this equation is linear and has so many symmetries, we can solve it exactly.

3.4.1 Solving the Poisson Equation

Consider functions $\phi(\vec{x})$ and $\eta(\vec{x})$ (the analog of $\frac{\rho}{\epsilon}$) so that ϕ satisfies the Poisson equation with η as its “source”:

$$-\nabla^2\phi(\vec{x}) = \eta(\vec{x}). \quad (3.4.20)$$

The motivation for this renaming of symbols will be so that we can replace ϕ and η with different symbols in different contexts as the solution to this problem will be useful multiple times. Then, define the Green's function $G(\vec{x}, \vec{x}')$ as the solution of ϕ when η is a “point-source” located at the position $\vec{x}'$. That is, by $G(\vec{x}, \vec{x}')$

³All of this points to a subtle issue we will return to in Part II. When we assume that a symmetry exists for a theory we also often assume that there exists at least one solution of the system which shares that symmetry. This is a stronger requirement. Equations of motion having a symmetry means there is a transformation which takes solutions to solutions. A particular solution having a symmetry means that we assume that there is a transformation which takes solutions to solutions that also takes that particular solution to itself. The reason we tend to assume this stronger requirement is that if we observe a symmetry in “empty space” then not only must the equations of motion have that symmetry but the “empty space” also has to have that symmetry. If it did not we would not have observed the symmetry experimentally to begin with. Here we can see that the Lagrangian density has rotational and translational symmetry but there are no solutions which have either symmetry unless $\rho_0 = 0$. If we allow $\rho_0 \neq 0$ then because $\vec{E}_0$ will be non-zero, it will effectively select a preferred direction and origin within space thus effectively breaking rotational and translational symmetry for our other variables. If ρ_0 was not 0, effective theories produced from this theory would not inherit the translational and rotational symmetries that we observe. When the equations of motion of a theory have a symmetry but no solutions of those equations have that symmetry, the symmetry is said to be “spontaneously broken”.

is defined so that:

$$-\nabla'^2 G(\vec{x}, \vec{x}') = \delta(\vec{x} - \vec{x}') \quad (3.4.21)$$

where ∇' indicates differentiation with respect to $\vec{x}'$. Notice that G is only defined up to adding to it a function $f(\vec{x}, \vec{x}')$ such that $\nabla'^2 f = 0$. Then, by direct calculation:

$$\nabla' \cdot (\phi(\vec{x}') \nabla' G(\vec{x}, \vec{x}') - G(\vec{x}, \vec{x}') \nabla' \phi(\vec{x}')) = \phi \nabla'^2 G - G \nabla'^2 \phi \quad (3.4.22)$$

$$= -\phi(\vec{x}') \delta(\vec{x} - \vec{x}') + G(\vec{x}, \vec{x}') \eta(\vec{x}'). \quad (3.4.23)$$

$$\implies \int_{\partial \mathbb{V}} (\phi \nabla' G - G \nabla' \phi) \cdot d\vec{\mathbb{A}} = -\phi(\vec{x}) + \int_{\mathbb{V}} G(\vec{x}, \vec{x}') \eta(\vec{x}') d\mathbb{S}'. \quad (3.4.24)$$

In going to (3.4.24) we have assumed $\vec{x}$ is in the region $\mathbb{V}$. Thus, solving for $\phi(\vec{x})$ we have:

$$\phi(\vec{x}) = \int_{\mathbb{V}} G(\vec{x}, \vec{x}') \eta(\vec{x}') d\mathbb{S}' + \int_{\partial \mathbb{V}} (G(\vec{x}, \vec{x}') \nabla' \phi(\vec{x}') - \phi(\vec{x}') \nabla' G(\vec{x}, \vec{x}')) \cdot d\vec{\mathbb{A}} \quad (3.4.25)$$

So, if we have the Green's function then the function ϕ in a volume is given by this formula in terms of η within the volume and the values of ϕ and $\nabla \phi$ on the boundary of the volume. As we found, the Green's function is not uniquely defined. The Green's function of interest is generally dictated by the boundary conditions of interest for the relevant problem. We will not have much to say about different common choices of Green's function (Dirichlet, Von Neumann, Robin) but it should be noted that different choices may make a particular problem more or less easily solved.

There is a Green's function of particular interest for solving the Poisson equation on all of space. Let $G_0(\vec{x}, \vec{x}')$ be the potential $\phi(\vec{x}')$ produced by a point charge of charge ϵ at location $\vec{x}$. We can find this Green's function by construction. Because the physical scenario has translational symmetry under shifting the position of the source $\vec{x}$ and the point at which the potential is evaluated $\vec{x}'$, we have:

$$G_0(\vec{x} + \vec{\epsilon}, \vec{x}' + \vec{\epsilon}) = G_0(\vec{x}, \vec{x}'). \quad (3.4.26)$$

Consequently:

$$G_0(\vec{x}, \vec{x}') = G_0(\vec{x} + (-\vec{x}), \vec{x}' + (-\vec{x})) = G_0(0, \vec{x}' - \vec{x}) = G_0(\vec{x}' - \vec{x}) \quad (3.4.27)$$

where in the last step we introduce a common abuse of notation because G_0 only depends on the difference $\vec{x}' - \vec{x}$. Similarly, a point charge has rotational symmetry about rotations treating the location of that point as the origin. Thus G_0 should have rotational symmetry and so must satisfy:

$$G_0(\hat{R}(\vec{x}' - \vec{x})) = G_0(\vec{x}' - \vec{x}). \quad (3.4.28)$$

Because of this, G_0 can only depend on properties of $\vec{x}' - \vec{x}$ which are rotationally invariant. The only such property is the magnitude $|\vec{x}' - \vec{x}|$ because any two vectors of the same magnitude can be rotated into each other. Thus, furthering our abuse of notation:

$$G_0(\vec{x}, \vec{x}') = G_0(|\vec{x} - \vec{x}'|). \quad (3.4.29)$$

With these requirements we can explicitly compute G_0 by starting with the Poisson equation and recalling that it should be the solution when the charge density is set to $\rho(\vec{x}') = \epsilon \delta(\vec{x} - \vec{x}')$:

$$-\nabla'^2 G_0 = \delta(\vec{x} - \vec{x}'). \quad (3.4.30)$$

Thus G_0 is in fact a Green's function. Now integrate both sides over a ball of radius R centered at $\vec{x}$, $\mathbb{B}(\vec{x}, R)$, and use the divergence theorem:

$$-\int_{\mathbb{B}(\vec{x}, R)} \nabla'^2 G_0(\vec{x}, \vec{x}') d\mathbb{S}' = \int_{\mathbb{B}(\vec{x}, R)} \delta(\vec{x} - \vec{x}') d\mathbb{S}' \quad (3.4.31)$$

$$\implies -\int_{\partial \mathbb{B}(\vec{x}, R)} \nabla' G_0(\vec{x}, \vec{x}') \cdot d\vec{\mathbb{A}}' = 1. \quad (3.4.32)$$

Because G_0 only depends on $r' = |\vec{x} - \vec{x}'|$:

$$\nabla' G_0(\vec{x}, \vec{x}') = \nabla' G_0(r') = \frac{\partial G_0}{\partial r'} \nabla' r' = \frac{\partial G_0}{\partial r'} \vec{n} \quad (3.4.33)$$

where $\vec{n}$ is the outward pointing unit vector from $\vec{x}$ to $\vec{x}'$. As well, $d\vec{\mathbb{A}}' = d\mathbb{A}' \vec{n}$ and so:

$$\int_{\partial \mathbb{B}(\vec{x}, R)} \nabla' G_0(\vec{x}, \vec{x}') \cdot d\vec{\mathbb{A}}' = \int_{\partial \mathbb{B}(\vec{x}, R)} \frac{\partial G_0}{\partial r'}(R) \vec{n} \cdot \vec{n} d\mathbb{A} = \frac{\partial G_0}{\partial r'}(R) \int_{\partial \mathbb{B}(\vec{x}, R)} d\mathbb{A} = 4\pi R^2 \frac{\partial G_0}{\partial r'}(R). \quad (3.4.34)$$

Then, (3.4.32) becomes:

$$-4\pi R^2 \frac{\partial G_0}{\partial r'}(R) = 1. \quad (3.4.35)$$

Because this is true for all $R > 0$, we can replace it by r' and integrate:

$$-4\pi r'^2 \frac{\partial G_0}{\partial r'} = 1 \implies \frac{\partial G_0}{\partial r'} = -\frac{1}{4\pi r'^2} \implies G_0(r') = \frac{1}{4\pi r'} + C. \quad (3.4.36)$$

Here C is just an integration constant. We define G_0 to be the Green's function which goes to 0 at large r and so we take $C = 0$ by definition (if $C \neq 0$ then there is a gauge transformation which sets $C' = 0$ by taking the gauge function $-Ct$). Then, we have:

$$G_0 = \frac{1}{4\pi r'} = \frac{1}{4\pi |\vec{x} - \vec{x}'|}. \quad (3.4.37)$$

Now let us return to (3.4.25). That equation holds for any Green's function on the region $\mathbb{V}$. We would like to take $\mathbb{V}$ to be all of space. In order to do so carefully we really have to take $\mathbb{V}$ to be a very large region and take the limit that that region becomes all of space. For calculations it is nicest to take $\mathbb{V}$ to be a ball of radius R centered at the origin and to take $R \rightarrow \infty$ at the end. The Green's function we will use is G_0 . Explicitly evaluating (3.4.25) using G_0 and spherical coordinates yields:

$$\phi(\vec{x}) = \int_{\mathbb{V}} \frac{\eta(\vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d^3\vec{x}' + \int_0^\pi \int_0^{2\pi} \left(\frac{R \frac{\partial \phi}{\partial r}(R, \theta', \varphi')}{\sqrt{1 - 2 \frac{\vec{x} \cdot \vec{x}'}{R} + \frac{|\vec{x}|^2}{R^2}}} + \frac{\left(1 - \frac{\vec{x} \cdot \vec{x}'}{R}\right) \phi(R, \theta', \varphi')}{\left(1 - 2 \frac{\vec{x} \cdot \vec{x}'}{R} + \frac{|\vec{x}|^2}{R^2}\right)^{\frac{3}{2}}} \right) \frac{\sin \theta'}{4\pi} d\theta' d\varphi' \quad (3.4.38)$$

In order to evaluate this further we need to understand how ϕ and $\nabla \phi$ behave on the boundary of $\mathbb{V}$, in this case the sphere of radius R .

When using the Poisson equation we are generally interested in solutions which are due to charged distributions that are only in a finite region of space and which have finite charge⁴. Because we want our theory to be local, we demand that the effect of any localized charge distribution on any other such distributions goes to 0 when the separation between the distributions goes to infinity. The interaction term in the Lagrangian for a charge due to ϕ is given by $q\phi$; this means that ϕ should go to a constant as one gets arbitrarily far away from any charges so that this interaction term becomes just a surface term that can be removed from the Lagrangian in the limit of large separation. We take this as a boundary condition. That is, we require:

$$\lim_{|\vec{x}| \rightarrow \infty} \phi(\vec{x}) = C \text{ is finite} \quad (3.4.39)$$

for the scalar potential produced by a localized charge distribution. We can use the gauge freedom remaining in the definition of ϕ to choose the gauge function $-Ct$ so that instead ϕ limits to 0 as $|\vec{x}|$ limits to infinity. Requiring the total charge of the distribution to be finite requires from Gauss' law:

$$q = \int_{\mathbb{S}} \rho d\mathbb{S} = \epsilon \int_{\mathbb{S}} \nabla \cdot \vec{E} d\mathbb{S} = -\epsilon \int_{\partial \mathbb{S}} \nabla \phi \cdot d\vec{\mathbb{A}} = \text{finite} \quad (3.4.40)$$

$$\implies \lim_{R \rightarrow \infty} R^2 \frac{\partial}{\partial R} \int_0^\pi \int_0^{2\pi} \phi(R, \theta, \varphi) \sin \theta d\theta d\varphi = \text{finite}. \quad (3.4.41)$$

So, we require that for some functions $\psi_0(\theta, \varphi)$ and $\psi_1(r, \theta, \varphi)$:

$$\frac{\partial \phi}{\partial r}(r, \theta, \varphi) = \frac{\psi_0(\theta, \varphi) + \psi_1(r, \theta, \varphi)}{r^2} \quad (3.4.42)$$

where:

$$\lim_{r \rightarrow \infty} \psi_1(r, \theta, \varphi) = 0. \quad (3.4.43)$$

Then, it immediately follows that:

$$\lim_{r \rightarrow \infty} r \frac{\partial \phi}{\partial r}(r, \theta, \varphi) = 0. \quad (3.4.44)$$

⁴Later we will consider some systems which have infinity extending charge distributions. These are highly unrealistic models which are under some certain limited appropriate circumstances reasonable idealizations of some real systems, at least in describing some of their basic properties. However, it should be clear that these are just toys for understanding some ideas and not scenarios you could build in a lab. No infinitely extending line of charge has ever been built, nor does it make sense as a real physical distribution of charge.

With these as boundary conditions we can take the $R \rightarrow \infty$ limit of (3.4.38) and notice that the surface integrals disappear in that limit. Thus, the potential produced by a localized distribution η is:

$$\phi(\vec{x}) = \int_{\mathbb{S}} \frac{\eta(\vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.4.45)$$

This result is known as **Coulomb's Law** and as we see it gives us the solution to the Poisson equation on all space assuming our potential decays to 0 at large distances. Thus we have:

Theorem 3.2: Solution of Poisson's Equation

The solution $\phi(\vec{x})$ for a given $\eta(\vec{x})$ to the equation:

$$-\nabla^2 \phi = \eta \quad (3.4.46)$$

in a region $\mathbb{V}$ is given by

$$\phi(\vec{x}) = \int_{\mathbb{V}} \eta(\vec{x}') G(\vec{x}, \vec{x}') d\mathbb{S}' + \int_{\partial\mathbb{V}} (G(\vec{x}, \vec{x}') \nabla' \phi(\vec{x}') - \phi(\vec{x}') \nabla' G(\vec{x}, \vec{x}')) \cdot d\vec{\mathbb{A}}' \quad (3.4.47)$$

where $G(\vec{x}, \vec{x}') = \frac{1}{4\pi|\vec{x} - \vec{x}'|} + f(\vec{x}, \vec{x}')$ for f any function satisfying $\nabla'^2 f = 0$ for all $\vec{x}, \vec{x}'$ in $\mathbb{V}$. If $\mathbb{V}$ is taken to be all of space and ϕ is required to decay to 0 at large distances then:

$$\phi(\vec{x}) = \int_{\mathbb{S}} \frac{\eta(\vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.4.48)$$

It is interesting to note that although we only placed loose requirements on the behavior of ϕ at spatial infinity, we can make a much stronger statement now. If η is a localized distribution then outside of a finite volume $\mathbb{V}_\eta$, it is 0. Then, we can analyze the large $r = |\vec{x}|$ behavior of the potential it produces:

$$\phi(\vec{x}) = \int_{\mathbb{V}_\eta} \frac{\eta(\vec{x}')}{4\pi\sqrt{r^2 - 2r\vec{r} \cdot \vec{x}' + |\vec{x}'|^2}} d^3\vec{x}' = \frac{1}{4\pi r} \int_{\mathbb{V}_\eta} \eta(\vec{x}') d^3\vec{x}' + \mathcal{O}\left(\frac{1}{r^2}\right). \quad (3.4.49)$$

Thus, actually the potential of any localized charge distribution decays like $\frac{1}{r}$ or faster when very far away. With some mathematical effort, we can loosen the requirement that the source distribution should be 0 outside of a finite region to a weaker statement that sufficiently far away it should decay suitably quickly so that its integral over all space exists and is finite.

3.4.2 Effective Equations of Motion

Applying the Poisson's equation solution to (3.4.19), we have:

$$\phi(t, \vec{x}) = \int_{\mathbb{S}} \frac{\rho(t, \vec{x}')}{4\pi\epsilon|\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.4.50)$$

Now that we have solved for the scalar potential in terms of the distribution of particles, we can put it back into the equations of motion for the particles to see how particles react in response to the potential in the scalar theory. Recalling the relationship between the charge density and the point particles, for N point particles we have:

$$\phi(t, \vec{x}) = \int_{\mathbb{S}} \frac{\sum_{n=1}^N q_n \delta(\vec{x}' - \vec{x}_n(t))}{4\pi\epsilon|\vec{x} - \vec{x}'|} d\mathbb{S}' = \sum_{n=1}^N \frac{q_n}{4\pi\epsilon|\vec{x} - \vec{x}_n(t)|}. \quad (3.4.51)$$

Then, the $\vec{E}$ field produced by the particles is:

$$\vec{E} = -\nabla\phi = \sum_{n=1}^N \frac{q_n}{4\pi\epsilon} \frac{\vec{x} - \vec{x}_n(t)}{|\vec{x} - \vec{x}_n(t)|^3}. \quad (3.4.52)$$

Finally putting this into the equation of motion for the particles (equation (2.6.12)) and recalling that $\vec{B} = 0$:

$$m_n \ddot{\vec{x}}_n = q_n \vec{E}(t, \vec{x}_n) = q_n \sum_{k=1}^N \frac{q_k}{4\pi\epsilon} \frac{\vec{x}_n - \vec{x}_k}{|\vec{x}_n - \vec{x}_k|^3}. \quad (3.4.53)$$

We see an immediate problem whenever $n = k$: that term of the sum is just simply not well-defined. What is going on? This is actually the first sign that there is something fundamentally wrong with the idea of point

particles, but for now we can delay that issue. Instead of considering exactly point like particles, we consider the particles to be smeared out over a region of finite non-zero size. We will show that the smoothened theory has a well behaved point limit.

The only problematic term in (3.4.53) is the “self-force” term, meaning the term $n = k$. To analyze the problem more properly, let us instead consider the motion of a charge distribution with density $\rho(t, \vec{x})$ and current density $\vec{J}(t, \vec{x})$. After studying general well-behaved distributions, we will take the limit that we squeeze the distributions down to being point-like. We found in problem 2.19 that the force due to potentials on a charge q is given by the Lorentz force law. In the scalar theory $\vec{B} = 0$ and so the total force due to the scalar potential on a charge distribution M then is given by integrating this over the full distribution:

$$\vec{F} = \int_M \vec{E} dq = \int_S \rho(t, \vec{x}) \vec{E}(t, \vec{x}) d^3 \vec{x} = - \int_S \rho(t, \vec{x}) \nabla \phi(t, \vec{x}) d^3 \vec{x}. \quad (3.4.54)$$

It is useful to divide the potential ϕ into a part ϕ_{self} which is the potential due to the distribution M and a remainder ϕ_{ext} which is the potential due to everything else (this is possible because of the linearity of solutions to the Poisson equation):

$$\phi(t, \vec{x}) = \phi_{\text{self}}(t, \vec{x}) + \phi_{\text{ext}}(t, \vec{x}). \quad (3.4.55)$$

Because ϕ_{self} is the potential due to the distribution, it is defined to satisfy:

$$-\nabla^2 \phi_{\text{self}} = \rho(t, \vec{x}) \quad (3.4.56)$$

where ρ on the right hand side is the distribution of just the charge distribution under consideration (there may be other charges outside of this distribution and they are excluded from the meaning of ρ here). Using the solution to the Poisson equation, in particular we take:

$$\phi_{\text{self}}(t, \vec{x}) = \int_S \frac{\rho(t, \vec{x}')}{4\pi\epsilon|\vec{x} - \vec{x}'|} d^3 \vec{x}'. \quad (3.4.57)$$

Because the external potential ϕ_{ext} is due to everything but ρ , it is independent of $\rho(t, \vec{x})$. We can then decompose the total force on the distribution into a “self-force” and an “external force”:

$$\vec{F}_{\text{self}} = - \int_S \rho \nabla \phi_{\text{self}} d^3 \vec{x}, \quad \vec{F}_{\text{ext}} = - \int_S \rho \nabla \phi_{\text{ext}} d^3 \vec{x} \implies \vec{F} = \vec{F}_{\text{self}} + \vec{F}_{\text{ext}}. \quad (3.4.58)$$

We can compute the first term using the solution to the Poisson equation:

$$\vec{F}_{\text{self}} = - \int_S \rho(t, \vec{x}) \nabla \int_S \frac{\rho(t, \vec{x}')}{4\pi\epsilon|\vec{x} - \vec{x}'|} d^3 \vec{x}' d^3 \vec{x} = \int_S \int_S \rho(t, \vec{x}) \rho(t, \vec{x}') \frac{\vec{x} - \vec{x}'}{4\pi\epsilon|\vec{x} - \vec{x}'|^3} d^3 \vec{x} d^3 \vec{x}'. \quad (3.4.59)$$

If we swap the names of the integration variables we find that the self-force is equal to its own negative:

$$\vec{F}_{\text{self}} = \int_S \int_S \rho(t, \vec{x}) \rho(t, \vec{x}') \frac{\vec{x}' - \vec{x}}{4\pi\epsilon|\vec{x} - \vec{x}'|^3} d^3 \vec{x} d^3 \vec{x}' = -\vec{F}_{\text{self}} \quad (3.4.60)$$

$$\implies \vec{F}_{\text{self}} = 0. \quad (3.4.61)$$

The in the Galilean theory, **the total force of any charge distribution on itself is 0**. All that is left then is the contribution from the external potential:

$$\vec{F} = - \int_S \rho \nabla \phi_{\text{ext}} d^3 \vec{x}. \quad (3.4.62)$$

This has a completely well behaved point limit. ρ approaches a Dirac delta centered at the point charge and ϕ_{ext} , being independent of the charge distribution ρ , is unchanged during the limit. So, in the limit we shrink the distribution ρ down to a point charge of charge q :

$$\vec{F} = -q \nabla \phi_{\text{ext}}(t, \vec{x}(t)) = q \vec{E}_{\text{ext}}(t, \vec{x}(t)). \quad (3.4.63)$$

If we smoothen out the point particle at all, the effect of that charge on itself is 0. Then, using this appropriately smoothened Lorentz force, the equation of motion becomes:

$$m \ddot{\vec{x}} = q \vec{E}_{\text{ext}}(t, \vec{x}(t)). \quad (3.4.64)$$

If we consider particle n is a system of N particles then $\vec{E}_{\text{ext}}$ is the field due to all of the particles other than

n , by definition and so we have:

$$m_n \ddot{\vec{x}}_n = \sum_{\substack{k=1 \\ k \neq n}}^N \frac{q_n q_k}{4\pi\epsilon} \frac{\vec{x}_n - \vec{x}_k}{|\vec{x}_n - \vec{x}_k|^3}. \quad (3.4.65)$$

So, our smoothened equation of motion is simply given by (3.4.53) with the problematic term subtracted. Equation (3.4.65) is taken as the correct equation of motion for the particles when the theory is treated carefully. In the scalar theory “the effect of a point charge’s electric field on itself is 0”.

3.4.3 Effective Lagrangian

We can understand that the effect of a point charge’s electric field on itself is 0 nicely through the Lagrangian by directly inserting the solution of the Poisson equation into our Lagrangian for the particles in (3.3.1). This is legitimate because we are writing our solved ϕ as a function of the positions of each charge elements and thus the solution to the Poisson equation can be treated as a holonomic constraint on ϕ . By the Holonomic Constraint theorem this will produce the correct equations of motion for the $\vec{x}_n(t, \vec{\alpha})$. Let us now simplify the ϕ dependent terms in the Lagrangian using the Poisson equation:

$$\int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla \phi|^2 - \rho \phi \right) d\mathbb{S} = \int_{\mathbb{S}} \left(\frac{\epsilon}{2} \nabla \cdot (\phi \nabla \phi) - \frac{\epsilon}{2} \phi \nabla^2 \phi - \rho \phi \right) d\mathbb{S} \quad (3.4.66)$$

$$= -\frac{1}{2} \int_{\mathbb{S}} \rho \phi d\mathbb{S}. \quad (3.4.67)$$

Using the divergence theorem we rewrote the divergence as a surface integral which we set to 0 because the solution for the potential we found earlier goes to 0 sufficiently quickly for large r that this integral goes to 0 as the boundary of the volume of integration is taken to be large (ϕ decays like $1/r$ and so $\phi \frac{\partial \phi}{\partial r}$ as appears here decays like $\frac{1}{r^3}$ but the surface area of the surface only grows like r^2 and so the surface integral decays like $\frac{1}{r}$ when the surface is a sphere of radius r . In the $r \rightarrow \infty$ limit this goes to 0). We can now evaluate this integral using our solution to the Poisson equation for the smoothened charges. Let $\rho_k(t, \vec{x})$ be the smoothened charge density due to particle k at time t :

$$\rho(t, \vec{x}) = \sum_{n=1}^N \rho_n(t, \vec{x}). \quad (3.4.68)$$

Then:

$$\int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla \phi|^2 - \rho \phi \right) d\mathbb{S} = -\frac{1}{2} \int_{\mathbb{S}} \rho \phi d\mathbb{S} = -\frac{1}{2} \sum_{n=1}^N \int_{\mathbb{S}} \rho_n(t, \vec{x}) \phi(t, \vec{x}) d^3 \vec{x} \quad (3.4.69)$$

$$= -\sum_{\substack{n=1 \\ k=1}}^{N,N} \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\rho_n(t, \vec{x}) \rho_k(t, \vec{x}')}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' \quad (3.4.70)$$

Let us separate this double sum into terms for which $n = k$ and into terms for which $n \neq k$. Because the summand is symmetric under interchanging n and k , for each term such that $n < k$ there is an equal term so that $n > k$. As such, we only actually need to consider terms for which $n = k$ and twice the effect of terms for which $n < k$:

$$\int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla \phi|^2 - \rho \phi \right) d\mathbb{S} = -\sum_{n=1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\rho_n(t, \vec{x}) \rho_n(t, \vec{x}')}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\rho_n(t, \vec{x}) \rho_k(t, \vec{x}')}{4\pi\epsilon |\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}'. \quad (3.4.71)$$

When not in the point limit, we define $\vec{x}_n(t)$ by the center of mass of the charge distributions for each $\rho_n(t, \vec{x})$. That way, the value of $\vec{x}_n(t)$ is independent of the point limit (as in the point limit the whole distribution shrinks down to the center of mass). If we translate an entire distribution of charge and matter by $\delta \vec{x}$ in space, then the center of mass automatically shifts by $\delta \vec{x}$. As well, all of the charge which was at $\vec{x}$ would now be at $\vec{x} + \delta \vec{x}$ and so the new charge distribution $\rho'(t, \vec{x})$ would be related to the old one by:

$$\rho'(t, \vec{x} + \delta \vec{x}) = \rho(t, \vec{x}) \implies \rho'(t, \vec{x}) = \rho(t, \vec{x} - \delta \vec{x}). \quad (3.4.72)$$

For each particle's distribution $\rho_n(t, \vec{x})$, define $\bar{\rho}_n(t, \vec{x})$ by:

$$\bar{\rho}_n(t, \vec{x}) = \rho_n(t, \vec{x} + \vec{x}_n(t)). \quad (3.4.73)$$

This $\bar{\rho}_n$ automatically has the property that it is unchanged by shifting the charge distribution:

$$\bar{\rho}'_n(t, \vec{x}) = \rho'_n(t, \vec{x} + \vec{x}'_n(t)) = \rho_n(t, \vec{x} - \delta\vec{x} + \vec{x}_n(t) + \delta\vec{x}(t)) = \bar{\rho}_n(t, \vec{x}) \quad (3.4.74)$$

and that the actual charge distribution can be written as:

$$\rho_n(t, \vec{x}) = \bar{\rho}_n(t, \vec{x} - \vec{x}_n(t)). \quad (3.4.75)$$

By writing ρ_n in terms of $\bar{\rho}_n$ this way, we isolate the way in which ρ_n depends on the center of mass of the distribution because as established $\bar{\rho}$ is unchanged by shifting that center of mass. With this, the “self-field” contributions to the Lagrangian can be nicely written as:

$$\sum_{n=1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\rho_n(t, \vec{x}) \rho_n(t, \vec{x}')}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}' = \sum_{n=1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\bar{\rho}_n(t, \vec{x} - \vec{x}_n(t)) \bar{\rho}_n(t, \vec{x}' - \vec{x}_n(t))}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}' \quad (3.4.76)$$

$$= \sum_{n=1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\bar{\rho}_n(t, \vec{x}) \bar{\rho}_n(t, \vec{x}')}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}' \quad (3.4.77)$$

where in the last line we have shifted both integration variables by $\vec{x}_n(t)$ and the effects of that shift happen to cancel in the denominator. So, we see that the “self-field” contributions to the Lagrangian are actually independent of the location of the center of mass of the distribution (because they are written solely in terms of the $\bar{\rho}$). Therefore, for the purposes of computing equations of motion for the center of mass, they don't contribute (their variations when the center of mass is varied are 0). This is why the “self-force” term is 0 in the equations of motion. Let $E_n(t)$ be defined by:

$$E_n(t) = \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\bar{\rho}_n(t, \vec{x}) \bar{\rho}_n(t, \vec{x}')}{8\pi\epsilon |\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}'. \quad (3.4.78)$$

These $E_n(t)$ are functions of time but they are not functions of the positions of the centers of mass of the their respective distributions. In the point limit, the $E_n(t)$ will diverge. But, they never contribute to the motion of the centers of mass and so are removable as a surface term when writing an action for $\vec{x}_n(t)$. We have now:

$$\int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla\phi|^2 - \rho\phi \right) d\mathbb{S} = \sum_{n=1}^N E_n(t) - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \int_{\mathbb{S}} \int_{\mathbb{S}} \frac{\rho_n(t, \vec{x}) \rho_k(t, \vec{x}')}{4\pi\epsilon |\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}' \quad (3.4.79)$$

The double sum on the right hand side has a well-defined point limit. Now taking that limit:

$$\int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla\phi|^2 - \rho\phi \right) d\mathbb{S} = \lim_{\text{point}} \sum_{n=1}^N E_n(t) - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|}. \quad (3.4.80)$$

Then, returning to our full Lagrangian for the system of charges in (3.3.1):

$$\mathcal{L} = \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + \int_{\mathbb{S}} \left(\frac{\epsilon}{2} |\nabla\phi|^2 - \rho\phi \right) d\mathbb{S} \quad (3.4.81)$$

$$= \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - \lim_{\text{point}} \sum_{n=1}^N E_n(t) - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|} \quad (3.4.82)$$

$$\simeq \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|} \quad (3.4.83)$$

where this $\simeq$ sign indicates precisely that the two sides have equal variation when varying any of the $\vec{x}_n(t)$.

Hence this is the reduced Lagrangian for just the charges. One can verify by explicitly computing the Euler-Lagrange equations that it reproduces our equations of motion (3.4.65):

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}_n} = \frac{\partial \mathcal{L}}{\partial \vec{x}_n} \implies m_n \ddot{\vec{x}}_n = \sum_{\substack{k=1 \\ k \neq n}}^N \frac{q_n q_k}{4\pi\epsilon} \frac{\vec{x}_n - \vec{x}_k}{|\vec{x}_n - \vec{x}_k|^3}. \quad (3.4.84)$$

Now that we understand what happens in the point limit, consider precisely two charges. The equations

of motion simplify to:

$$m_1 \ddot{\vec{x}}_1 = \frac{q_1 q_2}{4\pi\epsilon} \frac{\vec{x}_1 - \vec{x}_2}{|\vec{x}_1 - \vec{x}_2|^3}, \quad m_2 \ddot{\vec{x}}_2 = \frac{q_1 q_2}{4\pi\epsilon} \frac{\vec{x}_2 - \vec{x}_1}{|\vec{x}_1 - \vec{x}_2|^3}. \quad (3.4.85)$$

Notice that if q_1 and q_2 have the same sign (and so their product is positive) and ϵ is positive, then the acceleration of each charge is directed along the line between them and points outward from each other. And so, in this case, the charges repel each other. If on the other hand ϵ is negative, the acceleration of each charge is direct along the line between them and points inward toward each other and so the charges attract. Because of this, theories with positive ϵ are called repulsive theories and theories with negative ϵ are called attractive theories. All of this together gives us our first self-contained theory of physics. That is, we finally have a Lagrangian (other than the free particle) in which we have equations of motion for every variable in the theory:

Theorem 3.3: Galilean Scalar Theory

The Lagrangian of GCM particles interacting with the scalar field ϕ is given by:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - q_n \phi(t, \vec{x}_n) \right) + \frac{\epsilon}{2} \int_{\mathbb{S}} |\nabla \phi|^2 d\mathbb{S}. \quad (3.4.86)$$

The equation of motion for the potential can be solved to give the effective Lagrangian for the particles as:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|} \right) \quad (3.4.87)$$

when the point-particle limit is treated by appropriately. $\epsilon > 0$ for repulsive theories and $\epsilon < 0$ for attractive theories.

Exercises

Problem 3.9: Consistency check. Without using electrostatic gauge, compute the equation of motion for $\vec{A}$ from (3.4.14) and show that it is consistent with what is predicted by Gauss' law and the continuity equation.

Problem 3.10: The Hamiltonian for the scalar theory. Without applying electrostatic gauge, compute the Hamiltonian corresponding to (3.4.14) and show that it reproduces the equation of motion for ϕ (Gauss' Law) and the equation of motion found in the previous question for $\vec{A}$. Explain why applying electrostatic gauge before computing the Hamiltonian is mathematically incorrect.

Problem 3.11: Integral form of Gauss' Law. Show, from Gauss' law, that the charge contained in a volume $\mathbb{V}$ is related to the integral of $\vec{E}$ over the boundary of that region by:

$$\int_{\partial\mathbb{V}} \vec{E} \cdot d\vec{\mathbb{A}} = \frac{q[\mathbb{V}]}{\epsilon}.$$

3.5 Ampere's Law

Let's now study the alternative to the scalar theory, the other possible lowest order Lagrangian we found in equation (3.3.93). In this theory, the full Lagrangian for the potentials is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-\frac{|\vec{B}|^2}{2\mu} + \vec{J} \cdot \vec{A} - \rho\phi \right) d\mathbb{S}. \quad (3.5.1)$$

Let us find the equation of motion for the vector potential:

$$\frac{\delta \mathcal{L}}{\delta \vec{A}} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\vec{A}}} = 0 \quad (3.5.2)$$

For the moment work without referring to our specific Lagrangian density so that we can have a general result for use later. Assume the Lagrangian density can depend on $\vec{A}$ directly or through $\vec{B}$ and $\vec{E}$ (which both by definition are expressions depending on $\vec{A}$). Then:

$$\delta \mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \vec{A}} \cdot \delta \vec{A} + \frac{\partial \mathcal{L}}{\partial \vec{B}} \cdot \delta \vec{B} + \frac{\partial \mathcal{L}}{\partial \vec{E}} \cdot \delta \vec{E} \right) d\mathbb{S}. \quad (3.5.3)$$

By the definition of $\vec{E}$ and $\vec{B}$, under a variation in $\vec{A}$:

$$\vec{B} = \nabla \times \vec{A} \implies \delta \vec{B} = \nabla \times \delta \vec{A}, \quad \vec{E} = -\nabla \phi - \dot{\vec{A}} \implies \delta \vec{E} = -\delta \dot{\vec{A}}. \quad (3.5.4)$$

With these the variation of the Lagrangian becomes:

$$\delta \mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \vec{A}} \cdot \delta \vec{A} + \frac{\partial \mathcal{L}}{\partial \vec{B}} \cdot \nabla \times \delta \vec{A} - \frac{\partial \mathcal{L}}{\partial \dot{\vec{A}}} \cdot \delta \dot{\vec{A}} \right) d\mathbb{S}. \quad (3.5.5)$$

To continue, the following vector calculus identity will be useful:

$$\nabla \cdot (\vec{f} \times \vec{g}) = \vec{g} \cdot \nabla \times \vec{f} - \vec{f} \cdot \nabla \times \vec{g}. \quad (3.5.6)$$

Using this with $\vec{f} = \frac{\partial \mathcal{L}}{\partial \vec{B}}$ and $\vec{g} = \delta \vec{A}$:

$$\int_{\mathbb{S}} \frac{\partial \mathcal{L}}{\partial \vec{B}} \cdot (\nabla \times \delta \vec{A}) d\mathbb{S} = \int_{\mathbb{S}} \delta \vec{A} \cdot \left(\nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}} \right) d\mathbb{S} - \int_{\partial \mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \vec{B}} \times \delta \vec{A} \right) \cdot d\vec{A}. \quad (3.5.7)$$

By taking the variations on the interior of the integration region, not on the boundary, the integrand of the surface integral is 0 and so throughout space we get:

$$\int_{\mathbb{S}} \frac{\partial \mathcal{L}}{\partial \vec{B}} \cdot (\nabla \times \delta \vec{A}) d\mathbb{S} = \int_{\mathbb{S}} \delta \vec{A} \cdot \left(\nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}} \right) d\mathbb{S}. \quad (3.5.8)$$

Making this replacement in (3.5.5) we have:

$$\delta \mathcal{L} = \int_{\mathbb{S}} \left(\frac{\partial \mathcal{L}}{\partial \vec{A}} \cdot \delta \vec{A} + \delta \vec{A} \cdot \left(\nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}} \right) - \frac{\partial \mathcal{L}}{\partial \dot{\vec{A}}} \cdot \delta \dot{\vec{A}} \right) d\mathbb{S} \quad (3.5.9)$$

$$\implies \frac{\delta \mathcal{L}}{\delta \vec{A}} = \frac{\partial \mathcal{L}}{\partial \vec{A}} + \nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}}, \quad \frac{\delta \mathcal{L}}{\delta \dot{\vec{A}}} = -\frac{\partial \mathcal{L}}{\partial \dot{\vec{A}}}. \quad (3.5.10)$$

Thus, the Euler-Lagrange equation of motion for $\vec{A}$ becomes:

$$\frac{\partial \mathcal{L}}{\partial \vec{A}} + \nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}} + \partial_t \frac{\partial \mathcal{L}}{\partial \dot{\vec{A}}} = 0. \quad (3.5.11)$$

For our specific Lagrangian in equation (3.5.1), we then see:

$$\boxed{\nabla \times \vec{B} = \mu \vec{J}}. \quad (3.5.12)$$

Equation (3.5.12) is called **Ampere's Law**. It can be cast nicely in terms of the vector potential by using our favorite cross product identity:

$$\nabla \times \vec{B} = \nabla \times (\nabla \times \vec{A}) = \nabla (\nabla \cdot \vec{A}) - \nabla^2 \vec{A} \quad (3.5.13)$$

$$\implies \nabla (\nabla \cdot \vec{A}) - \nabla^2 \vec{A} = \mu \vec{J}. \quad (3.5.14)$$

This equation is a bit messy but recall that we haven't actually defined a gauge for the vector potential yet and so this equation is true in all gauges. Consider a gauge transformation of the vector potential:

$$\vec{A}' = \vec{A} + \nabla f \implies \nabla \cdot \vec{A}' = \nabla \cdot \vec{A} + \nabla^2 f. \quad (3.5.15)$$

By choosing $\nabla^2 f = -\nabla \cdot \vec{A}$ (this can be done by considering $\nabla \cdot \vec{A}$ as η and f as ϕ in the Poisson equation, which we know we can solve), we make $\nabla \cdot \vec{A}' = 0$. Thus, it is always possible to go to a gauge in which:

$$\nabla \cdot \vec{A} = 0. \quad (3.5.16)$$

Such a gauge is called the **Coulomb gauge**. Then, in this gauge our equation of motion simplifies to:

$$-\nabla^2 \vec{A} = \mu \vec{J}. \quad (3.5.17)$$

This is simply the Poisson equation again and so the solution for the vector potential on all space in this gauge is:

$$\vec{A} = \int_{\mathbb{S}} \frac{\mu \vec{J}(t, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.5.18)$$

It seems we could now repeat the steps of the previous section for the vector potential and find the effective Lagrangian for just the charges. However, it turns out there is a road block we must address first.

In principle, equation (3.5.1) ought to give us the equations of motion for ϕ as well. Using (3.4.8),

$$\frac{\partial \mathcal{L}}{\partial \phi} + \nabla \cdot \frac{\partial \mathcal{L}}{\partial \vec{E}} = 0 \implies \rho = 0. \quad (3.5.19)$$

Hence, (3.5.1) is only possibly valid when there is no charge density anywhere! Recall that (3.5.1) is only the lowest order Lagrangian density consistent with our symmetries. If we included higher order terms (such as $(\vec{E} \cdot \vec{B})^2$) then $\frac{\partial \mathcal{L}}{\partial \vec{E}}$ would not be 0 and we would not receive such a damning equation of motion. So, this hiccup doesn't completely destroy the validity of what we are doing. However, it does tell us that equation (3.5.1) can only possibly be an effective theory, because certainly charge density is not 0 everywhere in space. When viewed as an effective theory, (3.5.19) tells us that (3.5.1) can only be a valid effective theory under circumstances with negligible charge density in the region of consideration. So, in contrast to the lowest order scalar theory (which was fully self-contained and self-consistent, after a bit of work), the lowest order vector theory is necessarily an effective theory and has no hope of being fundamental. In fact, it is not possible to have $\vec{J}$ be nonzero when $\rho = 0$ everywhere for any countable number of point particles. In order to apply the vector theory we will have to assume we have a continuous distribution of flowing charges so that the charge density can be 0 without setting $\vec{J}$ to 0. The vector theory is incompatible with point particles (this is more of an issue with the point particles than the vector theory).

We can only properly apply our vector theory when there is no appreciable charge density accumulated in our system. This means that through any region of space, the rate at which charge flows into that region must match the rate at which charge flows out (so that there is no charge build-up). That is, we need a continuous stream of flowing charge so that at any point we have no net charge. While point charges were viable objects of study in the scalar theory, they are not so in the vector theory because no finite number of discrete charges could make a continuous stream of flowing charge. However, current carrying wires (a wire with charge steadily flowing down it) are allowed in the vector theory if the charge flow in the wire is so that no charge accumulates anywhere.

To build the effective equations of motion for wires, we will need an expression for the Lorentz force on a wire. The total force on a set of discrete charges is, as we have found:

$$\vec{F} = \sum_{n=1}^N q_n \dot{\vec{x}}_n \times \vec{B}(t, \vec{x}_n) = \int_{\mathbb{S}} \sum_{n=1}^N q_n \dot{\vec{x}}_n \delta(\vec{x} - \vec{x}_n) \times \vec{B}(t, \vec{x}) d\mathbb{S}. \quad (3.5.20)$$

This last expression is precisely the current density $\vec{J}$. Thus, we have:

$$\vec{F} = \int_{\mathbb{S}} \vec{J}(t, \vec{x}) \times \vec{B}(t, \vec{x}) d\mathbb{S}. \quad (3.5.21)$$

Because this expression only references the current density and not individual charges, it is suitable for a continuous flow of current as well. Using our expression for the vector potential, we can identify the corresponding $\vec{B}$ field:

$$\vec{B} = \nabla \times \vec{A} = \nabla \times \int_{\mathbb{S}} \frac{\mu \vec{J}(t, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}' \quad (3.5.22)$$

$$\implies \vec{B} = \int_{\mathbb{S}} \frac{\mu \vec{J}(t, \vec{x}') \times (\vec{x} - \vec{x}')}{4\pi |\vec{x} - \vec{x}'|^3} d\mathbb{S}'. \quad (3.5.23)$$

Equation (3.5.23) is known as the **Biot-Savart law**.

We now perform the same division of $\vec{A}$ into a part due to a particular current of interest $\vec{A}_{\text{self}}$ and a part due to everything else $\vec{A}_{\text{ext}}$ that we did for the scalar potential in section 3.4. Then, the self/external decomposition extends immediately to $\vec{B}$. As well, it extends immediately to the force on our current density of interest:

$$\vec{F}_{\text{self}} = \int_{\mathbb{S}} \vec{J} \times \vec{B}_{\text{self}} d^3\vec{x}, \quad \vec{F}_{\text{ext}} = \int_{\mathbb{S}} \vec{J} \times \vec{B}_{\text{ext}} d^3\vec{x} \implies \vec{F} = \vec{F}_{\text{self}} + \vec{F}_{\text{ext}}. \quad (3.5.24)$$

The self force contribution is then given by the Biot-Savart law (with some help of the double cross product identity):

$$\vec{F}_{\text{self}} = \int_{\mathbb{S}, \mathbb{S}} \frac{\mu \vec{J}(t, \vec{x}) \times (\vec{J}(t, \vec{x}') \times (\vec{x} - \vec{x}'))}{4\pi |\vec{x} - \vec{x}'|^3} d^3\vec{x}' d^3\vec{x} \quad (3.5.25)$$

$$= \int_{\mathbb{S}, \mathbb{S}} \frac{\mu}{4\pi |\vec{x} - \vec{x}'|^3} \left(\vec{J}(t, \vec{x}') \vec{J}(t, \vec{x}) \cdot (\vec{x} - \vec{x}') - (\vec{x} - \vec{x}') \vec{J}(t, \vec{x}) \cdot \vec{J}(t, \vec{x}') \right) d^3\vec{x}' d^3\vec{x} \quad (3.5.26)$$

$$= -\frac{\mu}{4\pi} \int_{\mathbb{S}, \mathbb{S}} \left(\vec{J}(t, \vec{x}') \vec{J}(t, \vec{x}) \cdot \nabla \frac{1}{|\vec{x} - \vec{x}'|} + \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} \vec{J}(t, \vec{x}) \cdot \vec{J}(t, \vec{x}') \right) d^3\vec{x}' d^3\vec{x} \quad (3.5.27)$$

$$= \frac{\mu}{4\pi} \int_{\mathbb{S}, \mathbb{S}} \left(\vec{J}(t, \vec{x}') \frac{\nabla \cdot \vec{J}(t, \vec{x})}{|\vec{x} - \vec{x}'|} - \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} \vec{J}(t, \vec{x}) \cdot \vec{J}(t, \vec{x}') \right) d^3\vec{x}' d^3\vec{x}. \quad (3.5.28)$$

The surface term that would be gotten from integrating by parts is 0 because for any localized charge distribution (meaning charge is only contained in and moving around a finite region of space), $\vec{J}$ is strictly 0 as one goes out far enough space. By Ampere's law:

$$\nabla \cdot \vec{J} = \frac{1}{\mu} \nabla \cdot \nabla \times \vec{B} = 0. \quad (3.5.29)$$

Therefore:

$$\vec{F}_{\text{self}} = -\frac{\mu}{4\pi} \int_{\mathbb{S}, \mathbb{S}} \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} \vec{J}(t, \vec{x}) \cdot \vec{J}(t, \vec{x}') d^3\vec{x}' d^3\vec{x}. \quad (3.5.30)$$

Under renaming the integration variables $\vec{x}$ to $\vec{x}'$ and $\vec{x}'$ to $\vec{x}$ this integral goes to its own negative and so:

$$\vec{F}_{\text{self}} = -\vec{F}_{\text{self}} \implies \vec{F}_{\text{self}} = 0. \quad (3.5.31)$$

Thus, **the total force of any current distribution on itself is 0**. Because of this, just like with the scalar theory, we can use the external field in computing the force rather than the full field:

$$\vec{F} = \int_{\mathbb{S}} \vec{J} \times \vec{B}_{\text{ext}} d\mathbb{S}. \quad (3.5.32)$$

Just like with point charges, we don't need to consider the force of a wire on itself, only the effect on it due to other wires. Now that we know the force on a current distribution, consider a straight wire extending from $z = -\ell$ to $z = \ell$ which carries a current I . Then, the vector potential at a distance r away from the axis of the wire is:

$$\vec{A} = \int_{\mathbb{S}} \frac{\mu \vec{J}(t, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}' = \int_{-\ell}^{\ell} \frac{\mu I \vec{t}_z}{4\pi \sqrt{r^2 + (z - z')^2}} dz'. \quad (3.5.33)$$

With the u-substitution $z' = z + r \tan \theta$ this integral is manageable:

$$\vec{A} = \int_{-\arctan(\frac{\ell+z}{r})}^{\arctan(\frac{\ell-z}{r})} \frac{\mu I \vec{t}_z}{4\pi} \sec \theta d\theta = \frac{\mu I \vec{t}_z}{4\pi} \ln |\sec \theta + \tan \theta| \Big|_{-\arctan(\frac{\ell+z}{r})}^{\arctan(\frac{\ell-z}{r})} \quad (3.5.34)$$

$$= \frac{\mu I \vec{t}_z}{4\pi} \ln \left(\frac{\sqrt{r^2 + (\ell - z)^2} + \ell - z}{\sqrt{r^2 + (\ell + z)^2} - \ell - z} \right). \quad (3.5.35)$$

It is a common idealization to consider a very long wire by taking $\ell \rightarrow \infty$; this limit can be a useful approximation for some purposes. One does have to be a bit careful with the limit. From our finite ℓ vector potential:

$$\vec{A} = \frac{\mu I \vec{t}_z}{4\pi} \left(\ln \left(\sqrt{\frac{r^2}{\ell^2} + \left(1 - \frac{z}{\ell}\right)^2} + 1 - \frac{z}{\ell} \right) - \ln \left(\sqrt{\frac{r^2}{\ell^2} + \left(1 + \frac{z}{\ell}\right)^2} - 1 - \frac{z}{\ell} \right) \right). \quad (3.5.36)$$

In this first term, the $\ell \rightarrow \infty$ limit is easy enough by series expansion in $\frac{1}{\ell}$:

$$\ln \left(\sqrt{\frac{r^2}{\ell^2} + \left(1 - \frac{z}{\ell}\right)^2} + 1 - \frac{z}{\ell} \right) = \ln 2 + \mathcal{O}\left(\frac{1}{\ell}\right). \quad (3.5.37)$$

The second term is slightly more complicated:

$$\ln \left(\sqrt{\frac{r^2}{\ell^2} + \left(1 + \frac{z}{\ell}\right)^2} - 1 - \frac{z}{\ell} \right) = -\ln 2 + 2 \ln r - 2 \ln \ell + \mathcal{O}\left(\frac{1}{\ell}\right). \quad (3.5.38)$$

Combining our results, the vector potential for a long wire is:

$$\vec{A} = -\frac{\mu I \vec{t}_z}{2\pi} \left(\ln r - \ln(2\ell) + \mathcal{O}\left(\frac{1}{\ell}\right) \right). \quad (3.5.39)$$

It seems the vector potential is divergent in the $\ell \rightarrow \infty$ limit. However, because the vector potential is only defined up to gauge transformation, if the term which causes the divergence can be removed by a gauge transformation then it isn't really part of the theory, just an artifact of the choice of gauge. Nicely, the $\ln \ell$ term which causes the problem above can be removed:

$$\vec{A} = -\frac{\mu I \vec{t}_z}{2\pi} \ln \left(\frac{r}{R} \right) + \nabla \left(\frac{\mu I \ln(2\ell)}{2\pi} \ln \left(\frac{2\ell}{R} \right) z \right) + \mathcal{O}\left(\frac{1}{\ell}\right) \quad (3.5.40)$$

$$\simeq -\frac{\mu I \vec{t}_z}{2\pi} \ln \left(\frac{r}{R} \right) + \mathcal{O}\left(\frac{1}{\ell}\right). \quad (3.5.41)$$

Here R is any constant with dimensions of length. We have included it because it is bad form to write the logarithm of a quantity unless it is dimensionless. Thus, in the new gauge the limit $\ell \rightarrow \infty$ gives that the vector potential for an infinite wire is:

$$\vec{A} = -\frac{\mu I \vec{t}_z}{2\pi} \ln \left(\frac{r}{R} \right). \quad (3.5.42)$$

Certainly current carrying wires in everyday life are not infinite but this expression can still be a good approximation for many cases. The associated $\vec{B}$ field is:

$$\vec{B} = \nabla \times \vec{A} = \frac{\mu I \vec{t}_\varphi}{2\pi r}. \quad (3.5.43)$$

Now we can compute the motion of one wire due to another. For this we will need to simplify (3.5.21) for the case of a wire. Because the wire only has current along the z axis from $-\ell$ to ℓ :

$$\vec{F} = \int_{\mathbb{S}} \vec{J} \times \vec{B} d\mathbb{S} = \int_{-\ell}^{\ell} I \vec{t}_z dz \times \vec{B} = I \vec{t}_z \times \int_{-\ell}^{\ell} \vec{B} dz. \quad (3.5.44)$$

Suppose the wire has mass per unit length λ so that it has total mass $m = 2\lambda\ell$. Then, because the wire is a rigid body, by (2.9.123):

$$m \ddot{\vec{x}} = \int_{\mathbb{S}} \vec{J} \times \vec{B} d\mathbb{S} \implies 2\lambda\ell \ddot{\vec{x}} = I \vec{t}_z \times \int_{-\ell}^{\ell} \vec{B} dz \quad (3.5.45)$$

$$\implies \lambda \ddot{\vec{x}} = I \vec{t}_z \times \left(\frac{1}{2\ell} \int_{-\ell}^{\ell} \vec{B} dz \right). \quad (3.5.46)$$

In the limit $\ell \rightarrow \infty$, the integral just becomes over average value of $\vec{B}$ over all z :

$$\lambda \ddot{\vec{x}} = I \vec{t}_z \times \text{Avg}_z(\vec{B}). \quad (3.5.47)$$

Take wire 1 to be carrying current I_1 in the z direction with mass per unit length λ_1 and experiencing the field of wire 2 which carries current I_2 and has mass per unit length λ_2 . Then, the $\vec{B}$ field due to I_2 has no z dependence and so the average is trivial:

$$\vec{B} = \frac{\mu I_2 \vec{t}_\varphi}{2\pi r} \implies \text{Avg}_z(\vec{B}) = \frac{\mu I_2 \vec{t}_\varphi}{2\pi r}. \quad (3.5.48)$$

With this, the equation of motion for the position of wire 1 in the (x, y) plane becomes:

$$\lambda_1 \ddot{\vec{x}}_1 = I_1 \vec{t}_z \times \left(\frac{\mu I_2 \vec{t}_\varphi}{2\pi r} \right) = -\frac{\mu I_1 I_2}{2\pi} \frac{\vec{t}_r}{r} \quad (3.5.49)$$

$$\implies \lambda_1 \ddot{\vec{x}}_1 = -\frac{\mu I_1 I_2}{2\pi} \frac{\vec{x}_1 - \vec{x}_2}{|\vec{x}_1 - \vec{x}_2|^2}. \quad (3.5.50)$$

By the symmetry of the problem, just replace indices of 1's with 2's and 2's with 1's to get the equation of motion for wire 2. We can see that wires carrying currents in the same direction in a theory with negative μ repel each other and wires carrying currents in the same direction in a theory with positive μ attract each other. Thus, negative μ is repulsive and positive μ is attractive in this theory.

Exercises

Problem 3.12: Integral form of Ampere's Law. Using Ampere's Law, show that the current through a surface $\mathbb{A}$, $I[\mathbb{A}]$, is related to the integral of the $\vec{B}$ field around the boundary of that surface by:

$$\int_{\partial\mathbb{A}} \vec{B} \cdot d\vec{x} = \mu I[\mathbb{A}].$$

Problem 3.13: Symmetry approach to the field of a wire. Using the integral form of Ampere's law, consider an infinite wire carrying current I along the z axis and an integration surface that is a circle of radius R concentric with the wire. Argue by symmetry considerations that $\vec{B} = B(r)\vec{e}_\varphi$ and thus use the integral form of Ampere's law to derive (3.5.43).

3.6 Newtonian Gravity

Now that we have a reasonable understanding of the possible Galilean theories, we will look into some of their major successes. So far all of these fields theories interact with our particles through some property called charge. And so, the charge with which a particle couples to the potentials is a property of that particle. We have encountered only one other particle property so far, mass. There is no reason mass cannot also be a charge. So, what if we let it be so? Then the first question is scalar or vector theory (because as we know we cannot do both at the same time). As we saw, the vector theory can only apply when the charge density is essentially 0 everywhere unless we consider a higher order theory. Thus, because mass density is not everywhere 0, we will choose the scalar theory. The next question is attractive or repulsive, which has to be settled experimentally. We see in experiment that masses attract each other and so according to our theories so far the only possible theory at lowest order for the interaction of just masses is:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - m_n \phi(t, \vec{x}_n) \right) - \int_{\mathbb{S}} \frac{|\nabla \phi|^2}{8\pi G} d\mathbb{S}. \quad (3.6.1)$$

Here ϕ is the scalar potential for the theory of attracting masses, known as the gravitational scalar potential, and $\epsilon = -\frac{1}{4\pi G}$ where G is a positive constant called Newton's gravitational constant. Typically, instead of $\vec{E}$ in this theory one calls it the gravitational field:

$$\vec{g} = -\nabla \phi. \quad (3.6.2)$$

Equation (3.6.1) is the Lagrangian for Newtonian gravity. It is good enough for the gravitation between almost everything in our solar system. A more sophisticated theory will turn out to be needed eventually, but this one is quite good. In terms of ϕ and $\vec{g}$, Gauss' law (3.4.15) becomes:

$$\nabla \cdot \vec{g} = -\nabla^2 \phi = -4\pi G \rho \quad (3.6.3)$$

where ρ is the mass density of the particles. It will often be useful to solve for and eliminate the potential to get the effective theory of just the masses:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + G \sum_{k=n+1}^N \frac{m_n m_k}{|\vec{x}_n - \vec{x}_k|} \right). \quad (3.6.4)$$

Exercises

Problem 3.14: Field of a Sphere Consider a uniformly massive sphere of radius R and total mass m .

- (a) Show using a symmetry argument and the integral form of Gauss' law that the gravitational field due to this mass is:

$$\vec{g}(\vec{x}) = \begin{cases} 0, & \text{if } |\vec{x}| < R \\ -Gm \frac{\vec{x}}{|\vec{x}|^3}, & \text{if } |\vec{x}| > R \end{cases}.$$

Thus, outside of a sphere, it acts gravitationally exactly like a point-mass.

- (b) Integrate $\vec{g}$ to show in electrostatic gauge ($\vec{g} = -\nabla \phi$) that the scalar potential is given by:

$$\phi(t, \vec{x}) = C(t) + \begin{cases} -\frac{Gm}{R}, & \text{if } |\vec{x}| \leq R \\ -\frac{Gm}{|\vec{x}|}, & \text{if } |\vec{x}| > R \end{cases}$$

for some arbitrary $C(t)$ which can be taken however (as part of the definition of the gauge).

- (c) Show using Coulomb's law directly that the potential is given by the result found in the previous part with $C(t) = 0$.

Problem 3.15: Field of a Ball Consider a uniformly massive ball of radius R and total mass m .

- (a) Show using a symmetry argument and the integral form of Gauss' law that the gravitational field due to this mass is:

$$\vec{g}(\vec{x}) = \begin{cases} -\frac{Gm}{R^3} \vec{x}, & \text{if } |\vec{x}| < R \\ -Gm \frac{\vec{x}}{|\vec{x}|^3}, & \text{if } |\vec{x}| > R \end{cases}.$$

Thus, outside of a sphere, it acts gravitationally exactly like a point-mass.

- (b) Integrate $\vec{g}$ to show in electrostatic gauge ($\vec{g} = -\nabla\phi$) that the scalar potential is given by:

$$\phi(t, \vec{x}) = C(t) + \begin{cases} \frac{Gm}{2R^3}|\vec{x}|^2 - \frac{3Gm}{2R}, & \text{if } |\vec{x}| \leq R \\ -\frac{Gm}{|\vec{x}|}, & \text{if } |\vec{x}| > R \end{cases}$$

for some arbitrary $C(t)$ which can be taken however (as part of the definition of the gauge).

- (c) Show using Coulomb's law directly that the potential is given by the result found in the previous part with $C(t) = 0$.

Problem 3.16: Symmetry of Gravitational force. Show, using Coulomb's law, that the force due to gravity of a mass distribution ρ_1 on another ρ_2 , $\vec{F}_{1 \rightarrow 2}$ and force due to gravity of ρ_2 on ρ_1 , $\vec{F}_{2 \rightarrow 1}$ are related by:

$$\vec{F}_{1 \rightarrow 2} + \vec{F}_{2 \rightarrow 1} = 0.$$

Problem 3.17: Gravitational force between spherically symmetric bodies. Consider two bodies with non-overlapping mass distributions $\rho_1(\vec{x})$ (spherically symmetric about a point $\vec{x}_1$ and with a radius of extent R_1) and $\rho_2(\vec{x})$ (spherically symmetric about a point $\vec{x}_2$ and with a radius of extent R_2).

- (a) Show using a symmetry argument and the integral form of Gauss' law that the gravitational field due to either of the masses is exactly like if it were a point-mass on the outside.
 (b) Use the previous part and the previous question to show then that the gravitational force between the bodies is exactly as if they were point masses.

Problem 3.18: Mass Conversation. Show that the combination of the continuity equation and the use of mass as a type of interaction charge implies that mass is locally conserved (that it is neither created nor destroyed but simply flows around).

Problem 3.19: Motion under a Central Potential. Consider two bodies interacting due to a potential energy depending only on the distance between them. That is, the bodies have a Lagrangian of the form:

$$\mathcal{L} = \frac{1}{2}m_1|\dot{\vec{x}}_1|^2 + \frac{1}{2}m_2|\dot{\vec{x}}_2|^2 - U(|\vec{x}_1 - \vec{x}_2|).$$

Define the center of mass position $\vec{X}$ of the system and relative position $\vec{x}$ within the system as:

$$\vec{X} \stackrel{\text{def}}{=} \frac{m_1\vec{x}_1 + m_2\vec{x}_2}{m_1 + m_2}, \quad \vec{x} \stackrel{\text{def}}{=} \vec{x}_2 - \vec{x}_1.$$

- (a) Show that the original positions can be rewritten as:

$$\vec{x}_1 = \vec{X} - \frac{m_2}{m_1 + m_2}\vec{x}, \quad \vec{x}_2 = \vec{X} + \frac{m_1}{m_1 + m_2}\vec{x}.$$

- (b) Input the new coordinates into the Lagrangian to show that it becomes:

$$\mathcal{L} = \frac{1}{2}M|\dot{\vec{X}}|^2 + \frac{1}{2}\mu|\dot{\vec{x}}|^2 - U(|\vec{x}|)$$

where $M = m_1 + m_2$ is called the total mass and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is called the reduced mass. Notice that M is larger than either m_1 or m_2 and that μ is smaller than either m_1 or m_2 .

- (c) Show that $\vec{X}$ and $\vec{x}$ do not interact with each other. Solve the equation of motion for $\vec{X}$ and show that we can take:

$$\mathcal{L} = \frac{1}{2}\mu|\dot{\vec{x}}|^2 - U(|\vec{x}|)$$

as the effective Lagrangian for just the relative position. This result is called the “center of mass decomposition”. Equivalently, one can view this as the Lagrangian in which we have applied a boost so that $\vec{X} = 0$ (which is possible because $\vec{X}$ is constant). Thus, this is the Lagrangian in the “center of mass frame”.

- (d) Show that the angular momentum of the relative position is conserved and that this implies that the plane spanned by the relative position and its velocity remains constant in time. Thus, show that the motion of the relative position lies purely in this plane.
 (e) Parameterize the plane of motion of the relative position by polar coordinates: $\vec{x} = (r \cos \varphi, r \sin \varphi)$.

Show that in these coordinates, the Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2}\mu\dot{\mathbf{r}}^2 + \frac{1}{2}\mu r^2\dot{\varphi}^2 - U(r).$$

- (f) Use the Legendre transform to show that the Hamiltonian is:

$$\mathcal{H} = \frac{p_r^2}{2\mu} + \frac{p_\varphi^2}{2\mu r^2} + U(r).$$

Show that the φ equation of motion gives that its conjugate momentum is conserved and that φ is an ignorable coordinate. Show that the conjugate momentum to φ matches the magnitude of angular momentum from before.

- (g) The path that $\vec{x}$ makes in the plane will define some geometric curve. Consider the area $\mathbb{A}$ swept by the line segment connecting the origin to $\vec{x}$ as a function of time. Show that:

$$d\mathbb{A} = \frac{1}{2}r^2 d\varphi$$

and that the rate at which the area is swept out per unit time is constant (use the equation of motion for φ). The fact that central force motion sweeps out area at a constant rate in time is called **Kepler's Second Law**. (We will encounter Kepler's first and third laws soon.)

- (h) Let L be the magnitude of angular momentum. Show that after the reduction of φ from the Hamiltonian, the effective Hamiltonian and Lagrangian for r become:

$$\mathcal{H} = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} + U(r), \quad \mathcal{L} = \frac{1}{2}\mu\dot{r}^2 - \frac{L^2}{2\mu r^2} - U(r).$$

- (i) Finally, show that the equations of motion for $r(t)$ and $\varphi(t)$ are:

$$\frac{d\varphi}{dt} = \frac{L}{\mu r^2}, \quad \frac{d^2 r}{dt^2} - \frac{L^2}{\mu^2 r^3} + \frac{1}{\mu} \frac{\partial U}{\partial r} = 0.$$

If you want to solve them, $r(t)$ can be solved in terms of an integral expression depending on the function U , if you wish to try.

Problem 3.20: Gravity near the Earth's Surface Consider a point-particle of mass m_{obj} interacting gravitationally with the Earth (of mass m_E which is much larger than m_{obj} and which we assume to have a spherically symmetric mass distribution). By (3.6.4), the Lagrangian is:

- (a) Show using the result of problem 3.19 that the Lagrangian is:

$$\mathcal{L} = \frac{1}{2}m_{\text{obj}}|\dot{\vec{x}}_{\text{obj}}|^2 + \frac{1}{2}m_E|\dot{\vec{x}}_E|^2 + \frac{Gm_{\text{obj}}m_E}{|\vec{x}_{\text{obj}} - \vec{x}_E|}.$$

- (b) Show using the center of mass decomposition the following equations to lowest order in powers of m_{obj}/m_E (recall the Earth is quite massive):

$$\begin{aligned} \vec{x}_E &= \vec{X} + \mathcal{O}\left(\frac{m_{\text{obj}}}{m_E}\right), & \vec{x}_{\text{obj}} &= \vec{X} + \vec{x} + \mathcal{O}\left(\frac{m_{\text{obj}}}{m_E}\right), \\ M &= m_E \left(1 + \mathcal{O}\left(\frac{m_{\text{obj}}}{m_E}\right)\right), & \mu &= m_{\text{obj}} + \mathcal{O}\left(\frac{m_{\text{obj}}}{m_E}\right). \end{aligned}$$

Thus conclude that the large mass of the Earth compared to our object allows us to think of $\vec{X}$ as the position of the Earth, M as the mass of the Earth, and μ as the mass of the object.

- (c) Use the previous part to show that at lowest order in m_{obj}/m_E the Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2}m_E|\dot{\vec{X}}|^2 + \frac{1}{2}m_{\text{obj}}|\dot{\vec{x}}|^2 + \frac{Gm_E m_{\text{obj}}}{|\vec{x}|}.$$

Thus, conclude that the object moves relative to the Earth by a central potential and that the Earth just keeps moving with no meaningful effect due to the object.

- (d) Consider the object to be near the surface of the Earth so that its position is $\vec{x} = (x, y, R + z)$ where R is the radius of the Earth and $(0, 0, 1)$ is the outward pointing unit vector of the Earth's surface near where the object is. Let $r = \sqrt{x^2 + y^2 + z^2}$ and show that the effective Lagrangian for the object to lowest order in r/R (the Earth's radius is much larger than how far off the Earth the object is) is:

$$\mathcal{L} = \frac{1}{2}m_{\text{obj}}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \frac{Gm_E m_{\text{obj}}}{R^2}z + \mathcal{O}\left(\frac{r}{R}\right)^2.$$

Thus, conclude that near the surface of the Earth the object moves as observed by Galileo and show that the gravitational acceleration near the Earth's surface is given by:

$$g = \frac{Gm_E}{R^2}.$$

Problem 3.21: The Binet Equation. Consider again motion under a central potential. Let us start from the equations of motion for φ and r . Define $s = \frac{1}{r}$.

- (a) Rewrite the equations of motion in terms of s and φ to show:

$$\frac{1}{s^4} \frac{d^2 s}{dt^2} - \frac{2}{s^5} \left(\frac{ds}{dt} \right)^2 + \frac{L^2}{\mu^2} s + \frac{1}{\mu} \frac{\partial U}{\partial s} = 0, \quad \frac{d\varphi}{dt} = \frac{L}{\mu} s^2.$$

- (b) Using the equation of motion for φ , one can implicitly define t as a function of φ so that time derivatives can be rewritten as φ derivatives. Do so in the s equation of motion to show that it becomes:

$$\frac{d^2 s}{d\varphi^2} + s + \frac{\mu}{L^2} \frac{\partial U}{\partial s} = 0.$$

This equation is called the **Binet equation**. Thus, the Binet equation gives the trajectory $r(\varphi)$ and Kepler's second law gives the time dependence for the central potential problem.

- (c) Show that the Energy of the motion corresponding to the effective Hamiltonian for r becomes, in terms of s and φ :

$$E = \frac{L^2}{2\mu} \left(\left(\frac{ds}{d\varphi} \right)^2 + s^2 \right) + U.$$

Problem 3.22: The Kepler Problem. Consider two non-overlapping spherically symmetric bodies experiencing each other's gravity.

- (a) Show that because the bodies are spherically symmetric, the Lagrangian is:

$$\mathcal{L} = \frac{1}{2} m_1 |\dot{\vec{x}}_1|^2 + \frac{1}{2} |\dot{\vec{x}}_2|^2 + \frac{Gm_1 m_2}{|\vec{x}_1 - \vec{x}_2|}.$$

- (b) Show that the effective Lagrangian for the distance between the bodies is:

$$\mathcal{L} = \frac{1}{2} \mu \dot{r}^2 - \frac{L^2}{2\mu r^2} + \frac{GM\mu}{r}.$$

- (c) Show that the Binet equation becomes:

$$\frac{d^2 s}{d\varphi^2} + s = \frac{GM\mu^2}{L^2}.$$

- (d) Solve the Binet equation to show that the trajectories of the Kepler problem are:

$$\frac{1}{r(\varphi)} = \frac{GM\mu^2}{L^2} (1 + \varepsilon \cos(\varphi - \varphi_0))$$

where ε and φ_0 are constants determined by initial conditions.

- (e) Define the coordinate axes so that $\varphi_0 = 0$ (return to the original derivation of the central potential problem to see this is possible). Let $\ell = \frac{L^2}{GM\mu^2}$ for simplicity. Show that if $\varepsilon = 0$, the trajectory is a circle (and find its radius and center), that if $0 < \varepsilon < 1$ the trajectory is an ellipse (and find its semi-major axis length, semi-minor axis length, and foci), that if $\varepsilon = 1$ the trajectory is a parabola (and find its focus and directrix), and that if $\varepsilon > 1$ the trajectory is a hyperbola (and find its foci and vertices). Thus conclude **Kepler's First Law**, that the solutions to motion in the Coulomb potential are conic sections.
- (f) Express the parameters ℓ and ε in terms of the energy and angular momentum of the orbit (using the energy expression from the Binet equation) to show that:

$$\varepsilon = \sqrt{1 + \frac{2L^2 E}{G^2 M^2 \mu^3}}$$

and restate the conic section conditions on ε in terms of E and L . This ε is called the eccentricity of the orbit and this ℓ is called the semi-latus rectum.

- (g) Assume the energy and angular momentum are so that the orbit is elliptical. Show that the semi-major

axis length of the ellipse a and the period of the orbit τ are related by **Kepler's Third Law**:

$$a^3 = \frac{GM}{4\pi^2} \tau^2.$$

To derive this it will be useful to use that the area of an ellipse is πab where b is the semi-minor axis length and also recall Kepler's second law.

Problem 3.23: The Inverse Kepler Problem. Suppose that by looking at the data of trajectories of celestial objects, one has noticed they follow elliptical paths so that $r(\varphi)$ is known ahead of time to be:

$$r(\varphi) = \frac{\ell}{1 + \varepsilon \cos \varphi}$$

for some parameters ℓ and ε . By using the Binet equation and that U does not depend on L^2 , show that for some constant α independent of L , $U = -\frac{\alpha}{r}$ and thus we recover the Keplerian potential.

Problem 3.24: Escape Speed. Consider a mass m which is so much lighter than the Earth we consider its mass negligible and which is leaving the ground with speed v away from the Earth. Show, using the results of the Kepler problem, that the minimum speed the mass must leave with to never get pulled back down to the ground by gravity (called the escape speed) is:

$$v = \sqrt{\frac{2GM}{R}}$$

where M is the mass of the Earth and R is the radius of the Earth. Thus, what goes up need not come down if it goes up fast enough.

Problem 3.25: Gravitational Slingshot. Consider a spacecraft of mass m launching from Earth with velocity $v_0(0, 0, 1)$ relative to the Earth toward a very distant celestial body (like another planet) of velocity $v_p(\sin \alpha, 0, \cos \alpha)$ and a very large mass compared to the spacecraft. So that the spacecraft interacts with the planet as much as possible, assume its launch velocity is designed to lie in the plane spanned by the planet's velocity and the initial displacement between the planet and the spacecraft.

- Let $\vec{u}_0$ be the initial velocity of the spacecraft relative to the distant planet and let $\vec{u}_f$ be the asymptotic final velocity of the spacecraft relative to the distant planet. Explain why (using the solution of the Kepler problem) such an asymptotic final velocity exists and justify that $|\vec{u}_0| = |\vec{u}_f|$.
- Explain why $|\vec{u}_0| = |\vec{u}_f|$ implies there exists a rotation matrix so that $\vec{u}_f = \hat{R}\vec{u}_0$. Let χ , called the deflection angle, be the angle of that rotation matrix. Using our previous results on rotation matrices, show that the rotation $\hat{R}$ is given by:

$$\hat{R} = \begin{pmatrix} \cos \chi & 0 & \sin \chi \\ 0 & 1 & 0 \\ -\sin \chi & 0 & \cos \chi \end{pmatrix}.$$

- Show that the final velocity of the spacecraft in the original frame $\vec{v}_f$ is given by

$$\vec{v}_f = \vec{v}_p + \hat{R}(\vec{v}_0 - \vec{v}_p) = \begin{pmatrix} v_p(1 - \cos \chi) \sin \alpha - v_p \sin \chi \cos \alpha + v_0 \sin \chi \\ 0 \\ v_p(1 - \cos \chi) \cos \alpha + v_p \sin \chi \sin \alpha + v_0 \cos \chi \end{pmatrix}.$$

- Finally then, show that the final speed of the spacecraft is given by:

$$v_f^2 = 2v_p^2(1 - \cos \chi) + v_0^2 + 2v_0v_p(\cos \alpha - \cos(\alpha + \chi)).$$

Thus, notice that one can make the spacecraft come out of its interaction with the planet going much faster than it went in. This technique has been used many times to assist the travel of spacecraft.

Problem 3.26: Harmonic Central Potential. Consider the spherical harmonic oscillator:

$$\mathcal{H} = \frac{|\vec{p}|^2}{2m} + \frac{m\omega^2}{2}|\vec{x}|^2.$$

- Use that the potential is central to conclude that the motion is planar and therefore that the solution can be written as $\vec{x} = (x(t), y(t), 0)$. As well, find and solve the equations of motion to show:

$$x(t) = a \cos(\omega t - \varphi_1), \quad y(t) = b \sin(\omega t - \varphi_2)$$

for appropriate constants $a, b, \varphi_1, \varphi_2$ determined by initial conditions.

- (b) Suppose a or b is 0. Show that the path of the motion is a line segment.
- (c) Suppose neither a nor b is 0. Show that the path of the motion satisfies:

$$\frac{x^2}{a^2} - 2\frac{xy}{ab} \sin \varphi + \frac{y^2}{b^2} = \cos^2 \varphi$$

where $\varphi = \varphi_1 - \varphi_2$.

- (d) Suppose $\cos \varphi = 0$. Show that the path of the motion is a line segment.
- (e) Suppose $\cos \varphi \neq 0$. Show that the path of the motion is an ellipse.

Problem 3.27: Inverse Square Potential. Consider the Lagrangian:

$$\mathcal{L} = \frac{1}{2}m|\dot{\vec{x}}|^2 + \frac{k}{2|\vec{x}|^2}.$$

- (a) Consider the scale transformation $\vec{x}' = e^\varepsilon \vec{x}$ and $t' = e^{2\varepsilon} t$. Show that this system has symmetry under this transformation, find the associated generator of the transformation from Noether's theorem, and verify that it is conserved.
- (b) Write the Binet equation for this system and solve the orbits, both the shape of trajectory $\mathbf{r}(\varphi)$ and time dependence $\mathbf{r}(t)$ for all four cases of $L^2 > mk$, $L^2 = mk$ with $\frac{ds}{d\varphi}(1) \neq 0$, $L^2 = mk$ with $\frac{ds}{d\varphi}(1) = 0$, and $L^2 < mk$.
- (c) Show that the circular orbits found in the previous part are unstable (if they are perturbed by any amount they will not survive).

Problem 3.28: Existence of Circular Orbits for Attractive Potentials. Consider a central potential $U(r)$ which is attractive. That is, the direction of acceleration caused by this potential is inward toward $r = 0$.

- (a) Show that $\frac{\partial U}{\partial s} < 0$.
- (b) From the Binet equation, show that for any positive constant s_0 there exists an L so that $s = s_0$ solves the Binet equation for this potential U and angular momentum L . Thus, conclude that any attractive central potential possesses circular orbits of any radius.

Problem 3.29: Non-existence of Bound Orbits for Repulsive Potentials. Consider a central potential $U(r)$ which is repulsive. That is, the direction of acceleration caused by this potential is outward away from $r = 0$.

- (a) Show that $\frac{\partial U}{\partial s} > 0$.
- (b) From the Binet equation, show that $\frac{d^2 s}{d\varphi^2} < 0$. Integrate this twice to show that for $\varphi > 0$:

$$s < s(0) + \frac{ds}{d\varphi}(0)\varphi.$$

- (c) Use the above result to show that there exists a φ for which $r \rightarrow \infty$. Thus, conclude that there can be no bound orbit for a repulsive potential.

Problem 3.30: Bertrand's Theorem. Based on symmetry considerations, one could have likely guessed that when interacting, two otherwise isolated bodies in the Galilean theory interact via a central potential. However, by this method one would not have known what central potential to use. All one would know is it should be attractive so that the bound orbits of planets can exist. Here we will see how special the Keplerian potential really is. For the purposes of this question, define $J(s) = -\frac{\mu}{L^2} \frac{\partial U}{\partial s}$ so that the Binet equation becomes:

$$\frac{d^2 s}{d\varphi^2} + s = J(s).$$

- (a) Consider perturbing a circular solution to the Binet equation. That is, consider:

$$s(\varphi) = s_0 + \varepsilon s_1(\varphi) + \varepsilon^2 s_2(\varphi) + \varepsilon^3 s_3(\varphi) + \mathcal{O}(\varepsilon^4)$$

where s_0 is a constant, ε is a parameter which captures the strength of the perturbation, and s_a are the resulting perturbations to the solution and are by definition independent of ε . By inserting this form into the Binet equation, show (by matching terms at each order in ε) that the perturbations must

satisfy:

$$\begin{aligned} s_0 &= J(s_0), & \frac{d^2 s_2}{d\varphi^2} + s_2 &= J'(s_0)s_2 + \frac{1}{2}J''(s_0)s_1^2, \\ \frac{d^2 s_1}{d\varphi^2} + s_1 &= J'(s_0)s_1, & \frac{d^2 s_3}{d\varphi^2} + s_3 &= J'(s_0)s_3 + J''(s_0)s_1s_2 + \frac{1}{6}J'''(s_0)s_1^3. \end{aligned}$$

- (b) Explain that, because the solution $s(\varphi)$ is valid for all ε , in order for $s(\varphi)$ to describe a function which does not spiral into the origin then $s(\varphi)$ must be bounded and each $s_a(\varphi)$ must be bounded.
- (c) Show, using the equation for s_1 , that in order for s to be bounded, $1 - J'(s_0) > 0$. Then, let $\alpha \geq 0$ be defined by $\alpha^2 = 1 - J'(s_0)$ and show that s_1 is given by:

$$s_1(\varphi) = A \cos(\alpha(\varphi - \varphi_0))$$

for some constants A and φ_0 . As well, explain how A can be absorbed into the definition of ε and φ_0 can be absorbed into the definition of φ so that s_1 is given without loss of generality by:

$$s_1(\varphi) = \cos(\alpha\varphi).$$

- (d) The equations for s_2 and s_3 are of the form of a driven harmonic oscillator with frequency α . Use the integral solution to the driven harmonic oscillator to show then that s_2 is given by:

$$s_2(\varphi) = A_2 \cos(\alpha\varphi) + B_2 \sin(\alpha\varphi) + \int_0^\varphi \frac{1}{2} J''(s_0) s_1^2(\varphi') \sin(\alpha(\varphi - \varphi')) \frac{d\varphi'}{\alpha}.$$

Using the solution for s_1 , evaluate the integral and observe that s_2 is bounded for all φ . Choose the initial conditions to simplify the resulting expression for s_2 as much as possible to show that a particular possible solution for s_2 is:

$$s_2(\varphi) = \frac{J''(s_0)}{4\alpha^2} - \frac{J''(s_0)}{12\alpha^2} \cos(2\alpha\varphi).$$

- (e) Repeat the above process for s_3 to show it is given by:

$$s_3(\varphi) = A_3 \cos(\alpha\varphi) + B_3 \sin(\alpha\varphi) + \int_0^\varphi \left(J''(s_0) s_1(\varphi') s_2(\varphi') + \frac{1}{6} J'''(s_0) s_1^3(\varphi') \right) \sin(\alpha(\varphi - \varphi')) \frac{d\varphi'}{\alpha}.$$

Using the solutions for s_1 and s_2 , evaluate the integral and observe that s_3 is not generically bounded. Choose the initial conditions to simplify the resulting expression for s_3 as much as possible to show that a particular possible solution for s_3 is:

$$s_3(\varphi) = \frac{5J''(s_0)^2 + 3\alpha^2 J'''(s_0)}{48\alpha^3} \varphi \sin(\alpha\varphi) + \frac{J''(s_0)^2 - \alpha^2 J'''(s_0)}{192\alpha^4} \cos(3\alpha\varphi).$$

Thus, conclude that in order for the solution to remain bounded, it is necessary that:

$$5J''(s_0)^2 + 3\alpha^2 J'''(s_0) = 0.$$

- (f) In addition to being bounded, orbits may also be closed. The shape of the trajectory traced out in space may or may not close (repeat itself in space) in general. Assume our solution is required to close. Explain that, because the solution $s(\varphi)$ is valid for all ε , in order for $s(\varphi)$ to be a closed it must close at each order in ε . Then, show using the solution for s_1 that in order for s to be closed, there must be natural numbers p and q so that $p\alpha = q$. Thus, closure of the orbit implies α must be rational.
- (g) Show that the angular momentum L is given by:

$$L^2 = -\frac{\mu}{s_0} \frac{\partial U}{\partial s}(s_0)$$

and thus from the definition of α that α is given by:

$$\alpha^2 = 1 - s_0 \frac{\frac{\partial^2 U}{\partial s^2}(s_0)}{\frac{\partial U}{\partial s}(s_0)}.$$

Then, conclude that because the right hand side is a continuous function of s_0 and α must always be rational (to keep the orbits closed) and the only continuous function which takes only rational values is the constant function, we must have that α is independent of s_0 . Thus, the above is true for all s_0 and we have:

$$\alpha^2 = 1 - s \frac{\frac{\partial^2 U}{\partial s^2}(s)}{\frac{\partial U}{\partial s}(s)}.$$

Integrate this differential equation to show that in an appropriate choice of gauge, for some constant N :

$$U(s) = Ns^{2-\alpha^2}.$$

So, for bound closed orbits the potential must be a rational power law.

(h) From this form of U and how L is related to s_0 , show that:

$$J'(s_0) = 1 - \alpha^2, \quad J''(s_0) = -\frac{\alpha^2(1 - \alpha^2)}{s_0}, \quad J'''(s_0) = \frac{(1 - \alpha^2)\alpha^2(1 + \alpha^2)}{s_0^2}.$$

Use these expressions in the necessary condition for bounded orbits derived in part (e) to show that it becomes:

$$\alpha^4(1 - \alpha^2)(4 - \alpha^2) = 0.$$

Thus, conclude that in order for the orbits to be both bounded and closed, it is necessary that $\alpha \in \{0, 1, 2\}$. From the allowed values of α , we see that in order for all bounded orbits produced by a potential to be closed, it is necessary that the potential be ($\alpha = 0$) the inverse square potential, ($\alpha = 1$) the Keplerian potential, or ($\alpha = 2$) the spherical harmonic oscillator. Then, recall that the only bound orbits of the inverse square potential are unstable. Certainly planetary orbits must be stable (otherwise the effect of a distant passing comet or the other planets would cause us to spiral into the Sun), so the instability of the inverse square potential rules out its viability for planetary orbits. Finally then we have **Bertrand's Theorem**: The only central potentials which possess stable bound orbits and for which all bound orbits are closed are the Keplerian potential and the harmonic oscillator. The Keplerian potential is the unique potential which (1) is central (2) gets weaker with increasing separation (3) possesses stable bound orbits and (4) has its bound orbits close.

Problem 3.31: ★ The Cavendish Experiment. Consider a circular protractor marked in detail with angles whose origin is at $(0,0)$ on the ground ($z = 0$). Then, consider two very heavy spheres, each of mass M (measured on a scale) placed at the same height above the ground and held in place at coordinates $(\ell \cos \alpha, \ell \sin \alpha)$ and $(-\ell \cos \alpha, -\ell \sin \alpha)$ (the distance ℓ can be determined by comparing to sticks and the angle α can be read from above by looking down at where the spheres project onto the protractor). Next, consider two very light spheres, each of mass m (measured on a scale) placed at the same height above the ground as the heavy spheres and connected by a very light rod of length 2ℓ which has a string through its center connected to the ceiling so that the two light spheres and rod system are suspended and can only move by rotation in the plane of the spheres. Thus, the coordinates of the two light spheres are given by $(\ell \cos \theta, \ell \sin \theta)$ and $(-\ell \cos \theta, -\ell \sin \theta)$ where θ changes with time as the masses move. Again, θ can be measured by projection onto the protractor. Finally, the string which connects the rod to the ceiling resists twisting so that at $\theta = 0$ it is untwisted and by Hooke's law, near $\theta = 0$, there is an effective potential of $U(\theta) = \frac{1}{2}\kappa\theta^2$ to give that resistance to twisting. The constant κ is called the torsion of the string.

(a) Starting from the Lagrangian for all of the four masses gravitating and including the effect of the torsion potential, show that the Lagrangian for θ becomes:

$$\mathcal{L} = m\ell^2\dot{\theta}^2 + \frac{GmM}{\ell} \left(\frac{1}{\sin\left(\frac{\alpha-\theta}{2}\right)} + \frac{1}{\cos\left(\frac{\alpha-\theta}{2}\right)} \right) - \frac{1}{2}\kappa\theta^2.$$

(b) Consider the heavy spheres to be removed so that the Lagrangian becomes:

$$\mathcal{L} = m\ell^2\dot{\theta}^2 - \frac{1}{2}\kappa\theta^2.$$

Show that θ then evolves as:

$$\ddot{\theta} + \frac{\kappa}{2m\ell^2}\theta = 0.$$

Thus, show that the torsion constant of the string can be measured by comparing it to m , ℓ , and τ , the period of this motion (measurable by counting swings of a Huygens pendulum) by:

$$\kappa = \frac{8\pi^2 m\ell^2}{\tau^2}.$$

(c) Attaching again the heavy spheres, show that the evolution of θ is now given by:

$$\ddot{\theta} + \frac{\kappa}{2m\ell^2}\theta + \frac{GM}{4\ell^3} \left(\frac{\sin\left(\frac{\alpha-\theta}{2}\right)}{\cos^2\left(\frac{\alpha-\theta}{2}\right)} - \frac{\cos\left(\frac{\alpha-\theta}{2}\right)}{\sin^2\left(\frac{\alpha-\theta}{2}\right)} \right) = 0.$$

(One may also add a velocity dependent term to account for air resistance, but it will have no effect for us.)

- (d) Thus, show (using the previous expression for κ) that G is related to the angle θ_{eq} at which the masses sit still in equilibrium, the rod radius ℓ , the angle between the heavy masses and the untwisted orientation of the rod α , the heavy mass M , and the non-gravitating period τ by:

$$G = \frac{16\pi^2\ell^3}{M\tau^2} \theta_{\text{eq}} \frac{\sin^2\left(\frac{\alpha-\theta_{\text{eq}}}{2}\right) \cos^2\left(\frac{\alpha-\theta_{\text{eq}}}{2}\right)}{\cos^3\left(\frac{\alpha-\theta_{\text{eq}}}{2}\right) - \sin^3\left(\frac{\alpha-\theta_{\text{eq}}}{2}\right)}.$$

Hence, using this technique we can calculate G from directly measurable quantities, as originally done by Cavendish. Currently, the experimental value is $G = 6.67430(15) \times 10^{-11} \frac{\text{m}^3}{\text{kg s}^2}$.

Problem 3.32: Virial Theorem. Consider a system of N masses moving around due to each other's gravity so that the Lagrangian is:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + \sum_{k=n+1}^N \frac{Gm_n m_k}{|\vec{x}_n - \vec{x}_k|} \right).$$

- (a) Define the dynamic inertia I :

$$I = \sum_{n=1}^N m_n |\vec{x}_n|^2.$$

Show that:

$$\frac{dI}{dt} = \sum_{n=1}^N 2m_n \vec{x}_n \cdot \dot{\vec{x}}_n, \quad \frac{d^2 I}{dt^2} = \sum_{n=1}^N 2m_n |\dot{\vec{x}}_n|^2 + \sum_{n=1}^N 2m_n \vec{x}_n \cdot \ddot{\vec{x}}_n.$$

Then, use the equations of motion given by the Lagrangian to show that:

$$\frac{d^2 I}{dt^2} = 2 \sum_{n=1}^N m_n |\dot{\vec{x}}_n|^2 - \sum_{n=1}^N \sum_{\substack{k=1 \\ k \neq n}}^N \frac{Gm_n m_k}{|\vec{x}_n - \vec{x}_k|}.$$

To do so, it may be useful to use the clever but simple identity:

$$\vec{x}_n = \frac{\vec{x}_n + \vec{x}_k}{2} + \frac{\vec{x}_n - \vec{x}_k}{2}.$$

- (b) Define the time average of a function by:

$$\mathbb{T}[f] \stackrel{\text{def}}{=} \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau f(t) dt.$$

Time averaging naturally smooths out any oscillatory behavior and is insensitive to the short-term behavior of the function. Thus, it is said to capture “steady-state” (long term) as opposed to “transient” (short term) behavior. Assume that all of the orbits of the masses in our system remain bounded with finite bounded velocity. Show then that $\frac{dI}{dt}$ is always bounded and that this implies that the time average of $\frac{d^2 I}{dt^2}$ vanishes. Thus, under this condition, conclude:

$$\mathbb{T} \left[\sum_{n=1}^N m_n |\dot{\vec{x}}_n|^2 \right] = \mathbb{T} \left[\sum_{n=1}^N \sum_{\substack{k=1 \\ k \neq n}}^N \frac{Gm_n m_k}{2|\vec{x}_n - \vec{x}_k|} \right].$$

As well, explain that it is only possible that all of the orbits remain perpetually bound in the center of mass frame. This time averaged equation is known as the Virial Theorem.

- (c) Define the average body mass m and total system mass M :

$$M = \sum_{n=1}^N m_n, \quad m = \frac{M}{N}.$$

In the left hand side of the Virial Theorem, there are N terms in the sum, and so the “typical”

speed-squared v^2 (v is called the virial speed) appearing in the sum is defined by:

$$Nmv^2 = \mathbb{T} \left[\sum_{n=1}^N m_n |\dot{\vec{x}}_n|^2 \right].$$

Show that if all of the individual body speeds are the same, then v^2 is also that same speed. As well, show that in general heavier bodies have a more significant effect on the numerical value of v^2 . In the right hand side of the Virial Theorem, there are $N(N-1)$ terms in the sum, and so the “typical” interbody separation R (called the virial radius) appearing in the sum is defined by:

$$N(N-1) \frac{Gm^2}{2R} = \mathbb{T} \left[\sum_{n=1}^N \sum_{\substack{k=1 \\ k \neq n}}^N \frac{Gm_n m_k}{2|\vec{x}_n - \vec{x}_k|} \right].$$

Show that if all of the interbody separations are the same, then R is also that same separation. As well, show that in general heavier bodies have a more significant effect on the numerical value of R .

- (d) From the above definitions, show that the total mass of the system is given by:

$$M = \frac{2Rv^2}{G} \frac{N}{N-1}.$$

Often this equation is applied to systems with a very large number of bodies so that $\frac{N}{N-1}$ is very well approximated as 1. As well, we of course cannot wait forever to measure the time averages of systems. But, if we wait at least long enough for the behavior of a system to stabilize (“virialize”) we can use measurements made after that stabilization as good approximations of the time average. Further, we often can only estimate R and v^2 by sampling a few bodies in the system (though because they are most significantly impacted by the more massive bodies in a system, if we sample the most massive bodies we can often get a good measurement). All of this is to say, this equation, while very useful for determining the total mass of a gravitating system (such as galaxies, to which it is often applied in astrophysics) is usually restricted to only being precise within a factor 2 (or more likely, a factor of 10). For the astrophysical applications, the interbody distances and velocities can be measured from Earth just by observations made with telescopes and so this equation allows one to infer the total mass of a distant gravitating system from direct measurements made on Earth.

Problem 3.33: Gravitational Multipole Expansion. Far from a gravitating body its gravitational field will be very nearly that of a point of equivalent mass. However, sometimes one needs to keep a better approximation. In this question we will develop how to systematically approximate the gravitational field due to a mass distribution for observations made far from that distribution.

- (a) Use that the mass density $\rho(\vec{x})$ can be written by definition of the Dirac delta as:

$$\rho(\vec{x}) = \int_{\mathbb{S}} \rho(\vec{x}') \delta(\vec{x} - \vec{x}') d^3 \vec{x}'$$

and use Taylor’s theorem on the Dirac delta (valid when it is integrated against an analytic function):

$$\delta(\vec{x} - \vec{x}') = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (\vec{x}' \cdot \nabla)^n \delta(\vec{x})$$

to show that the mass distribution can be rewritten as:

$$\rho(\vec{x}) = \sum_{n=0}^{\infty} \int_{\mathbb{S}} \rho(\vec{x}') \frac{x'^{a_1} \dots x'^{a_n}}{n!} d^3 \vec{x}' (-1)^n \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

Thus, the distribution can be expanded as a series in the Dirac delta and its derivatives.

- (b) Consider the lowest order term in this series. Show that it is:

$$\rho_0(\vec{x}) = m \delta(\vec{x}), \quad m = \int_{\mathbb{S}} \rho(\vec{x}') d^3 \vec{x}'$$

and explain that this means the lowest order term approximates the whole distribution by a point mass at the origin where that point mass has the total mass of the full distribution. This is called the “monopole” term because there is only 1 spike in the distribution.

- (c) Consider the next to lowest order term in the series. Show that it is:

$$\rho_1(\vec{x}) = -\vec{\varphi} \cdot \nabla \delta(\vec{x}), \quad \vec{\varphi} = \int_{\mathbb{S}} \rho(\vec{x}') \vec{x}' d^3 \vec{x}'.$$

This $\vec{\varphi}$ appearing here is called the “dipole moment” of the distribution. Graphically, draw a Dirac delta and take its derivative to understand that the derivative will have 2 equal and opposite spikes. This is why the corresponding distribution is called a “dipole”, for 2 spikes.

- (d) Explain by the above reasoning that each higher term, involving another derivative on the Dirac delta, will double the number of spikes in the distribution. Thus, $\delta^{(n)}(\vec{x})$ when graphed has 2^n spikes. This is why the next term after the dipole is called the “quadrupole”, follow by “octopole”, and so on. Graph what these would look like as distributions. In general then, the n^{th} raw multipole moment of a distribution is defined by:

$$Q_n^{a_1 \dots a_n} = \int_{\mathbb{S}} \rho(\vec{x}) x^{a_1} \dots x^{a_n} d^3 \vec{x}.$$

Thus, show that the total distribution is given by:

$$\rho(\vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} Q_n^{a_1 \dots a_n} \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

- (e) Now, use our series for the mass distribution in the Coulomb’s law solution to the Poisson equation to show that the potential due to the mass distribution is given by:

$$\phi(\vec{x}) = -G \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} Q_n^{a_1 \dots a_n} \partial_{a_1 \dots a_n}^n \frac{1}{|\vec{x}|}.$$

Explain that each term in this series is proportional to consecutively higher powers of $\frac{1}{|\vec{x}|}$ and thus that the first few terms of this series dominate when “far away” from the distribution.

- (f) Expand the expression for the potential to the first two corrections terms to show that it is given by:

$$\phi(\vec{x}) = -\frac{Gm}{r} - \frac{G\vec{\varphi} \cdot \vec{r}}{r^2} - \frac{G\vec{r} \cdot \hat{Q} \cdot \vec{r}}{2r^3} + \mathcal{O}\left(\frac{1}{r^4}\right)$$

where $r = |\vec{x}|$, $\vec{r} = \frac{\vec{x}}{r}$, and:

$$(\hat{Q})^{a_1 a_2} = 3Q_2^{a_1 a_2} - \text{Tr}(Q_2)\delta^{a_1 a_2}.$$

Thus, the raw quadrupole moment Q_2 does not appear in the potential but instead the traceless “true” quadrupole moment does. For each of the higher moments, a similar phenomena happens in which not all of the components of the raw multipole moments contribute to the potential. The part which does contribute is called the true multipole moment as opposed to the raw moment we have so far defined. The fact that only certain parts of the raw moment contribute is actually due to the rotational symmetry of the Poisson equation⁵. The first 1, 2, or 3 terms in our expansion for the potential are sufficient for an extremely wide variety of applications and this method can be directly used to compute all higher effects as needed.

Problem 3.34: Measuring the Radius of the Earth (method 1). The Earth defines a natural set of spherical coordinates of latitude θ , the angle above the equator, longitude φ , the angle rotated around the equator relative to a given great circle (called the prime meridian) perpendicular to the equator, and altitude h , the distance off of the Earth so that any point in this coordinate system is given by:

$$\vec{x}_e = \begin{pmatrix} (R+h) \cos \varphi \cos \theta \\ (R+h) \sin \varphi \cos \theta \\ (R+h) \sin \theta \end{pmatrix}$$

where R is the radius of the Earth, which we will now determine⁶. Consider another coordinate system in which the Sun is directly to the positive x direction from the Earth. In the Earth’s coordinate system, we defined the z direction as North, and thus along the axis of the Earth’s rotation. So, as the Earth rotates

⁵For the interested reader, check [52] to see that the n^{th} moment can be expressed in spherical harmonics with only $2n+1$ independent components.

⁶There are many independent and precise modern ways of determining the Earth’s radius, but we will describe a crude method simple enough for you to do at home.

about its axis it experiences a rotation $\hat{R}_z(\beta)$ with β covering a full 2π over the course of a day. However, the Earth's North is tilted by an angle α relative to the normal direction of the plane of orbit of the Earth about the Sun. Thus, apply an x axis rotation to the Earth's coordinate system by α to account for the tilt so that after rotation, the new z direction is the normal to the plane of orbit. As the Earth orbits the Sun, the direction of the Earth's North-South axis basically does not change⁷ (why? Think about conservation laws). Thus, all one has left to account for is that after going through an orbital angle of τ , the angle between the tilt and the line separating the Earth from the Sun will have rotated on the z axis by τ . τ will cover 2π over the course of 1 year. So, the position of a point on Earth in the fixed Sun coordinate system accounting for the orbital angle which develops throughout the year and the fixed tilt is:

$$\vec{x} = \hat{R}_z(\tau)\hat{R}_x(\alpha)\hat{R}_z(\beta)\vec{x}_e.$$

- (a) Explain that a point on (or above) Earth can see the Sun (and thus experiences daytime⁸.) whenever $x > 0$ or $y^2 + z^2 > R^2$. As well, explain that this second condition is equivalent to $(R + h)^2 - x^2 > R^2$ by using that rotations do not change the magnitude of a vector.
- (b) Show by calculating the above matrix multiplication that the x component is given by:

$$x = (R + h)(\cos(\varphi + \beta) \cos \theta \cos \tau - \sin(\varphi + \beta) \cos \theta \cos \alpha \sin \tau + \sin \theta \sin \alpha \sin \tau).$$

- (c) Whenever the North-South axis of the Earth is orthogonal to the Earth's displacement from the Sun, it is said to be an equinox. Show that equinox occurs when $\tau = 0$ or $\tau = \pi$ and that on equinox whether a point on the Earth sees the Sun or not is determined solely by $\varphi + \beta$. Then, explain that because τ does not change appreciably over 1 day and each point on Earth rotates through a full range of β in 1 day, over the course of the day of the equinox (about March 21 and September 22), everywhere on Earth gets an equal amount of daytime and nighttime⁹. As well, this gives a measure of the duration of one full day by adding the amount of daytime and amount of nighttime on the equinox. Call the duration of one day T .
- (d) Consider a person whose eyes are a height h off the ground when standing to be laying down on the ground watching the sunset over a clear and flat horizon on the day of equinox. When the bottom of the Sun first touches the horizon, they quickly start a timer and stand up. Because they are higher up, they can see the Sun just a little higher so that for a few seconds it has not yet touched the horizon from this higher perspective. When the bottom of the Sun first touches the horizon again from their higher location, they stop the timer and record the time that elapsed δt . Show that when the Sun first went down, $\cos(\varphi + \beta(t)) = 0$. Then, show that because the Earth rotates about its axis at a constant rate, $\beta(t + \delta t) = \beta(t) + \frac{2\pi\delta t}{T}$. Then, show that the Sun hits the horizon for the second time when:

$$1 - \cos^2(\varphi + \beta(t + \delta t)) \cos^2 \theta = \frac{R^2}{(R + h)^2}.$$

- (e) Finally, consider that δt will be very small (because a person is quite short compared to the radius of the Earth) and Taylor expand the above for small h and δt to show that the radius of the Earth is given by:

$$R \approx \frac{T^2 h}{2\pi^2 \delta t^2 \cos^2 \theta}.$$

- (f) The only remaining detail to determine is your latitude. Conveniently, this can also be determined easily on the equinox. Explain why on the equinox, using that the Sun is very far from the Earth compared to the Earth's radius, when the Sun is highest in the sky, the angle of the Sun above the horizon is $\frac{\pi}{2} - \theta$. Thus, by pointing directly at the Sun when it is at its highest in the sky on the day of the equinox and measuring the angle made with the ground, one can determine their latitude, completing what is needed to determine the radius of the Earth. Now the hardest things to do are to measure the time δt accurately and to not look at the Sun directly for too long while doing the experiment. The Earth is not a perfect sphere, but its averaged radius is experimentally 6371000 m.

⁷There are small effects which cause it to change, for example from the Moon and the Sun, but we will neglect them.

⁸In principle one also would want to account for atmospheric refraction. The light from the Sun is scattered significantly by interactions with particles in the atmosphere so that the apparent position of the Sun in the sky is not quite the actual position. This adds a few minutes of daylight to each day because the light from the Sun at the horizon is bent by these interactions in the atmosphere in a way which makes it visible even when physically the Sun is slightly below the horizon. The effect at the horizon is about half of a degree in the sky, which is also approximately the apparent diameter of the Sun.

⁹At least, almost everywhere on Earth it very nearly meets this criterion.

Problem 3.35: Measuring the Radius of the Earth (method 2). This method relies on even less technology than the previous method (no need to measure time), but it relies on more convenient geography (you will need more than a clear flat place to watch the sunset). Suppose you have a level (a stick partly filled with visible fluid so that you can see the surface line of the fluid), a very good protractor, and the ability to measure distances on flat ground.

- (a) Suppose there is a mountain cliff overlooking a flat region of land. The mountain has an unknown height h . You lay on the ground on the flat region and point directly at the mountain top, measuring an angle above horizontal of θ_1 . You then walk a distance d further away from the mountain and measure an angle above horizontal to the mountaintop of θ_2 . Show that the height of the mountain is given by:

$$h = d \frac{\tan \theta_1 \tan \theta_2}{\tan \theta_1 - \tan \theta_2}.$$

- (b) Now that you know the height of the mountain, you hike to the mountaintop. Using your level at the mountaintop you determine the direction tangent to the Earth pointing off the cliff. You then use your protractor to measure the angle α below level that points directly to the horizon. Show that the radius R of the Earth is given by:

$$R = \frac{h \cos \alpha}{1 - \cos \alpha}.$$

The Iranian scientist Abu Rayhan Muhammad ibn Ahmad al-Biruni (al Biruni for short) used this method in the 11th century to determine the radius of the Earth within 2% of the correct value [110].

Problem 3.36: Measuring the Mass of the Earth. Use the determined value of G , g , and the radius of the Earth R and their relationship with the mass of the Earth M to calculate the mass of the Earth. Experimentally, the value is 5.97237×10^{24} kg.

Problem 3.37: Measuring the Distance to the Moon. By observing the location of the Moon each night, one can find that it takes $\tau = 27.321$ days for the Moon to return to the same location in the sky relative to those stars which do not appear to move from night to night. Thus, explain that the orbital period of the Moon around the Earth is this time τ . Then, using Kepler's third law and that the Earth is much heavier than the moon, determine the semi-major axis distance of the Moon from the Earth. The experimental value is $\ell = 384748000$ m.

Problem 3.38: Measuring the Radius of the Moon. Once the distance to the moon is known, one can determine the radius of the Moon by measuring its angular size in the sky. Suppose the Moon has angular size θ in the sky (which you can measure by pointing at two ends of a diameter of the Moon on a full Moon and measuring the angle between those two lines, the experimental value varies between 29.3 and 34.1 arcminutes¹⁰). Show then that the radius of the Moon is given by $r = d \sin \frac{\theta}{2}$ where d is the distance to the Moon. The angular size of the Moon varies with time because the Moon's orbit is elliptical, not circular, and so its distance from Earth changes. Explain how using this method one can determine the eccentricity of the Moon's orbit by measuring the angular size of the Moon many different nights over a long period of time to find the minimum and maximum angular size of the Moon. Show in particular that the eccentricity is given by:

$$\varepsilon = \frac{\sin \left(\frac{\theta_{\max}}{2} \right) - \sin \left(\frac{\theta_{\min}}{2} \right)}{\sin \left(\frac{\theta_{\max}}{2} \right) + \sin \left(\frac{\theta_{\min}}{2} \right)}.$$

Experimentally, the eccentricity of the Moon's orbit is found to be .0549 and so the orbit is quite nearly circular. Show that the radius of the moon is given by:

$$r = \ell \frac{\sin \left(\frac{\theta_{\max}}{2} \right) + \sin \left(\frac{\theta_{\min}}{2} \right)}{2}.$$

where ℓ is defined as in the Kepler problem. Experimentally, the Moon's radius is found to be 1737400 m.

Problem 3.39: Measuring the Distance to the Sun. Consider the day of a half-moon, when precisely half of the Moon is illuminated by the Sun as seen on Earth.

- (a) Explain that at a half-moon, the triangle formed by the centers of the Earth, Moon, and Sun is a right

¹⁰An arcminute is $1/60^{\text{th}}$ of 1 degree (a degree in the sense of $1/360^{\text{th}}$ of 1 full revolution of 2π radians).

triangle with the right angle at the center of the Moon.

- (b) Consider an observer looking up at the sky at the time of day at which the line in the sky connecting the Sun and the Moon runs directly overhead on the day of a half moon. Draw the line connecting them to the Earth's center and let θ be the angle between that line and the line from the Earth's center to the Moon. Then, draw the line connecting the center of the Moon to the observer to form a triangle. Draw another line connecting the Sun's center to the Earth's center and let φ be the angle between that line and the line connecting the observer to the Earth's center. As well, draw the line connecting the center of the Sun to the observer to form another triangle. Then, let α be the angle the observer sees the Sun above the horizon and β be the angle the observer sees the Moon above the horizon. Using the law of sines, show that:

$$\frac{\cos(\beta + \theta)}{R} = \frac{\cos \beta}{\ell}, \quad \frac{\cos(\alpha + \varphi)}{R} = \frac{\cos \alpha}{d}$$

where R is the radius of the Earth, ℓ is the distance from the Earth to the Moon, and d is the distance from the Earth to the Sun.

- (c) Show using the right triangle formed by Earth, Moon, and Sun that:

$$\ell = d \cos(\theta + \varphi).$$

- (d) Eliminate θ and φ and solve for d using the above results to show that the distance from the Earth to the Sun is given by:

$$d = \sqrt{R^2 \cos^2 \alpha + \left(\frac{R^2 \cos \alpha \cos \beta \cos(\alpha + \beta) + R \sqrt{\ell^2 - R^2 \cos^2 \beta} \cos \alpha \sin(\alpha + \beta) - \ell^2}{\sqrt{\ell^2 - R^2 \cos^2 \beta} \cos(\alpha + \beta) - R \cos \beta \sin(\alpha + \beta)} \right)^2}.$$

Then, use that ℓ is much larger than R to show that at lowest order in R/ℓ ,

$$d \approx \frac{\ell}{\cos(\alpha + \beta)}.$$

Thus, with this we can determine the distance to the Sun, which has an experimental value of 149597870700 m.

Problem 3.40: Measuring the Radius of the Sun. Similarly to the Moon, once the distance to the Sun is known, one can determine the radius of the Sun by measuring its angular size in the sky. Suppose the Sun has angular size θ in the sky (which you can measure by pointing at two ends of a diameter of the Sun and measuring the angle between those two lines, the experimental value is between 31.6 and 32.7 arcminutes). Using the distance to the Sun we found and the angular size of the Sun on that same day, find the radius of the Sun. As well, find the eccentricity of the Earth's orbit around the Sun. Experimentally, the Sun's radius is found to be 696342000 m and the eccentricity of the Earth's orbit is found to be 0.0167086 and so the orbit is quite nearly circular.

Problem 3.41: Measuring the Mass of the Sun. Use the determined value of G , the distance from the Earth to the Sun d found above, the duration of one orbit of the Earth around the Sun (1 year), and the fact that the Sun is much heavier than anything else in the solar system to determine the mass of the Sun from Kepler's 3rd law. Experimentally, the mass of the Sun is found to be approximately 1.9885×10^{30} kg. Then, explain how given the mass of the Sun and the ability to determine the orbital periods of the other planets (just by observing their location each night in the sky), one can use Kepler's 3rd law to determine the distances to the other planets.

Problem 3.42: The Gravity Train Model the Earth as a uniformly massive ball of radius R and mass M . Consider a tunnel dug through the Earth between two points on it A and B without removing any meaningful amount of mass.

- (a) Without loss of generality, define the plane made by A , B , and the Earth's center as the xy plane and the y direction as the direction which bisects the angle formed by the line segments joining A and B to the center of the Earth. Let the angle between the y direction and the line segment joining A to the center of the Earth be φ . Then, show that in these coordinates, $A = (R \sin \varphi, R \cos \varphi, 0)$ and $B = (-R \sin \varphi, R \cos \varphi)$ (or, the two are swapped in which case rename A and B so this is true).
- (b) Thus, in these coordinates if a mass were to move within the tunnel from A to B it would move solely in the x -direction. Using the potential inside a uniformly massive sphere, show then that the Lagrangian

of a mass m moving within this tunnel is:

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{GMm}{2R^3}x^2.$$

- (c) Show that the mass moves through the tunnel exactly as a harmonic oscillator with angular frequency $\omega = \sqrt{\frac{g}{R}}$ independent of the distance between A and B . So, conclude that a “train” dropped into the tunnel from A will reach B in a time of $t = \pi\sqrt{\frac{R}{g}}$ independent of the distance between A and B . Show that this time using the parameters of Earth is only 42 minutes. This sounds almost like it would be a great way to get around on Earth but it is horribly impractical to actually make and would not operate nearly as simply as the model would suggest. This problem is a case of simplifying approximations taken too far, way beyond the point of usefully helping us study the real world. Think about why this gravity train would be entirely dysfunctional in reality.

Problem 3.43: Gravitational vs. Inertial mass. In our gravitational workings so far, we have assumed that the “gravitational charge” is mass. However, in principle, we could have taken the gravitational charge to be any function of the mass $f(m)$. Then, $f(m)$ is typically called the “gravitational mass” and m the “inertial mass”.

- (a) Explain that with the gravitational mass, the Lagrangian (3.6.1) would become:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2}m_n|\dot{\vec{x}}_n|^2 - f(m_n)\phi'(t, \vec{x}_n) \right) - \int_{\mathbb{S}} \frac{|\nabla\phi'|^2}{8\pi G'} d\mathbb{S}$$

- (b) Explain that because low mass objects are observed to move under the influence of gravity in a way which is independent of their mass, $f(0) = 0$. Then, Taylor expanding $f(m)$ (let us assume we can do so), show that by appropriate definition of ϕ' and G' we can take $f'(0) = 1$ without loss of generality. Thus, show that with this definition:

$$f(m) = m + am^2 + \mathcal{O}(m^3)$$

for some constant a .

- (c) Find the equations of motion for a mass experiencing gravity with $f(m)$ expanded to the previously mentioned order and describe how one could experimentally observe the effects of a from this modified equation of motion. The assumption $f(m) = m$ holds to very high experimental precision. The would-be effects of this parameter a have never been observed. Gravitational mass really is inertial mass.

3.7 Electrostatics

The next major success of Galilean mechanics comes from adding a new kind of charge separate from mass. We call it electric charge. The corresponding scalar potential ϕ is called the electric potential and the $\vec{E}$ field is called the electric field. Again settled by experiment, in this theory like charges are seen to repel and so ϵ is positive for this theory. So, the interacting theory has Lagrangian:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - q_n \phi(t, \vec{x}_n) \right) + \int_{\mathbb{S}} \frac{\epsilon_0}{2} |\nabla \phi|^2 d\mathbb{S}. \quad (3.7.1)$$

This theory is called electrostatics and $\epsilon = \epsilon_0$ is a constant officially called the vacuum permittivity but everyone just says “epsilon-naught”. It will also often be useful to solve for the potential and eliminate it to get the effective theory of just the charges:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - \sum_{k=n+1}^N \frac{q_n q_k}{4\pi \epsilon_0 |\vec{x}_n - \vec{x}_k|} \right). \quad (3.7.2)$$

It may seem at first glance that ϵ_0 is a “fundamental constant” of the theory, meaning a constant for which the only way to determine its value is by experiment. However, this is incorrect. We have so far no definition of electric charge other than that it measures the strength with which charges interact with the electric potential. Only the product $q\vec{E}$ appears in the equation of motion or correspondingly $q\phi$ in the Lagrangian. This does not define the overall scale of q in the sense that we can define $q' = \alpha q$ for α some constant and use q' as our new meaning of charge as long as we scale ϕ correspondingly so that the term in the Lagrangian is unchanged. That is, $q'\phi' = q\phi$ and so if $q' = \alpha q$ then $\phi' = \frac{1}{\alpha}\phi$. Putting this rescaled ϕ into the Lagrangian:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - q'_n \phi'(t, \vec{x}_n) \right) + \int_{\mathbb{S}} \frac{\epsilon_0}{2} \alpha^2 |\nabla \phi'|^2 d\mathbb{S}. \quad (3.7.3)$$

This looks the exact same as our original Lagrangian but with a new ϵ_0 :

$$\epsilon'_0 = \epsilon_0 \alpha^2. \quad (3.7.4)$$

By choosing the value of α , you can make the value of ϵ_0 whatever positive number you want. Choosing α is called “defining your units of charge”. The reason for this name is that it implicitly selects a charge q so that $q' = \alpha q$ has numerical value 1. Then, that selection acts like a “reference value” in the sense that the numerical value of any other charge would equal how strong it is compared to that reference. One can take an arbitrary particular reference charge of their choice (like when we have a reference length by a stick) to be 1 which then implicitly defines a numerical value for ϵ_0 which one needs to measure in an experiment. However, it is conceptually and mathematically clearer to define the value of ϵ_0 to be 1, as then one has 1 fewer unnecessary quantity appearing in all equations. It is always possible to do this from an initial value of ϵ_0 by selecting $\alpha = \frac{1}{\sqrt{\epsilon_0}}$. Then, one has no reference charges but can measure any charge without a reference. Either way, ϵ_0 is **NOT** fundamental to the theory, it is an artifact of your choice of units of charge. It’s numerical value is always decided by convention. For now we will keep factors of ϵ_0 explicit so that this book is maximally useful for comparing against sources written in SI units which due to historical baggage are cursed with a value of ϵ_0 which is not 1. Later in Part II we will switch permanently to using units of charge so that $\epsilon_0 = 1$ because not doing produces too much clutter to be reasonable. We will see clearly in the homework and in Appendix B how to restore factors of ϵ_0 after you have set it to 1 if you ever want to compare against someone using clunky units; you can always do so and no information at all is ever lost by setting $\epsilon_0 = 1$.

One can see that because ϵ_0 goes like the square of our scaling, no scaling can change the sign of ϵ_0 and so we cannot rescale an attractive theory to a repulsive one or vice versa. You could ask why we didn’t do the same scaling process to rescale our G in the gravitational theory to make $G = 1$. In principle, you could. But, mass is a little different than electric charge. If we set $G = 1$, then mass would have to be measured by gravitational experiments to get numerical values in this unit system. Unlike charge, mass appears in two different ways. It appears not only in the theory of gravity but the equations of motion in general. Thus, one would have to do gravitational experiments first to use mass measurements for anything else if one chose units in which G took a predefined value. Consequently, all experiments would have experimental uncertainty contributions from uncertainties in gravitational experiments. It turns out gravity is very weak for objects in daily life and gravitational experiments are correspondingly very hard to make precise. So, this is a very

impractical way to define units of mass; the error bars in every experiment would be unnecessarily large. We will see later that there are further good theoretical reasons not to define units of mass this way which would be valid no matter how precise gravitational experiments were. Electric charge on the other hand only shows up in the theories of electricity/magnetism and so there is no drawback when the value of ϵ_0 is chosen because nothing else is affected. Thus, by convention (with practical motivation), we do not and will never define our unit of mass to make G become 1. There is nothing we are currently able to measure more precisely than electricity/magnetism and so using experiments based on electricity/magnetism to define our unit system is optimal.

Exercises

Problem 3.44: Common Electrostatic Fields

- (a) Show using a symmetry argument and the integral form of Gauss' law that the $\vec{E}$ field due to a uniform spherical shell of charge q and radius R is:

$$\vec{E}(\vec{x}) = \begin{cases} 0, & |\vec{x}| < R \\ \frac{q\vec{x}}{4\pi\epsilon_0|\vec{x}|^3}, & |\vec{x}| > R \end{cases}$$

and that one can take as the potential corresponding to this electric field:

$$\phi(\vec{x}) = \begin{cases} \frac{q}{4\pi\epsilon_0 R}, & |\vec{x}| \leq R \\ \frac{q}{4\pi\epsilon_0|\vec{x}|}, & |\vec{x}| > R \end{cases}.$$

- (b) Show using a symmetry argument and the integral form of Gauss' law that the $\vec{E}$ field due to a uniform cylindrical shell of charge per unit length λ , radius R , and infinite length running in the z direction is:

$$\vec{E}(\vec{x}) = \begin{cases} 0, & \sqrt{x^2 + y^2} < R \\ \frac{\lambda(x, y, 0)}{2\pi\epsilon_0(x^2 + y^2)}, & \sqrt{x^2 + y^2} > R \end{cases}$$

and that one can take as the potential corresponding to this electric field:

$$\phi(\vec{x}) = \begin{cases} 0, & \sqrt{x^2 + y^2} \leq R \\ \frac{\lambda}{2\pi\epsilon_0} \ln\left(\frac{R}{\sqrt{x^2 + y^2}}\right), & \sqrt{x^2 + y^2} > R \end{cases}.$$

- (c) Show using a symmetry argument and the integral form of Gauss' law that the $\vec{E}$ field due to a uniform plane of charge per unit area σ and infinite extent with normal vector in the z direction is:

$$\vec{E}(\vec{x}) = \frac{\sigma}{2\epsilon_0} \text{sgn}(z) \vec{e}_z$$

and that one can take as the potential corresponding to this electric field:

$$\phi(\vec{x}) = -\frac{\sigma}{2\epsilon_0} |z|.$$

- (d) Consider a ball of radius R with uniform charge density ρ_0 except for a ball shaped cavity with no charge of smaller radius a with its center a distance $d < R - a$ off of the center of the larger ball. Using a symmetry argument and the linearity of Gauss' law, find the potential everywhere due to this charge distribution.

Problem 3.45: Electric Fringe Fields. The above infinite cylinder and infinite plane of charge above are obviously idealizations not realizable in the world. In practice, they are useful as approximations to the cases of a finite cylinder or finite plane, which have much more complicated fields. The difference in field between the finite case and the idealized cases is called the fringe field. Consider a line segment of length 2ℓ running along the z axis and centered on the origin carrying a uniform charge per unit length of λ . Use the cylindrical coordinates r, φ, z .

- (a) Using Coulomb's law, integrate to get that the exact potential is:

$$\phi(\vec{x}) = C + \frac{\lambda}{4\pi\epsilon_0} \ln\left(\frac{\sqrt{r^2 + (\ell - z)^2} + \ell - z}{\sqrt{r^2 + (\ell + z)^2} - \ell - z}\right).$$

To do so, the integration substitution $z' = z + r \tan \varphi'$ will be useful. Here C is an arbitrary constant due to gauge invariance.

- (b) Taylor expand the above potential in inverse powers of ℓ to get that:

$$\phi = C + \frac{\lambda}{4\pi\epsilon_0} \ln(4\ell^2) - \frac{\lambda}{2\pi\epsilon_0} \ln r + \frac{\lambda}{4\pi\epsilon_0\ell^2} \left| \frac{r^2}{2} - z^2 \right| + \mathcal{O}\left(\frac{1}{\ell^4}\right).$$

To do so, you will need an unfortunately high order of Taylor expansion for the square-root terms. Choose the constant C to cancel the constant term which otherwise would diverge as $\ell \rightarrow \infty$. Thus, identify the lowest order correction due to finite size to the potential.

Problem 3.46: ★ Measuring Charge with a Coulomb Balance. Consider two spherically symmetric charged bodies with charges q_1 and q_2 and masses m_1 and m_2 . The charge q_1 is attached to one end of a very light rod of length ℓ which is suspended by a string of torsion κ so that the position of q_1 is given by $\vec{x}_1 = (\ell \cos \theta, \ell \sin \theta, 0)$ and the rod-charge system can rotate by twisting the string. Thus, the effective potential due to twisting the string is $U = \frac{1}{2}\kappa\theta^2$ by Hooke's law. The charge q_2 is held fixed on a stand so that its position is given by $\vec{x}_2 = (\ell, -d, 0)$.

- (a) Show that the Lagrangian for the charges is then:

$$\mathcal{L} = \frac{1}{2}m_1\ell^2\dot{\theta}^2 - \frac{1}{2}\kappa\theta^2 - \frac{q_1q_2}{4\pi\epsilon_0\sqrt{d^2 + 2\ell d \sin \theta + 2\ell^2(1 - \cos \theta)}}$$

and that the equation of motion is then:

$$m_1\ell^2\ddot{\theta} = -\kappa\theta + \frac{q_1q_2}{4\pi\epsilon_0} \frac{\ell d \cos \theta + \ell^2 \sin \theta}{(d^2 + 2\ell d \sin \theta + 2\ell^2(1 - \cos \theta))^{\frac{3}{2}}}.$$

- (b) Show that the equilibrium deflection angle θ_{eq} satisfies:

$$\frac{q_1q_2}{\epsilon_0} = 4\pi\kappa \frac{(d^2 + 2\ell d \sin \theta_{\text{eq}} + 2\ell^2(1 - \cos \theta_{\text{eq}}))^{\frac{3}{2}}}{\ell d \cos \theta_{\text{eq}} + \ell^2 \sin \theta_{\text{eq}}} \theta_{\text{eq}}$$

and that for small deflection angle this becomes:

$$\frac{q_1q_2}{\epsilon_0} = \frac{4\pi\kappa d^2}{\ell} \theta_{\text{eq}} + \mathcal{O}(\theta_{\text{eq}}^2).$$

- (c) Suppose the charges are produced the exact same way so that $q_2 = q_1$ and that that charge is taken as the “reference charge” to define a unit of charge, q . Show then that the deflection angle allows one to measure ϵ_0 as:

$$\epsilon_0 = \frac{q^2}{4\pi\kappa\theta_{\text{eq}}} \frac{\ell d \cos \theta_{\text{eq}} + \ell^2 \sin \theta_{\text{eq}}}{(d^2 + 2\ell d \sin \theta_{\text{eq}} + 2\ell^2(1 - \cos \theta_{\text{eq}}))^{\frac{3}{2}}} = \frac{q^2\ell}{4\pi\kappa d^2\theta_{\text{eq}}} + \mathcal{O}(1).$$

One common choice of reference charge is the unit of the Coulomb, which is extremely large for most daily applications but for historical reasons is the SI unit of charge. The unit of Coulombs, written C, is defined so that the magnitude of the charge of an electron is exactly $1.602176634 \times 10^{-19}\text{C}$. If one takes the unit of Coulombs for their charges, the corresponding value of ϵ_0 will be $\epsilon_0 = 8.8541878128(13) \times 10^{-12} \frac{\text{C}^2\text{s}^2}{\text{kgm}^3}$. Because we will not define our charges by reference values, we will not have any need for the Coulomb.

- (d) Suppose instead that one wisely uses units in which $\epsilon_0 = 1$ by definition but again that the charges are produced in the same way so that $q_1 = q_2 = q$. Show then that:

$$q = \pm \sqrt{4\pi\epsilon_0\kappa \frac{(d^2 + 2\ell d \sin \theta_{\text{eq}} + 2\ell^2(1 - \cos \theta_{\text{eq}}))^{\frac{3}{2}}}{\ell d \cos \theta_{\text{eq}} + \ell^2 \sin \theta_{\text{eq}}} \theta_{\text{eq}}} = \sqrt{\frac{4\pi\epsilon_0\kappa d^2\theta_{\text{eq}}}{\ell}} + \mathcal{O}(\theta_{\text{eq}}).$$

Hence, this apparatus can measure q . Explain that the sign is not determined by $\epsilon_0 = 1$ because $q \rightarrow -q$ leaves the theory, including the value of ϵ_0 , unchanged. Thus, one picks by convention which charge counts as positive and which counts as negative. (Once such a convention is set, it is fixed for any future experiments by attraction or repulsion to the charge with defined sign.)

- (e) Suppose one is not fortunate enough to have two identical charges and instead has three unknown charges q_1, q_2, q_3 and the ability to swap which charges are attached to the Coulomb balance at will. Explain how by taking measurements from the Coulomb balance, one can determine the products:

$$f_{12} = q_1q_2, \quad f_{13} = q_1q_3, \quad f_{23} = q_2q_3$$

and that from these products one can determine the charges as:

$$q_1 = \pm \sqrt{\frac{f_{12}f_{13}}{f_{23}}}, \quad q_2 = \frac{f_{12}}{q_1}, \quad q_3 = \frac{f_{13}}{q_1}.$$

Thus, one can determine q_1 (up to defining the sign by convention) and then use it to determine q_2 and q_3 .

- (f) Suppose now that one has determined a specific charge q by the above three charge procedure and now attaches a new unknown charge q' with it to the Coulomb balance. Show that q' is given by:

$$q' = \frac{4\pi\kappa}{q} \frac{(d^2 + 2\ell d \sin \theta_{\text{eq}} + 2\ell^2(1 - \cos \theta_{\text{eq}}))^{\frac{3}{2}}}{\ell d \cos \theta_{\text{eq}} + \ell^2 \sin \theta_{\text{eq}}} \theta_{\text{eq}} = \frac{4\pi\kappa d^2}{\ell q} \theta_{\text{eq}} + \mathcal{O}(\theta_{\text{eq}}^2).$$

Thus, the Coulomb balance allows us to measure the values of other charges from a known charge.

Problem 3.47: Establishing properties of Electrostatics. In order to measure charges by the method of the Coulomb balance, we need a consistent way to prepare q_1 to measure other charges against. As well, we ought to see how to determine that in fact electrostatics is a repulsive theory.

- Almost all every day objects do not seem to attract or repel each other under everyday circumstances. Thus, conclude that every day objects are typically charge neutral (or at least nearly so).
- It is observed that if two glass rods are each rubbed against wool then each touched to a different metal ball, the two metal balls will repel each other. Then, if the metal balls are touched to a large metal surface and then brought back near each other, there will be no more repulsion. Thus, explain that rubbing the glass rod on the wool accumulates charge on it and that touching the glass rod to the metal transfers the excess charge from it (“discharges” it) to the metal.
- Explain that the fact that the metal balls after being touched by the glass rods which had been rubbed on the wool repel each other implies that electrostatics is a repulsive theory.
- It is observed that if the above procedure is repeated but the wool is rubbed on silk, then the results are the same. Explain how this is what is predicted by the previous part.
- It is observed that if one of the glass rods is rubbed on wool and the other is rubbed on silk and then each is touched to their respective metal balls, then those two metal balls will attract each other. Thus, conclude that rubbing on wool and rubbing on silk accumulate different signs of charge. Which one is decided to be positive or negative is a historical convention. Benjamin Franklin set the convention that the charge accumulated on the glass by rubbing it on silk is called positive while the charge accumulated by rubbing the glass on wool is negative. The fact that charge can be accumulated on certain surfaces due to rubbing them on other specific surfaces is called **triboelectricity** (electricity due to friction). The theoretical explanation for such is actually quite intricate.
- Explain then that by “charging up” metal balls using wool, silk, and glass we can accumulate the charges necessary to calibrate the Coulomb balance by the three charge method in the previous problem. Then, explain how keeping one of these charged metal balls on the Coulomb balance allows on to test the charge of a desired external charge.

Problem 3.48: Electric Boundary Conditions. Consider a surface which has a not necessarily uniform surface charge density σ on it.

- (a) Take Faraday’s law and integrate it over an at the moment arbitrary area $\mathbb{A}$ to show that:

$$\int_{\partial\mathbb{A}} \vec{E} \cdot d\vec{x} = -\frac{d}{dt} \int_{\mathbb{A}} \vec{B} \cdot d\vec{\mathbb{A}}.$$

Then, take the integration region to be a rectangle of length ℓ which is parallel to the charged surface and thickness w which is perpendicular to the charged surface and for which one side of the rectangle lies on each side of the charged surface. Call the side of the rectangle “below” the charged surface T_- , the side of the rectangle which crosses from below to above N_+ , the side of the rectangle “above” the charged surface T_+ , and the side of the rectangle which crosses from above to below N_- . Then, show that the above integral formula becomes:

$$\int_{T_-} \vec{E} \cdot d\vec{x} + \int_{N_+} \vec{E} \cdot d\vec{x} + \int_{T_+} \vec{E} \cdot d\vec{x} + \int_{N_-} \vec{E} \cdot d\vec{x} = -\frac{d}{dt} \int_{\mathbb{A}} \vec{B} \cdot d\vec{\mathbb{A}}.$$

- (b) Show that in the limit that the thickness of the rectangle is taken to 0, the area goes to 0 and N_+ and N_- go to 0. As well, that T_- and T_+ both make contact with the charged surface (but one on each side

of the surface). Let $\vec{E}^-$ be the limit of the electric field as one approaches the charged surface from below and $\vec{E}^+$ be the limit of the electric field as one approaches the charged surface from above. Show taking $w \rightarrow 0$ gives:

$$\int_{T_-} \vec{E}^- \cdot d\vec{x} + \int_{T_+} \vec{E}^+ \cdot d\vec{x} = 0.$$

- (c) Divide both sides of the above by ℓ and take the limit that $\ell \rightarrow 0$. Let $\vec{T}$ be the tangent vector to the charged surface in the direction of the side T_+ of the rectangle. Show that the above becomes:

$$-\vec{T} \cdot \vec{E}^- + \vec{T} \cdot \vec{E}^+ = 0.$$

Thus conclude that part of the electric field which is parallel to the charged surface, $\vec{E}_{\parallel}$, is continuous across the surface:

$$\vec{E}_{\parallel}^+ = \vec{E}_{\parallel}^-.$$

- (d) Consider now the integral form of Gauss' law. Let the volume of integration be a cylinder of height h and cross sectional area $\mathbb{A}$ for which one end cap ($\mathbb{A}_-$) is below the charged surface and one end cap ($\mathbb{A}_+$) is above the charged surface. Let S be the shell (without end caps) of the cylinder. Show that the integral form of Gauss' law then becomes:

$$\int_{\mathbb{A}_-} \vec{E} \cdot d\vec{\mathbb{A}} + \int_S \vec{E} \cdot d\vec{\mathbb{A}} + \int_{\mathbb{A}_+} \vec{E} \cdot d\vec{\mathbb{A}} = \frac{q[\mathbb{V}]}{\epsilon_0}.$$

- (e) Take the limit that $h \rightarrow 0$ to show that S goes to 0 and that $q[\mathbb{V}]$ goes to only the contribution from the charge on the charged surface. As well, show that in the limit both $\mathbb{A}_+$ and $\mathbb{A}_-$ make contact with the charged surface. Then, show that the above integrals become:

$$\int_{\mathbb{A}} \vec{E}^- \cdot d\vec{\mathbb{A}} + \int_{\mathbb{A}} \vec{E}^+ \cdot d\vec{\mathbb{A}} = \int_{\mathbb{A}} \frac{\sigma}{\epsilon_0} d\mathbb{A}.$$

- (f) Divide both sides of the above by $\mathbb{A}$ and take the limit that $\mathbb{A} \rightarrow 0$. Let $\vec{n}$ be the normal vector to the charged surface pointing out of the surface from above. Show that the above becomes:

$$-\vec{E}^- \cdot \vec{n} + \vec{E}^+ \cdot \vec{n} = \frac{\sigma}{\epsilon_0}.$$

Thus conclude that the component of the electric field which is perpendicular to the charged surface, $E_{\perp}$, is discontinuous across the surface where the discontinuity is precisely the surface charge density:

$$E_{\perp}^+ - E_{\perp}^- = \frac{\sigma}{\epsilon_0}.$$

- (g) Combine both components of the boundary conditions to show that:

$$\vec{E}^+ - \vec{E}^- = \frac{\sigma}{\epsilon_0} \vec{n}.$$

Problem 3.49: Properties of Conductors. An ideal conductor is a material through which charge can move perfectly freely. Metals are often well modeled as ideal conductors.

- Consider the interior of a conducting volume. Suppose the charges in the conductor have equilibrated so that they are not moving. Show then that the electric field in the interior must be 0 (by using the equation of motion for the charges). Thus, in equilibrium, the electric field inside any conducting volume is 0.
- Then, take Gauss' law combined with the previous conclusion to show that the charge density inside any conducting volume must vanish in equilibrium. So, we also see that all of the charge in a conductor accumulates on the surface.
- Consider now the bounding surface of the conducting volume. Suppose the charges in the conductor have equilibrated and show then that the part of the electric field parallel to the surface must be 0 (again use the equation of motion but note that because the charges don't leave the surface there may be normal constraint forces on the charge). Thus, in equilibrium the electric field parallel to the surface of a conductor is 0 (the normal component need not be 0).
- Using electrostatic gauge, show that the conclusion that the parallel components of the electric field on the surface vanish implies that the scalar potential ϕ takes the same value over the whole surface of the conductor. Thus, the surface of a conductor is said to be an equipotential.
- Consider then a conducting volume with thickness characterized by a length h which has an interior

cavity. Let σ_- be the surface charge density on the inner surface (the surface which bounds the cavity) and σ_+ be the surface charge density on the outer surface (the surface which faces the exterior of the volume). Show using the result of the previous problem that:

$$\sigma_- = -\epsilon_0 E_{\perp}^-, \quad \sigma_+ = \epsilon_0 E_{\perp}^+$$

where $E_{\perp}^-$ is the electric field pointing into the cavity on the inner surface of the conductor and $E_{\perp}^+$ is the electric field point out of the conductor on its outer surface. These results are independent of the thickness and so remain valid as we consider the limit of $h \rightarrow 0$ in which the volume becomes a closed conducting surface (such as a sphere).

Problem 3.50: Common Conductors and the Method of Images. The fact that the Poisson equation with appropriately specified boundary conditions has a unique solution allows us to find prospective solutions by intelligent guessing which by then verifying that such a prospect satisfies the desired equation and boundary conditions, guarantees it is in fact *the* solution. One common way of doing so for conductors is called the method of images. Because a conducting surface must be an equipotential, we can often find the equilibrium state of a conducting surface when it is exposed to an external charge by considering adding to the system one or more hypothetical charges on the other side of the conductor and choosing the positions and strengths of the charges so as to make the surface of the conductor an equipotential. These hypothetical charges are called image charges.

- Consider an infinite conducting plane at $z = 0$ and consider an external charge q to be placed at (x_0, y_0, z_0) with $z_0 > 0$. Identify the charge q' and position $\vec{x}' = (x'_0, y'_0, z'_0)$ which an image charge should have (it must be below the plane) to make the surface of the conductor an equipotential. Then, write the full potential of the conductor-charge system above the conducting plane and compute the induced charge density on the top of the conducting plane due to the external charge.
- Once you have found the potential on the conducting plane, use the Laplace equation with that potential as the boundary condition to find the potential below the conducting plane. As well, compute the induced charge density on the bottom of the conducting plane due to the external charge.
- Consider a conducting sphere of radius R with its center at the origin and a charge q placed inside the sphere at $\vec{x}_0$. Identify the charge q' and position $\vec{x}'_0$ which an image charge should have (it must be outside of the sphere) to make the surface of the conductor an equipotential. Then, write the full potential of the conductor-charge system and compute the induced charge density on the inner surface of the sphere.
- Once you have found the potential on the sphere, use the Laplace equation with the potential as the boundary condition to find the potential outside of the sphere. As well, compute the induced charge density on the outer surface of the sphere due to the external charge. You should find that the field outside of the sphere depends only on the total charge within the sphere but not where that charge is located within the sphere. This a general feature of the fields outside of conducting volumes.

Problem 3.51: Faraday Cages and Conductive Shielding. Consider a conducting volume with an interior cavity. Consider an external charge q placed outside of the conducting volume. Show that not only is the electric field throughout the conductor 0 but also that the electric field in the cavity is 0 as well. To do so, you may find it helpful to use theorem 3.2. Thus, wrapping a region of space in a conductor “shields” it from the electric fields on any external charges. Such a device, often called a Faraday cage (because a conducting mesh can essentially accomplish the same job and is more practical for many applications), is very useful for protecting sensitive electromagnetic equipment from potentially dangerous external factors.

Problem 3.52: Potential Difference and Electromotive Force. Consider a system of charges experiencing $\vec{E}$ and $\vec{B}$ fields. The Electromotive Force or commonly “EMF”, written $\mathcal{E}$, experienced by charges along a path is defined as the line integral of the Lorentz force per unit charge on the body. That is, along the path γ :

$$\mathcal{E}[\gamma] = \int_{\gamma} \left(\vec{E} + \dot{\vec{x}} \times \vec{B} \right) \cdot d\vec{x}.$$

Here $\vec{x}(t, s)$ is the position on the path $\gamma(t)$. s is some parameter which labels positions along the path. The path γ is allowed to be time dependent in general. One should be careful to note that $\dot{\vec{x}}$ is the velocity (the time derivative of $\vec{x}(t, s)$) and $d\vec{x}$ is the displacement along the path ($\frac{d\vec{x}}{ds} ds$) and not the displacement in time.

This is why $(\dot{\vec{x}} \times \vec{B}) \cdot d\vec{x} \neq 0$ generally. The practical usefulness of the EMF will be established over the following sections.

- (a) We found that in Galilean electrostatics, $\vec{B} = 0$ and $\vec{E} = -\nabla\phi$ in electrostatic gauge. Show that in this gauge if ϕ does not depend on time then the EMF depends only on the end points of the path γ and is given by the difference in ϕ at those end points. Thus, in electrostatics, the EMF is often called a “potential difference”.
- (b) Suppose that the path $\gamma(t)$ is the shape of a wire at time t in which charges move. Suppose that charges in the rest frame of the wire only move down the direction of the wire. As well, suppose that all of the charges in the wire move with the same speed relative to the wire and that $\vec{E}$ and $\vec{B}$ do not depend on time. Show that the work done on a charge q when moving through the wire is given by:

$$W = q\mathcal{E}[\gamma].$$

Thus, the emf can be under these conditions interpreted as the work done per unit charge on the charges flowing through the wire. These assumptions seem quite restrictive but in a more realistic sense, we could replace these exact assumptions with more achievable approximations. If one were to average over all of the charges moving in the wire, we would only need the average velocity over the charges to point down the wire. The condition that all of the charges move with the same speed can likewise be replaced by requiring that the net flow charge per time through any cross section of the wire is the same as any other cross section (this is equivalent to requiring no charge accumulates anywhere in the wire by the continuity equation). As well, if $\vec{E}$ and $\vec{B}$ are time dependent but merely change very little in the time that it takes a charge to flow down the wire (which is often true), then at least to very good approximation, emf retains the interpretation given.

Problem 3.53: Properties of Capacitors. Consider two conductors which together have a net charge of 0 and which are connected by a battery. A battery is a device which has two ends and provides a fixed EMF between those two ends. Let that EMF be called $\mathcal{E}$. If one takes a path starting at one end of the battery and ending at the other and receives a positive emf then the starting point is called the positive terminal of the battery and the end point is called the negative terminal of the battery. Charge is able to flow between the conductors through the battery. We will discuss a simple way to actualize a battery in a later question.

- (a) Show using the linearity of the Poisson equation that when the charges have equilibrated there will be a positive charge q accumulated on the conductor connected to the positive terminal of the battery and a negative charge $-q$ accumulated on the conductor connected to the negative terminal of the battery and that if the battery EMF is multiplied by a constant α : $\mathcal{E}' = \alpha\mathcal{E}$ then the induced charge is also scaled by that same factor: $q' = \alpha q$. Thus, conclude that the quantity:

$$C = \frac{q}{\mathcal{E}}$$

is independent of $\mathcal{E}$ and so an intrinsic property of the two conductor system. This quantity is called the “capacitance” of the system. It gives charge accumulated on one of the conductors per EMF applied between them.

- (b) Consider two concentric spherical conductors with the smaller one of radius R_1 and the larger one of radius R_2 . Suppose there is an emf of $\mathcal{E}$ between the two spheres and compute the induced charge on them. From this, find the capacitance of the system. Such a two conductor system is called a capacitor.
- (c) Consider two concentric cylindrical conductors with the smaller one of radius R_1 and the larger one of radius R_2 . Take both conductors to have infinite length. Suppose there is an emf of $\mathcal{E}$ between the two cylinders and compute the induced charge per unit length on them. From this, find the capacitance per unit length of the system. As well, from this find the lowest order expression for the capacitance of the system if the cylinders have finite but very large length ℓ .
- (d) Consider two parallel plate conductors which are separated by a distance d and both have infinite area. Suppose there is an emf of $\mathcal{E}$ between the two plates and compute the induced charge per unit area on them. From this, find the capacitance per unit area of the system. As well, from this find the lowest order expression for the capacitance of the system if the plates have finite but very large area A .

Problem 3.54: Energy stored by a Capacitor.

- (a) From the Lagrangian and using Gauss’ Law, show that in equilibrium (when all charges have become

stationary) the energy of a system of charges becomes:

$$E = \int_{\text{All } q} \frac{dq(\vec{x})dq(\vec{x}')}{8\pi\epsilon_0|\vec{x}-\vec{x}'|} = \frac{1}{2} \int_{\mathbb{S}} \phi(\vec{x})dq(\vec{x}).$$

- (b) Consider two non-overlapping charge distributions M_1 and M_2 . Show that the energy becomes:

$$E = \frac{1}{2} \int_{M_1} \phi(\vec{x})dq(\vec{x}) + \frac{1}{2} \int_{M_2} \phi(\vec{x})dq(\vec{x}).$$

- (c) Consider the two distributions to each be due to conductors so that on each distribution the potential is uniform. As well, assume the two conductors form a capacitor so that the charge q of distribution M_1 is balanced by a charge of $-q$ in distribution M_2 . Let $\mathcal{E}$ be the emf between the two conductors. Show that the energy becomes:

$$E = \frac{1}{2}q\mathcal{E}.$$

- (d) Show using the definition of capacitance that the energy of the capacitor can be written as:

$$E = \frac{q^2}{2C} = \frac{1}{2}C\mathcal{E}^2.$$

Problem 3.55: ★ Classical Scattering. Consider a mass m to have a Hamiltonian which is the free particle Hamiltonian everywhere except a finite region M of space called the collision region. In that region it may have some generic position dependence. That is, for $\vec{x}$ outside of M , $\mathcal{H} = \frac{|\vec{p}|^2}{2m}$ and for $\vec{x}$ inside of M , $\mathcal{H} = \mathcal{H}(\vec{x}, \vec{p})$. Let the origin of our coordinate system be some point within M (which we will typically set to be the “center” in some sense of M).

- (a) Suppose the particle starts at $(b \cos \alpha, b \sin \alpha, -w)$ for $w > 0$, $b > 0$ with initial velocity $v = v_0(0, 0, 1)$. The parameter b is called the impact parameter and the parameter α is called the beam angle. Because the collision region is finite, if b is sufficiently large the particle never enters the collision region and thus passes right through as a completely free particle. This persists if we consider the limit $w \rightarrow \infty$. However, if b is sufficiently small it will enter the interaction region and be affected by the Hamiltonian in that region. Often, by integrating the equations of motion, the particle will be found to eventually escape that region permanently. If it does so, the particle is said to have scattered. If it never leaves permanently, the particle is said to have become bound. Show that if a particle is scattered, then it will actually go arbitrarily far away from the collision region as $t \rightarrow \infty$. As well, express the position of the particle in spherical coordinates $\vec{x}(t) = (r(t) \cos \varphi(t) \sin \theta(t), r(t) \sin \varphi(t) \sin \theta(t), r(t) \cos \theta(t))$ and show that $\theta(t)$ and $\varphi(t)$ have well defined limits as $t \rightarrow \infty$.
- (b) Consider a scattered particle as above and suppose we have a probability distribution of initial conditions of the particle $f_{\text{in}}(b, \alpha)$ which is the probability per unit area that the particle has initial conditions b and α . Explain that by solving the equations of motion the $t \rightarrow \infty$ limits of θ and φ can be computed in terms of b and α and thus that as $t \rightarrow \infty$ this initial distribution of b and α allows us to define a final distribution of θ and φ satisfying:

$$f_{\text{in}}(b, \alpha) b db d\alpha = f_{\text{out}}(\theta, \varphi) \sin \theta d\theta d\varphi$$

where $f_{\text{out}}(\theta, \varphi)$ is the probability per unit solid angle that that particle limits to those values of θ and φ .

- (c) Define the interaction cross section $\frac{d\sigma}{d\Omega}$ by the ratio of the outgoing distribution per unit solid angle to the input distribution per unit cross section:

$$\frac{d\sigma}{d\Omega} = \frac{f_{\text{out}}(\theta, \varphi)}{f_{\text{in}}(b, \alpha)} = \left| \frac{b db d\alpha}{\sin \theta d\theta d\varphi} \right|$$

where $d\Omega = \sin \theta d\theta d\varphi$ is the differential solid angle. Similarly, define the integrated cross section by:

$$\sigma = \int_{\Omega} \frac{d\sigma}{d\Omega} d\Omega.$$

Now consider the incoming distribution to be a uniform distribution $f_{\text{in}}(b, \alpha) = \frac{1}{\mathbb{A}}$ over an area $\mathbb{A}$ such that when put into the equations of motion this area maps to covering the whole sphere of (θ, φ) . Show that in this case the outgoing distribution becomes:

$$f_{\text{out}}(\theta, \varphi) = \frac{1}{\mathbb{A}} \frac{d\sigma}{d\Omega}$$

and that then this area $\mathbb{A}$ must be the integrated cross section σ . Thus, explain that the integrated cross section σ has the interpretation of the incoming cross sectional area which gets mapped to cover the whole sphere and thus is the cross sectional area of the largest beam of incoming particles so that all particles in the beam get scattered.

- (d) In experimental applications, one typically has a beam of many particles with some incoming distribution which is fired at a target (the collision region) and a detector surrounding the collision region so that θ and φ can be measured by noting the point of impact on the detector. Explain that if one runs the beam without the collision region in place (meaning all the particles are free), by observing where the particles land on a wall placed opposite the beam, one can measure $f_{\text{in}}(b, \alpha)$. Then, explain that if one observes where particles land on the spherical detector one can measure f_{out} . Finally then explain that this allows us to experimentally measure the scattering cross section. Because the scattering cross section can be directly experimentally measured and directly theoretically computed from the Hamiltonian, it is a very common and essential way of comparing theory and experiment. While we treated the collision region M as being of finite size in this question, one can in principle take the collision region to become arbitrarily large and fill space as long as in the limit that one goes far away from the “center” the Hamiltonian limits to the free particle Hamiltonian sufficiently quickly.

Problem 3.56: Hard Spheres - the Kablamiltonian. Consider an impenetrable sphere of radius R fixed at the origin and a mass m which is fired at this sphere with speed v_0 , impact parameter b , and beam angle α .

- (a) Show that if $b > R$ then the particle is not scattered and if $b \leq R$ then it is.
 (b) Show that if $b \leq R$:

$$\alpha = \varphi, \quad b = R \cos \frac{\theta}{2}$$

where θ and φ are asymptotic final spherical coordinates of the mass.

- (c) Show that:

$$\frac{d\sigma}{d\Omega} = \frac{R^2}{4}, \quad \sigma = \pi R^2$$

and that σ matches the cross sectional area of the beam which is scattered by the target.

Problem 3.57: ★ Rutherford Scattering. Consider a charge Q fixed at the origin and a mass m with charge q which is fired at this target charge with speed v_0 , impact parameter b , and beam angle α .

- (a) Show that the Hamiltonian for this system is:

$$\mathcal{H} = \frac{|\vec{p}|^2}{2m} + \frac{qQ}{4\pi\epsilon_0 r}$$

Thus, we can apply the Binet equation to this problem.

- (b) Show using energy and angular momentum conservation that:

$$E = \frac{1}{2}mv_0^2, \quad L = mv_0 b.$$

- (c) Show using the Binet equation or solution to the Kepler problem that the trajectory is given by:

$$\frac{1}{r(\beta)} = -\frac{qQm}{4\pi\epsilon_0 L^2} + A \cos(\beta - \beta_0)$$

where A and β_0 are constants determined by initial conditions. We have used β as the polar coordinates angle to avoid notation confusion later.

- (d) Define the coordinate system so that at $\beta = 0$, the charge is the closest it will get to the target and let that minimum distance be called R . Show using energy conservation that:

$$E = \frac{L^2}{2mR^2} + \frac{qQ}{4\pi\epsilon_0 R}, \quad \frac{1}{R} = -\frac{qQm}{4\pi\epsilon_0 L^2} + A$$

and use these results together to show that the trajectory is given by:

$$\frac{1}{r(\beta)} = -\frac{\ell}{b^2} + \left(\frac{\ell}{b^2} + \frac{1}{\ell + \sqrt{\ell^2 + b^2}} \right) \cos \beta$$

where $\ell = \frac{qQ}{4\pi\epsilon_0 mv_0^2}$.

- (e) Let β_∞ be the polar angle that the particle asymptotically goes to in these coordinates as $t \rightarrow \infty$. Show

that:

$$\cos \beta_{\infty} = \frac{\ell}{\sqrt{\ell^2 + b^2}}.$$

- (f) Now consider the incoming charge in the context of scattering. Show that:

$$\varphi = \alpha, \quad \theta = \pi - 2\beta_{\infty}, \quad b = \frac{\ell}{\tan \frac{\theta}{2}}.$$

- (g) Finally then, show that the Coulomb interaction has scattering cross section:

$$\frac{d\sigma}{d\Omega} = \left(\frac{qQ}{16\pi\epsilon_0 E^2} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}}.$$

This is called the Rutherford formula. Because the scattering cross section can be directly experimentally observed, fitting those experimental findings to this functional form across a range of v_0 allows one to measure $\frac{qQ}{m\epsilon_0}$ and check that in fact the interaction of the two charges is well described by Coulomb's law.

Historically, this scattering experiment was originally done with a beam of positively charged particles known as “alpha-particles” scattering off of a very thin sheet of gold. Everyday matter is generally charge neutral. Before the Rutherford experiment, it was known that the current in electrical circuits was carried by a species of low mass negatively charged particles we now call electrons but it was believed that in everyday materials like gold the electrons were scattered randomly throughout the material while the rest of the material was an essentially continuous blob of positive charge. If this model were correct, the alpha-particle beam would pass straight through the gold because the alpha-particles are much heavier than the electrons and so deflect them away and the homogeneous positive charge background of the gold would have an averaged effect of basically nothing. Instead, what actually happened was that most of the beam passed straight through but some, a significant fraction, of the beam was deflected by a very large angle (greater than 90°). Explain using the Coulomb cross section how this is consistent with interpreting the positive charge of the gold as being contained in small separated regions, now called atomic nuclei, and that the parts of the beam that are deflected by a large angle are those that have very small impact parameter with one of the nuclei. Later experiments of course demonstrated that atomic nuclei themselves consist of positively charged protons and electrically neutral neutrons. The proton charge by all experiments is exactly equal in magnitude but opposite in sign to the electron charge (there is a theoretical reason why this must be true, but we will not get there until Part II) but the electron is much lighter than either the proton or neutron in mass, which is why it moves around more easily to do the charge carrying. Alpha-particles are now known to just be blobs of two protons and two neutrons, and gold nuclei are now known to be blobs of 79 protons and 118 neutrons. Quickly after the Rutherford experiment, it was established that the atomic number Z of an element in the periodic table is exactly equal to the number of protons in the nucleus of an atom of that element.

- (h) Show that the integrated cross section from the Rutherford formula diverges and explain why this is not surprising given that the Coulomb interaction has infinite range (is non-zero for all finite values of r and decays quite slowly with r).

Problem 3.58: Beam Attenuation. Consider a beam of particles which is fired at a material which has a uniform number density n of collision regions (or “targets”) per unit volume and for which the integrated cross section of the scattering of a beam particle off of any of the collision regions is σ .

- (a) Consider an individual beam particle. Suppose that we are firing that particle toward a slice of this material of area A with thickness δx . Suppose that δx is small enough so that none of the cross sections of the collision regions in this slice overlap each other. Show then that the probability that the particle is scattered in this slice is given by:

$$p = \frac{\text{Number of Targets in the Slice} \times \text{Cross Section of Each Target}}{\text{Cross Sectional Area of the Slice}} = n\sigma\delta x.$$

- (b) Suppose we align N such slices as above, each of the same thickness δx . Let P_k be the probability that the particle has not been scattered after going through k slices. Show that:

$$P_0 = 1, \quad P_{k+1} = (1 - n\sigma\delta x)P_k.$$

- (c) Let $P(x)$ be the probability that the particle has not been scattered after going a depth x into a

continuous medium containing these targets. Take the $\delta x \rightarrow 0$ limit of the previous part to show that:

$$P(0) = 1, \quad \frac{dP}{dx}(x) = -n\sigma P(x).$$

As well, solve this differential equation to show that:

$$P(x) = e^{-n\sigma x}.$$

- (d) Let $f(x)$ be the probability per unit length that the particle scatters at depth x . Show that:

$$f(x) = -\frac{dP}{dx} = n\sigma e^{-n\sigma x}.$$

- (e) Let λ , called the mean free path, be the average distance traveled between collisions for a particle in this material. Show that:

$$\lambda = \int_0^\infty x f(x) dx = \frac{1}{n\sigma}.$$

- (f) Define the relaxation time τ as the average time between collisions. Suppose the beam particle is moving with speed v . Show that:

$$\tau = \frac{\lambda}{v} = \frac{1}{nv\sigma}.$$

- (g) Suppose our beam enters the material with I_0 incident particles. Show that on average after going a depth x into the material the unscattered beam will only have:

$$I(x) = I_0 e^{-\frac{x}{\lambda}}$$

particles remaining. This is called the Beer-Lambert law.

Problem 3.59: Radiation Stopping Power. Consider a beam of particles so that each particle has an initial energy E_0 . The beam is fired into a material containing many charged particles (electrons specifically, of charge $-q_e$ and mass m_e) which may be scattered by the incoming beam particles. Because the beam instigates scattering of these electrons, some of the energy of the beam will be lost to them. The cross section of the electron scattering will generally depend on the energy of the incoming beam and of course on the recoil energy E_R which the electron is imparted with in the scattering event. Let $\frac{d\sigma}{dE_R}$ be the total cross section per amount of recoil energy delivered, so that the total scattering cross section of an electron of arbitrary final energy from a beam particle is:

$$\sigma = \int_0^\infty \frac{d\sigma}{dE_R} dE_R.$$

- (a) Let n be the number density of electrons in the material, assuming the material is essentially homogeneous show that the energy loss of a particle in the beam per unit length traveled (called the stopping power $S(E)$) into the material is given by:

$$S(E) = -\frac{dE}{dx} = n \int_0^\infty E_R \frac{d\sigma}{dE_R} dE_R.$$

- (b) Suppose the stopping power of the material is known. Show that the equation of motion for the beam particle's depth $x(t)$ into the material is given by:

$$m \frac{d^2 x}{dt^2} = -S(E(t))$$

where $E(t) = \frac{1}{2} m \dot{x}^2$. Explain how (if all relevant analytical steps could be performed or numerical method used) this equation of motion could be used to compute the penetration depth of the particle into the material (meaning the depth at which the particle will reach before stopping) and the amount of energy deposited per unit length $D(x)$ into the material. A precise understanding of the energy deposit curve is essential not only for the design of particle experiments but not also for medical applications of physics. Knowing the stopping power, it is possible to control beam parameters so that a particle beam can safely irradiate cancerous tumors within the body, depositing nearly all of its energy at the depth of the tumor, without harming healthy tissue.

- (c) Let us try to estimate the stopping power more directly. Assume the beam particle is much heavier than an electron so that during a single scattering event the beam particle can be treated as having approximately constant velocity and that each electron is able to be approximated as initially at rest.

Suppose the beam particle has charge Zq_e and show to lowest order in perturbation theory that by integrating the force due to the Coulomb potential in a single scattering event between the beam particle and an electron, the electron is imparted with an energy:

$$E_R \approx \frac{Z^2 q_e^4 M}{16\pi^2 \epsilon_0^2 m_e b^2 E}$$

where M is the mass of the beam particle, b is the impact parameter of the event (the smallest distance between the the beam particle and the electron), and E is the incoming energy of the beam particle. Rewrite the stopping power integral as an integral over impact parameter. Assume that Coulomb interactions only occur between particles separated by at least a minimum impact parameter $b_{\min}$ (because at sufficiently small close distances the microscopic fact that none of these particles are actually point-particles and there is significant small distance physics we haven't yet studied comes to dominate) and that Coulomb interactions only occur between particles separated by less than a maximum impact parameter $b_{\max}$ (because sufficiently far away particles will have their interactions swamped by the effects of all of the atoms in the matter), show that the stopping power can be estimated by:

$$S(E) \approx \frac{Z^2 q_e^4 M n}{8\pi \epsilon_0^2 m_e E} \ln \left(\frac{b_{\max}}{b_{\min}} \right).$$

The logarithm of the ratio of maximum to minimum relevant impact parameters is called the Coulomb logarithm and does vary gradually with energy though generally pretty slowly. This calculation can be made significantly more precise, but it should be taken to motivate that at leading order, the stopping power as a function of energy can be approximated as taking the form:

$$S(E) \approx \frac{A}{E}$$

for a constant A . More detailed calculations modify the very high and very low energy behavior of this formula.

- (d) Assuming the simple form of the stopping power found in the previous part, show that the beam deposits energy per unit length per beam particle $D(x)$ into the material according to:

$$D(x) = \frac{A}{\sqrt{E_0^2 - 2Ax}}$$

for $0 < x < \frac{E_0^2}{2A}$ and 0 otherwise. Notice that the deposit curve peaks sharply (called the Bragg peak) right before dropping to 0. Because of this, if the beam energy is tuned and the parameter A known, one can target a specific depth $\frac{E_0^2}{2A}$ with the bulk of the energy of the beam.

Problem 3.60: Kirchoff's Laws. Consider an interconnected system of conducting wires and circuit components. A circuit component is a device which can be connected to conducting wires in some number of places (most conventional components have two points of connection, called terminals, while some common components have more). Charge generically is capable of flowing through these conducting wires and circuit components. Such a network of interconnected wires and components is called a circuit. Take the whole system to be overall charge neutral.

- (a) Consider a point at which multiple wires meet. This is called a junction. Let I_n be the current carried out of this junction by wire n . That is:

$$I_n = \int_n \vec{J} \cdot d\vec{A}$$

where $\vec{J}$ is the current density in wire n and the integral measure is directed out of the junction. Show using that the wires are conducting and the conservation of charge that:

$$\sum_n I_n = 0.$$

This is called Kirchoff's junction rule. Conventionally, if the current I_n computed above would be negative one instead uses the current into the junction for that wire, which is given by the same integral but opposite convention for the measure's direction and thus is related by an overall minus sign. When this is done, Kirchoff's junction rule then splits into a sum of currents from wires carrying charge out of the junction minus a sum of currents from wires carrying charges into the junction to give 0. Thus,

Kirchoff's junction rule can also be said as "the net current through a junction is 0".

- (b) Consider our circuit components to be non-magnetic so that $\vec{B} = 0$ everywhere in our circuit. Consider a closed path γ which goes along a sequence of wires and through components. Show that the emf across any of the wires is 0 and that, if we take $\mathcal{E}_n$ to be the emf across the terminals of component n present in the loop γ , then:

$$\sum_n \mathcal{E}_n = 0.$$

This is called the non-magnetic version of Kirchoff's loop rule.

- (c) Consider two components side by side each with two terminals. Suppose that the right terminal of device 1 is connected by a wire to the left terminal of device 2 and that neither device develops a net accumulation of charge within itself during operation. Two such components are said to be "in series". Show Kirchoff's junction rule that the current through device 1 is the same as the current through device 2.
- (d) Consider two components side by side each with two terminals. Suppose that the left terminals of each device are connected by two wires which meet at junction (with potentially more wires connected at that junction) and that the right terminals of each device are connected by two wires which meet at another junction (which also may have more wires connected to it). Two such components are said to be "in parallel". Show using Kirchoff's loop rule that the emf through device 1 is the same as the emf through device 2.

Problem 3.61: Capacitors in Circuits.

- (a) Consider a capacitor for which each of the two conducting surfaces is connected to a wire. Let q be the charge on the left conducting surface. Suppose a current I flows through the wire attached to the left conducting surface into that surface. Show using charge conservation that:

$$\frac{dq}{dt} = I.$$

- (b) Show that the current which flows out of the right conducting surface is also given by I .
- (c) Show that the emf between the two conducting surfaces satisfies:

$$\frac{d\mathcal{E}}{dt} = \frac{I}{C}.$$

- (d) Consider two capacitors (of capacitances C_1 and C_2 respectively) which are connected in series experiencing a current I into the left terminal of the left capacitor. Let $\mathcal{E}$ be the emf between the left terminal of the left capacitor and the right terminal of the right capacitor. Show using Kirchoff's laws that:

$$\frac{d\mathcal{E}}{dt} = \left(\frac{1}{C_1} + \frac{1}{C_2} \right) I$$

and thus justify that two capacitors in series effectively act as a single capacitor with equivalent capacitance:

$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2}.$$

- (e) Consider two capacitors which are connected in parallel experiencing an emf $\mathcal{E}$ across either capacitor. Let I be the total current into the left terminals of the capacitors from the junction at which they are connected. Show that:

$$\frac{d\mathcal{E}}{dt} = \frac{I}{C_1 + C_2}$$

and thus justify that two capacitors in parallel effectively act as a single capacitor with equivalent capacitance:

$$C = C_1 + C_2.$$

Problem 3.62: Ohm's Law. Consider a material which contains a number density n of charges each of mass m and charge q which may move throughout it and which also contains many much more massive (and essentially stationary due to their large mass) objects which act as collision targets for the smaller charges with relaxation time τ . Suppose that the smaller charges have low enough density as to essentially neglect their interactions with one another (at least compared to their more significant interactions with the targets). This whole material experiences a constant and uniform electric field $\vec{E}$.

- (a) Show that between collisions with the targets, for any of the smaller charges:

$$m\ddot{\vec{x}} = q\vec{E}.$$

- (b) For charge k , let t_k be the time at which it had its most recent collision. Show that:

$$m\dot{\vec{x}}_k(t) = q(t - t_k)\vec{E} + m\dot{\vec{x}}_k(t_k).$$

- (c) Suppose that the interaction between any of the charges and the targets is sufficiently strong as to scatter the charge essentially uniformly in all directions off of the target. As well, suppose that each of the charges have independently uniformly at random chosen initial velocities and initial positions within the material. This is reasonable because in a real material we would not generally have control over the initial positions and velocities of the individual charges within it and these distributions are consistent with the symmetries of space. Let $\vec{v}$ be the sample average velocity:

$$\vec{v} = \frac{1}{N} \sum_{k=1}^N \dot{\vec{x}}_k(t).$$

Show by summing the result of the previous part over all n that on average:

$$m\vec{v} = q\vec{E}\tau.$$

- (d) Show then that the current density in the material is on average:

$$\vec{J} = qn\vec{v} = \frac{q^2 n \tau}{m} \vec{E} \stackrel{\text{def}}{=} \sigma \vec{E}$$

where the conductivity σ of the material is defined by the expression above to its left. The fact that the initial condition averaged, time averaged current density through the material is proportional to the applied electric field is called (the microscopic version of) Ohm's law. A material which satisfies this equation is called an Ohmic conductor; it is a much more realistic model than the idealized conductors we have considered so far as it accounts for the fact that it takes time for the system to equilibrate. Because this equation is local, it still works well for electric fields and current densities which are not constant and not uniform as long as they are approximately constant on the necessary scale for the time averaging to reach this equation and approximately uniform on the length scale associated to how far the relevant charges will travel in the time scale over which the time averaging is done. Thus, as long as $\vec{E}$ is well-approximated for our purposes as constant over a time of τ and uniform over a ball of radius λ where λ is the mean free path in the material, Ohm's law is still a good approximation. Because to derive this result we had to assume uniform scattering direction coming off of a collision with the fixed targets in the medium, Ohm's law is only really valid in the rest frame of that medium. In any other frame (meaning coordinate system boosted relative to the medium), the targets in the medium would be moving and the assumptions of our derivation would not apply. Thus, to apply Ohm's law to a moving medium one has to apply it in the rest frame of that medium and then apply a boost to see what it implies in other frames.

- (e) Show that in the limit $\sigma \rightarrow \infty$, if the current density in the material is finite then the electric field in the material must be 0. Thus, explain that in the $\sigma \rightarrow \infty$ limit, Ohm's law reproduces the previous behavior of the idealized conductor. As such, we can identify which materials are "good conductors" (act similarly to our idealized conductors) as those with sufficiently large σ and "bad conductors" (also known as insulators, materials in which charges are essentially fixed in place) as those with sufficiently small σ .
- (f) Consider our material to have at time $t = 0$ a charge density of $\rho_0(\vec{x})$ within it. Using the continuity equation, Ohm's law, and Gauss' law, show that the charge density in the material satisfies:

$$\frac{\partial \rho}{\partial t} = -\frac{\sigma}{\epsilon_0} \rho(t, \vec{x}).$$

Solve this differential equation to show that all of the charge density in the material exponentially flows to the surface of the material at a rate of $\frac{\sigma}{\epsilon_0}$. Thus, in the long run even for finite σ Ohmic matter reaches the same equilibrium state as ideal conducting matter.

- (g) Consider a straight region of Ohmic matter with conductivity σ , length ℓ , and cross sectional area $\mathbb{A}$. Let I be the current through the material and $\mathcal{E}$ be the emf between its two ends. Integrate (the microscopic version of Ohm's law) over the whole material to show:

$$\mathcal{E} = \frac{\ell}{\sigma \mathbb{A}} I.$$

Thus, the emf across the material is proportional to the current through the material. This is known as (the macroscopic version of) Ohm's law. The proportionality constant is called the resistance of the material:

$$R = \frac{\ell}{\sigma \mathbb{A}}.$$

A piece of Ohmic matter with resistance R is called a resistor. In real materials, the small charges are the free electrons in that material and the heavier targets the atoms/ions making up that material. If the material has a highly crystalline lattice structure so that the atoms are organized very predictably and periodically, then there are paths through the material which never hit an atom (one can just move parallel to a line of atoms in the lattice but offset so as not to hit that line). As such, in a perfectly regular material the relaxation time becomes arbitrarily high (as any charges which take these target-free paths pass right through) and so $\sigma \rightarrow \infty$ (this is known as superconductivity). It is thus the lattice defects (deviations from the regular repeating structure) present in every material which keep the relaxation time, and thus the conductivity, finite.

Problem 3.63: Resistors in Circuits.

- (a) Consider two resistors (of resistances R_1 and R_2 respectively) which are connected in series experiencing a current I into the left terminal of the left resistor. Let $\mathcal{E}$ be the emf between the left terminal of the left resistor and the right terminal of the right resistor. Show using Kirchoff's laws that:

$$\mathcal{E} = (R_1 + R_2)I$$

and thus justify that two resistors in series effectively act as a single resistor with equivalent resistance:

$$R = R_1 + R_2.$$

- (b) Consider two resistors which are connected in parallel experiencing an emf $\mathcal{E}$ across either resistor. Let I be the total current into the left terminals of the resistors from the junction at which they are connected. Show that:

$$\mathcal{E} = \frac{I}{\frac{1}{R_1} + \frac{1}{R_2}}$$

and thus justify that two resistors in parallel effectively act as a single resistor with equivalent resistance:

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}.$$

Problem 3.64: The RC Circuit. Consider a resistor of resistance R which is connected in series with a capacitor of capacitance of C .

- (a) Suppose the capacitor begins with no accumulated charge and that the circuit is completed by putting a battery of emf $\mathcal{E}$ in series with the resistor and capacitor and closing the loop of wire. Show that the charge accumulated on one of the conductors in the capacitor satisfies:

$$\mathcal{E} = R \frac{dq}{dt} + \frac{q}{C}, \quad q(t) = \mathcal{E}C \left(1 - e^{-\frac{t}{RC}}\right).$$

Thus, placing the battery in series with the capacitor "charges up" the capacitor at a rate determined by the time-constant RC .

- (b) Suppose the capacitor begins with accumulated charge q_0 and that the circuit is completed just by attaching the remaining terminal of the resistor to the remaining terminal of the capacitor. Show that the charge accumulated on one of the conductors in the capacitor satisfies:

$$0 = R \frac{dq}{dt} + \frac{q}{C}, \quad q(t) = q_0 e^{-\frac{t}{RC}}.$$

As well, show that the emf across the conductor is given by:

$$\mathcal{E} = \frac{q_0}{C} e^{-\frac{t}{RC}}.$$

- (c) Show that in the previous part if $\mathcal{E}_0 = \frac{q_0}{C}$ is held constant while taking $C \rightarrow \infty$ then the capacitor acts as a perfect battery of emf $\mathcal{E}_0$. Thus, a battery is an idealized limit of a capacitor with a large accumulated charge and high capacitance. Indeed, this is essentially how early batteries were made (now there are superior chemical methods by which to make a battery). From the various capacitance formulae found question 3.53, you should notice that a large capacitance can be made by putting the two conductors very close together and making them very large. As well, the effective capacitance

can be increased by placing multiple capacitors in parallel as in question 3.61. Then, to make this large capacitance capacitor a battery we only need to accumulate a large amount of charge. This can be done using triboelectricity through devices such as a Van de Graaff generator which in short is a device with a rubber belt rolling against a triboelectric material to accumulate charge and a connection to a conductor to transfer that charge. By rolling the belt sufficiently one can accumulate very large amounts of charge on the connected conductor. The very charged up very high capacitance capacitor then acts as a battery.

Problem 3.65: Power Dissipation in Circuits.

- (a) By integrating the Lorentz force law, show that the work done per unit time (called the power transferred) by $\vec{E}$ and $\vec{B}$ to a charge distribution moving is given by:

$$\mathcal{P} = \frac{dW}{dt} = \int_{\mathbb{S}} \vec{J} \cdot \vec{E} d\mathbb{S}.$$

- (b) Consider a region with fixed cross sectional area and length ℓ and suppose that $\vec{E}$ is uniform over each cross section with current flowing down the region so that the current through any cross section is the same. Show that the above integral becomes:

$$\mathcal{P} = I\mathcal{E}$$

Problem 3.66: Measuring resistance.

- (a) Suppose that a large conducting sheet of area $\mathbb{A}$ is charged by triboelectric methods such as the Van de Graaff generator. Approximate that the sheet is large enough and that we are near enough to the surface of the sheet to use the expressions for an infinite sheet. Suppose a known charge q (measured by say a Coulomb balance) is placed on a spring of known spring constant k a distance d (when the spring is in equilibrium) away from our charged conducting sheet. Let the x direction be the normal vector pointing from the sheet to the charge. Show that the electric field experience by the charge when it is a distance d away is:

$$\vec{E} = \left(\frac{\sigma}{2\epsilon_0} - \frac{q}{16\pi\epsilon_0 d^2} \right) \vec{i}_x.$$

(Because the sheet is conducting, do not forget the response of the sheet to an external charge.) Let Δx be the amount the spring is compressed when the charge q is in equilibrium. Show that the surface charge density σ on the conducting sheet is given by:

$$\sigma = \frac{q}{8\pi(d + \Delta x)^2} + \frac{2\epsilon_0 k}{q} \Delta x.$$

- (b) Suppose we have two same size conducting sheets which have been charged to surface charge densities σ_0 and $-\sigma_0$, determined by the previous method. (The second one you would have to tune, adjusting its charge by charging methods until it matches as precisely as you can get to the negative of the first.) If we now place these two plates parallel to each other with separation d then we have a parallel plate capacitor and thus we know its capacitance. As well, this gives us a method to prepare a known EMF. Take some amount of Ohmic material with unknown resistance R and connect it to one of the two plates. Take another wire and connect it to one of the plates. Then, connect it to the resistor for a fixed amount of time t and then disconnect it (to do this safely, one should use a switch). Afterward, go measure the surface charge density σ_f remaining on the sheet which initially had surface charge density σ_0 by the method of part (a). Show using the result of the RC circuit that the resistance of the unknown resistor is given by:

$$R = \frac{td}{\mathbb{A} \ln \left(\frac{\sigma_0}{\sigma_f} \right)}$$

Thus, this scheme gives us a way to measure the resistances of unknown resistors.

Problem 3.67: Electrostatic Multipole Expansion. Identically to the gravitational case, we can perform a multipole expansion for electrostatics to get simple approximations valid far from a charge distribution. It will be useful to refer to the results of the Gravitational Multipole Expansion.

- (a) Show that an arbitrary localized charge distribution can be rewritten as:

$$\rho(\vec{x}) = \sum_{n=0}^{\infty} \int_{\mathbb{S}} \rho(\vec{x}') \frac{x'^{a_1} \dots x'^{a_n}}{n!} d^3 \vec{x}' (-1)^n \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

Thus, the distribution can be expanded as a series in the Dirac delta and its derivatives.

- (b) Define the raw electric multipole moments by:

$$Q_n^{a_1 \dots a_n} = \int_{\mathbb{S}} \rho(\vec{x}) x^{a_1} \dots x^{a_n} d^3 \vec{x}.$$

Thus, show that the total distribution is given by:

$$\rho(\vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} Q_n^{a_1 \dots a_n} \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

- (c) Use this series to show that the total potential is given by:

$$\phi(\vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} Q_n^{a_1 \dots a_n} \partial_{a_1 \dots a_n}^n \frac{1}{4\pi\epsilon_0 |\vec{x}|}.$$

- (d) Consider the three lowest order terms in this series. Show that:

$$\phi(\vec{x}) = \frac{q}{4\pi\epsilon_0 r} + \frac{\vec{\varphi} \cdot \vec{\ell}}{4\pi\epsilon_0 r^2} + \frac{\vec{\ell} \cdot \hat{Q} \cdot \vec{\ell}}{8\pi\epsilon_0 r^3} + \mathcal{O}\left(\frac{1}{r^4}\right)$$

where $r = |\vec{x}|$, $\vec{\ell} = \frac{\vec{x}}{r}$, and:

$$q = \int_{\mathbb{S}} \rho(\vec{x}) d^3 \vec{x}, \quad \vec{\varphi} = \int_{\mathbb{S}} \rho(\vec{x}) \vec{x} d^3 \vec{x}, \quad (\hat{Q})^{ab} = \int_{\mathbb{S}} \rho(\vec{x}) (3x^a x^b - |\vec{x}|^2 \delta^{ab}) d^3 \vec{x}.$$

Just as with the gravitational case, q is called the monopole moment, $\vec{\varphi}$ the dipole moment, $\hat{Q}$ the quadrupole moment, and so on if one continues the series. Electrostatics is a bit more interesting than the gravitational case because while in gravity we always found mass to be positive and thus the monopole moment was never 0 and so dominated at large distances, for electrostatics any number of the multipole moments may be zero and so different distributions will have different dominant behaviors at large r based on their multipole moments. Note that the monopole distribution is given by:

$$\rho_{\text{mono}} = q\delta(\vec{x})$$

and that the dipole distribution is given by:

$$\rho_{\text{dip}} = -\vec{\varphi} \cdot \nabla \delta(\vec{x}).$$

- (e) Consider two charges q , located at $\frac{\ell}{2}\vec{n}$ where $|\vec{n}| = 1$, and $-q$, located at $-\frac{\ell}{2}\vec{n}$. Show that the monopole moment of this charge distribution is 0 and that the dipole moment of this distribution is $\vec{\varphi} = q\ell\vec{n}$. As well, show that the exact potential is:

$$\phi(\vec{x}) = \frac{q}{4\pi\epsilon_0 \left|\vec{x} - \frac{\ell}{2}\vec{n}\right|} - \frac{q}{4\pi\epsilon_0 \left|\vec{x} + \frac{\ell}{2}\vec{n}\right|}.$$

Consider taking the limit that $\ell \rightarrow 0$ while keeping $\vec{\varphi}$ fixed. Show that in this limit the potential becomes that of a perfect dipole with that dipole moment. Explain how this is what is expected from our analysis for the gravitational multipole.

- (f) Consider four charges $q_1, \dots, q_4$ at positions $\ell\vec{n}_1, \ell\vec{n}_2, \ell\vec{n}_3, \ell\vec{n}_4$. Assume the charges are so that the monopole and dipole moments of this distribution are 0. Let $q = q_1 + q_2 + q_3$. Keep the quadrupole moment of this distribution fixed while taking $q \rightarrow \infty$ and $\ell \rightarrow 0$ with $q_1/q, q_2/q, q_3/q$ fixed. Show that the result makes a perfect quadrupole.

Problem 3.68: Dipole in an Electric Field. Consider a perfect dipole of dipole moment $\vec{\varphi}$ located at a position $\vec{y}$ experiencing an electric field $\vec{E}(\vec{x})$.

- (a) Show using equation (2.9.123) and the expression for the charge density of a dipole that the net force on the dipole is:

$$\vec{F} = (\vec{\varphi} \cdot \nabla) \vec{E}(\vec{x}) \Big|_{\vec{x}=\vec{y}}$$

- (b) Show using equation (2.9.124) and the expression for the charge density of a dipole that the net torque

on the dipole about the point $\vec{y}$ is:

$$\vec{\tau} = \vec{\varphi} \times \vec{E}(\vec{y}).$$

- (c) Consider a mass m of charge q located at $\vec{y} + \frac{\ell}{2}\vec{n}$ where $\vec{n} = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$ and a second mass m of charge $-q$ located at $\vec{y} - \frac{\ell}{2}(\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$ where the z direction is defined to be the direction of $\vec{E}(\vec{y})$. Show that in electrostatic gauge the Lagrangian for this system becomes:

$$\mathcal{L} = \frac{m\ell^2}{2}(\dot{\theta}^2 + \dot{\varphi}^2 \sin^2 \theta) - q\phi\left(\vec{y} + \frac{\ell}{2}\vec{n}\right) + q\phi\left(\vec{y} - \frac{\ell}{2}\vec{n}\right).$$

- (d) Let I be the moment of inertia of the two charge system described in the previous part about any axis orthogonal to $\vec{n}$ and φ be the magnitude of the system's electric dipole moment. Keeping these two fixed in the $\ell \rightarrow 0$ limit, show that this Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2}I(\dot{\theta}^2 + \dot{\varphi}^2 \sin^2 \theta) + \varphi|\vec{E}(\vec{y})| \cos \theta.$$

Note the correspondence between this and the Lagrangian for a spherical pendulum.

- (e) Consider the special case that the dipole is not initially spinning around $\vec{E}$ (initially $\dot{\varphi} = 0$). Show that θ satisfies the equation of motion:

$$\ddot{\theta} + \frac{\varphi|\vec{E}(\vec{y})|}{I} \sin \theta = 0$$

and note that this equation is of the exact same form as a pendulum swinging in a uniform gravitational field. Thus, conclude that when an electric dipole is placed in an external electric field it will oscillate around aligning with that external field.

Problem 3.69: Interaction of Charge Distributions.

- (a) Show using equation (2.9.123) and Coulomb's law for the potential that the total force on any charge distribution due to the electric field which it generates is given by the integral:

$$\vec{F} = \int_{\mathbb{S}, \mathbb{S}'} \rho(t, \vec{x}) \rho(t, \vec{x}') \frac{\vec{x} - \vec{x}'}{4\pi\epsilon_0 |\vec{x} - \vec{x}'|^3} d\mathbb{S} d\mathbb{S}'$$

and show that this integral is identically 0.

- (b) Consider a charge distribution $\rho(t, \vec{x})$ in a region M . Show, using Gauss' Law and the expression for $\vec{E}$ in terms of ϕ in electrostatic gauge that the force on any such charge distribution due to any electrostatic field is:

$$\vec{F} = \int_{\partial M} \epsilon_0 \left(\vec{E} \vec{E}^T - \frac{1}{2} |\vec{E}|^2 \mathbb{1} \right) \cdot d\vec{A}$$

and thus the force on the distribution only depends on the electric field on its boundary. This integrand is called the electrostatic stress tensor.

- (c) Using the result of the previous part, consider a charge distribution alone in space which vanishes for distance greater than R_0 from the origin. Using a sphere of radius $R > R_0$ to define the integration region, show that the above integrand goes to 0 as $R \rightarrow \infty$. Explain why the result of the integral is independent of R for all $R > R_0$ and use this to show that $\vec{F} = 0$ for the distribution on itself by in an independent calculation to part (a).
- (d) Show that the electrostatic part of the Lagrangian (3.7.1), that is:

$$\mathcal{L}_{\text{Elec}} = \int_{\mathbb{S}} \left(-\rho\phi + \frac{\epsilon_0}{2} |\nabla\phi|^2 \right) d\mathbb{S}$$

becomes:

$$\mathcal{L}_{\text{Elec}} = -\frac{1}{2} \int_{\mathbb{S}} \rho\phi d\mathbb{S}$$

when the Coulomb's law solution for ϕ is inserted into it.

- (e) Consider two nonoverlapping charge distributions ρ_1 and ρ_2 . Show, using the linearity of Coulomb's law, that $\mathcal{L}_{\text{Elec}}$ becomes:

$$\mathcal{L}_{\text{Elec}} = -\frac{1}{2} \int_{\mathbb{S}} (\rho_1(t, \vec{x})\phi_1(t, \vec{x}) + \rho_2(t, \vec{x})\phi_1(t, \vec{x}) + \rho_1(t, \vec{x})\phi_2(t, \vec{x}) + \rho_2(t, \vec{x})\phi_2(t, \vec{x})) d\mathbb{S}$$

where ϕ_1 and ϕ_2 are the potentials due to solely ρ_1 or ρ_2 respectively. Show that the $\rho_1\phi_1$ and $\rho_2\phi_2$

terms in the Lagrangian/action have variation equal to 0 when the distributions are translated or rotated. Thus, conclude that for the purposes of computing the motion of the center of mass or overall orientation of the distributions, these terms do not contribute. Explain that for computing such equations of motion then we can take the effective contribution to the Lagrangian to be:

$$\mathcal{L}_{\text{Elec, eff}} = -\frac{1}{2} \int_{\mathbb{S}} (\rho_2(t, \vec{x}) \phi_1(t, \vec{x}) + \rho_1(t, \vec{x}) \phi_2(t, \vec{x})) d\mathbb{S}$$

(f) For the scenario described in the previous part, show by using Coulomb's law that:

$$\int_{\mathbb{S}} \rho_1(t, \vec{x}) \phi_2(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{S}} \rho_2(t, \vec{x}) \phi_1(t, \vec{x}) d\mathbb{S}.$$

This result is known as Green's Reciprocity Theorem. Thus, conclude that for computing the center of mass motion of two charge distributions, we can take their interaction term in the Lagrangian to be:

$$\mathcal{L}_{\text{Elec, eff}} = - \int_{\mathbb{S}} \rho_1(t, \vec{x}) \phi_2(t, \vec{x}) d\mathbb{S} = - \int_{\mathbb{S}, \mathbb{S}'} \frac{\rho_1(t, \vec{x}) \rho_2(t, \vec{x}')}{4\pi\epsilon_0 |\vec{x} - \vec{x}'|} d\mathbb{S} d\mathbb{S}'.$$

Problem 3.70: Electric Dipole-Dipole interaction. Consider two electric dipoles $\vec{\varphi}_1$ and $\vec{\varphi}_2$ separated by a distance r in the z direction with moments of inertia $I_1 \mathbb{1}$ and $I_2 \mathbb{1}$. Each dipole is allowed to rotate.

(a) Show using the result of the previous question that the electrostatic term in the Lagrangian for this system becomes:

$$\mathcal{L}_{\text{Elec}} = \frac{3\vec{\varphi}_1 \cdot \vec{\ell}_z \vec{\ell}_z \cdot \vec{\varphi}_2 - \vec{\varphi}_1 \cdot \vec{\varphi}_2}{4\pi\epsilon_0 r^3}.$$

(b) Show then that in spherical coordinates the full Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2} I_1 (\dot{\theta}_1^2 + \dot{\varphi}_1^2 \sin^2 \theta_1) + \frac{1}{2} I_2 (\dot{\theta}_2^2 + \dot{\varphi}_2^2 \sin^2 \theta_2) + \frac{\varphi_1 \varphi_2}{4\pi\epsilon_0 r^3} (2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\varphi_1 - \varphi_2)).$$

(c) Find the equilibria of this Lagrangian's equations of motion and classify their stability.

Problem 3.71: Interior Multipole Expansion. The multipole expansion we have done so far is more properly called the exterior multipole expansion; it gives iterative approximations for the potential due to a charge distribution when far away and outside of that charge distribution. Alternatively, one may also perform an interior multipole expansion which gives iterative approximations for the potential due to a charge distribution which surrounds you. That is, we will be looking at the potential near the origin of a distribution of charge which is located all around the origin but at large distances away.

(a) Consider Coulomb's law for the potential and show by doing a traditional Taylor expansion of the expression in terms of $\vec{x}$ around $\vec{x} = 0$, we get that the potential is given by the series:

$$\phi(\vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{4\pi\epsilon_0 n!} x^{a_1} \dots x^{a_n} \int_{\mathbb{S}} \rho(\vec{x}') \partial'_{a_1} \dots \partial'_{a_n} \frac{1}{|\vec{x}'|} d^3 \vec{x}'.$$

Thus, we can quite simply get a formula for the potential near the origin. When the charge density $\rho(\vec{x}')$ only has support for large $|\vec{x}'|$, the integrands appearing in the sum appear are suppressed due to the inverse powers of $|\vec{x}'|$ and so for such charge distributions one has convergence of this sum. Just as with the exterior multipole expansion, we now define the raw interior multipole moments:

$$Q_{a_1 \dots a_n}^{\text{int}, n} = \int_{\mathbb{S}} \rho(\vec{x}) (-\partial_{a_1}) \dots (-\partial_{a_n}) \frac{1}{|\vec{x}|} d^3 \vec{x}$$

so that the series becomes:

$$\phi(\vec{x}) = \sum_{n=0}^{\infty} \frac{Q_{a_1 \dots a_n}^{\text{int}, n}}{4\pi\epsilon_0 n!} x^{a_1} \dots x^{a_n}.$$

(b) Expand the first three terms of this series to show that the potential near the origin is given by:

$$\phi(\vec{x}) = \frac{K}{4\pi\epsilon_0} + \frac{\vec{L} \cdot \vec{x}}{4\pi\epsilon_0} + \frac{\vec{x} \cdot \hat{M} \cdot \vec{x}}{8\pi\epsilon_0} + \mathcal{O}(r^3)$$

where:

$$K = \int_{\mathbb{S}} \frac{\rho(\vec{x})}{|\vec{x}|} d^3 \vec{x}, \quad \vec{L} = \int_{\mathbb{S}} \rho(\vec{x}) \frac{\vec{x}}{|\vec{x}|^3} d^3 \vec{x}, \quad \hat{M} = \int_{\mathbb{S}} \rho(\vec{x}) \frac{3\vec{x}\vec{x}^T - |\vec{x}|^2 \mathbb{1}}{|\vec{x}|^5} d^3 \vec{x}.$$

(c) Consider a sphere of radius R and uniformly distributed charge q . Show that for this distribution, all of

the interior multipole moments except for $Q^{\text{int},0}$ vanish and that for this distribution $Q^{\text{int},0} = \frac{q}{R}$. As well, keeping that moment fixed, take $R \rightarrow \infty$ to show that this becomes a perfect interior monopole. Thus, an interior monopole can be understood as the potential due to a charged sphere at infinity. To do this, you may use the result of question 3.44(a).

- (d) Consider a point charge of charge q located at $\ell\vec{n}$ where $|\vec{n}| = 1$ and another point charge of charge $-q$ located at $-\ell\vec{n}$. Compute the interior multipole moments for this distribution. Keep $Q^{\text{int},1}$ fixed while taking the limit $\ell \rightarrow \infty$ and show that all interior multipole moments except this one vanish. Thus, an interior dipole potential is exactly the potential due to being between the ends of a regular dipole.
- (e) Generalize the arguments of the previous two parts to apply to arbitrarily high interior multipole moments to show that in general the N^{th} interior multipole potential is the potential due to being in the interior of a charge distribution with that corresponding exterior multipole distribution taken in the limit that its size goes to infinity.

3.8 Magnetostatics

The Galilean picture starts to become shaky when we talk about magnetism. Whereas in the previous section we considered a scalar theory of electric charge (which we called electrostatics), we could also consider a vector theory of electric charge (which is called magnetostatics). This may seem problematic because as we found, we cannot simultaneously have both the scalar and vector theories while preserving Galilean symmetry. Thus, the domains of validity cannot overlap. For the moment just saying we will only consider them individually but not at the same time, we proceed. The vector theory Lagrangian for $\vec{A}$ with its coupling to the current would be:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \frac{|\nabla \times \vec{A}|^2}{2\mu_0} \right) d\mathbb{S}. \quad (3.8.1)$$

Here μ_0 is a positive constant officially called the vacuum permeability but everyone just says “mu-naught”. μ_0 is decided to be positive by experimentally observing that two wires carrying current in the same direction attract, and so positive by the logic of section 3.5. While we could eliminate μ_0 by definition making it 1 in the same way we did to ϵ_0 , we cannot do so if we have already done so to ϵ_0 . This is because fixing the value ϵ_0 already determines our unit of charge and so leaves no more freedom to scale μ_0 independently. When the unit of charge is scaled, ϕ has to be scaled. Then due to the gauge interdependence between ϕ and $\vec{A}$, $\vec{A}$ must be scaled as well. Scaling $\vec{A}$ consequently scales the value of μ_0 . Let us consider for a moment the units of ϵ_0 and μ_0 . Recall that a quantity surrounded by square-brackets gives the units of that quantity (so far our independent unit scales are lengths L , for which we need a reference distance, times T for which we need a reference duration, and masses M for which we need a reference object). For now we are still being agnostic toward your choice of units of charge and so we will write our presently independent unit of charge as Q . (Later, when we permanently use $\epsilon_0 = 1$, the unit of charge will be fixed in terms of L , M , and T . Such a unit system is called **Galilean natural units** or **GNU**.) The different terms in equation (3.7.2) must have the same units and so:

$$\left[\frac{1}{2} m |\dot{\vec{x}}|^2 \right] = \left[\frac{q^2}{4\pi\epsilon_0 r} \right] \quad (3.8.2)$$

$$\implies M \frac{L^2}{T^2} = \frac{Q^2}{L[\epsilon_0]} \quad (3.8.3)$$

$$\implies [\epsilon_0] = \frac{T^2 Q^2}{ML^3}. \quad (3.8.4)$$

This gives the units of ϵ_0 . In units in which $\epsilon_0 = 1$ by definition, this then defines the unit of charge to be $Q = \frac{M^{\frac{1}{2}} L^{\frac{3}{2}}}{T}$. Now using equation (3.1.3), we can identify the units of the vector potential and consequently the magnetic field:

$$\left[\frac{1}{2} m |\dot{\vec{x}}|^2 \right] = \left[q \vec{A} \cdot \dot{\vec{x}} \right] \quad (3.8.5)$$

$$\implies M \frac{L^2}{T^2} = Q [\vec{A}] \frac{L}{T} \quad (3.8.6)$$

$$\implies [\vec{A}] = \frac{ML}{QT} \quad (3.8.7)$$

$$\implies [\vec{B}] = [\nabla \times \vec{A}] = \frac{[\vec{A}]}{L} = \frac{M}{QT}. \quad (3.8.8)$$

Finally, using equation (3.8.1) we can find the units of μ_0 :

$$\left[\frac{1}{2} m |\dot{\vec{x}}|^2 \right] = \left[\int_{\mathbb{S}} \frac{|\vec{B}|^2}{2\mu_0} d\mathbb{S} \right] \quad (3.8.9)$$

$$\implies M \frac{L^2}{T^2} = \frac{[\vec{B}]^2}{[\mu_0]} L^3 \quad (3.8.10)$$

$$\implies [\mu_0] = \frac{[\vec{B}]^2 L T^2}{M} = \frac{ML}{Q^2}. \quad (3.8.11)$$

Because both $[\epsilon_0]$ and $[\mu_0]$ depend on the unit of charge Q , we cannot scale them independently through

just the unit of charge. However, the product of the two of them has no dependence on the units of charge:

$$[\epsilon_0 \mu_0] = \frac{T^2}{L^2} \quad (3.8.12)$$

This product has units of the reciprocal of speed squared. As such, in lieu of μ_0 , we could also introduce a parameter c which has units of speed defined by:

$$c \stackrel{\text{def}}{=} \frac{1}{\sqrt{\mu_0 \epsilon_0}}. \quad (3.8.13)$$

That is, we could alternatively write our Lagrangian in (3.8.1) as:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \frac{\epsilon_0 c^2}{2} |\nabla \times \vec{A}|^2 \right) d\mathbb{S}. \quad (3.8.14)$$

At this point it isn't clear if this c introduced here can genuinely be interpreted as the speed of anything in particular, but soon we will see that it absolutely is.

This theory is successful for describing the attraction and repulsion of current carrying wires. But, as we said it can't be exact if $\rho \neq 0$. To make this theory consistent with $\rho \neq 0$, we need to change the equation of motion for ϕ and thus have to add terms into the Lagrangian which depend on ϕ . The only appropriately invariant quantity we have found which depends on ϕ is $\vec{E} \cdot \vec{B}$ but it is a surface term. Therefore the lowest order correction we could add is $(\vec{E} \cdot \vec{B})^2$. However, this term also depends on $\vec{B} = \nabla \times \vec{A}$ and so will also affect the equation of motion for $\vec{A}$. Thus, if this term is present to make a consistent theory with $\rho \neq 0$, it will have observable effects on the predictions of this theory which (if those corrections are correct) should be observed when $\rho \approx 0$. As well, it still couldn't have the $|\vec{E}|^2$ term in the Lagrangian which gives a successful theory of electrostatics. The scalar theory of electrostatics can't apply when $\vec{B} \neq 0$ as we found in section 3.4 even though it is also experimentally correct. The scalar theory can only apply when $\vec{B} \approx 0$ and the vector theory can only apply when $\rho \approx 0$. Neither can be exactly true. We need some way to **unify** these two theories into one...

Exercises

Problem 3.72: Integral form of the Solenoid Law. Using the Solenoid Law, show that the net magnetic field through any closed surface $\mathbb{A}$ is 0:

$$\int_{\mathbb{A}} \vec{B} \cdot d\vec{\mathbb{A}} = 0.$$

Problem 3.73: Common Magnetostatics Fields.

- (a) Show using a symmetry argument and the integral form of Ampere's Law that the magnetic field due to an infinitely long current carrying wire of current I in the z direction is:

$$\vec{B} = \frac{\mu_0 I}{2\pi r} \vec{e}_\varphi.$$

and that one can take the corresponding vector potential to be:

$$\vec{A} = -\frac{\mu_0 I \vec{e}_z}{2\pi} \ln\left(\frac{r}{R}\right)$$

for a constant R .

- (b) Show using a symmetry argument and the integral form of Ampere's Law that the magnetic field due to an infinitely long current carrying cylindrical shell of radius R carrying current I down the cylinder's length in the z direction is:

$$\vec{B} = \begin{cases} 0, & r < R \\ \frac{\mu_0 I}{2\pi r} \vec{e}_\varphi, & r > R \end{cases}$$

and that one can take the corresponding vector potential to be:

$$\vec{A} = \begin{cases} 0, & r < R \\ \frac{\mu_0 I \vec{e}_z}{2\pi} \ln\left(\frac{R}{r}\right), & r > R \end{cases}.$$

- (c) A solenoid of wire is a common device in magnetism in which a wire is coiled tightly to make a cylinder in which current I runs around the cylinder and the coil has a number density of n turns (or loops) per

unit length. Consider an infinitely long solenoid as described with radius R . Show using a symmetry argument and the integral form of Ampere's Law that the magnetic field due to the solenoid is:

$$\vec{B} = \begin{cases} \mu_0 n I \vec{e}_z, & r < R \\ 0, & r > R \end{cases}$$

and that one can take the corresponding vector potential to be:

$$\vec{A} = \begin{cases} \frac{\mu_0 n I r}{2} \vec{e}_\varphi, & r < R \\ \frac{\mu_0 n I R^2}{2r} \vec{e}_\varphi, & r > R \end{cases}.$$

- (d) It may be surprising that even though the magnetic field is 0 outside of the solenoid, the vector potential is not also 0 (or at least constant). Show that outside of the solenoid in any open region not enclosing the solenoid, it naively seems the vector potential can be written as the gradient:

$$\vec{A} \stackrel{?}{=} \nabla \left(\frac{\mu_0 n I R^2}{2} \varphi \right) = \nabla f$$

However, show that due to the degeneracy of cylindrical coordinates, the gauge function f implied above cannot be made continuous when enclosing the solenoid and that this discontinuity prevents this gradient from existing everywhere around the solenoid and so prevents $\vec{A}$ from actually being able to be transformed to 0 outside of the solenoid. Thus, yes, genuinely the vector potential of a solenoid is non-zero and non-uniform outside the solenoid even though the magnetic field in that region is 0. Show using the integral form of Ampere's law that this had to be the case.

Problem 3.74: Coaxial Cables. Consider a long (treat as infinitely long) cylindrical shell of radius R_1 concentric with a larger cylindrical shell of radius $R_2 > R_1$. Show that if the inner cylinder carries current I down its axis and the outer cylinder carries the same current in the opposite direction then (at least in a particular choice of gauge):

$$\vec{B} = \begin{cases} 0, & r < R_1 \\ \frac{\mu_0 I}{2\pi r} \vec{e}_\varphi, & R_1 < r < R_2 \\ 0, & r > R_2 \end{cases}, \quad \vec{A} = \begin{cases} \frac{\mu_0 I \vec{e}_z}{2\pi} \ln \left(\frac{R_2}{R_1} \right), & r < R_1 \\ \frac{\mu_0 I \vec{e}_z}{2\pi} \ln \left(\frac{R_2}{r} \right), & R_1 < r < R_2 \\ 0, & r > R_2 \end{cases}.$$

Problem 3.75: Magnetic Boundary Conditions. Consider a surface which has a not necessarily uniform surface current density $\vec{K}$ on it.

- (a) Consider the integral form of the Solenoid law with the volume under consideration being a cylinder of height h and cross sectional area $\mathbb{A}$ for which one end cap ($\mathbb{A}_-$) is below the current surface and one end cap ($\mathbb{A}_+$) is above the current surface. Let S be the shell (without end caps) of the cylinder. Show that the integral form of the Solenoid law then becomes:

$$\int_{\mathbb{A}_-} \vec{B} \cdot d\vec{\mathbb{A}} + \int_S \vec{B} \cdot d\vec{\mathbb{A}} + \int_{\mathbb{A}_+} \vec{B} \cdot d\vec{\mathbb{A}} = 0.$$

- (b) Take the limit that $h \rightarrow 0$ to show that S goes to 0. As well, show that in the limit both $\mathbb{A}_+$ and $\mathbb{A}_-$ make contact with the current surface. Then, show that the above integrals become:

$$\int_{\mathbb{A}} \vec{B}^- \cdot d\vec{\mathbb{A}} + \int_{\mathbb{A}} \vec{B}^+ \cdot d\vec{\mathbb{A}} = 0$$

where $\vec{B}^-$ is the limit of $\vec{B}$ when approaching the surface from below and $\vec{B}^+$ is the limit of $\vec{B}$ when approaching the surface from above.

- (c) Divide both sides of the above by $\mathbb{A}$ and take the limit that $\mathbb{A} \rightarrow 0$. Let $\vec{n}$ be the normal vector to the current surface pointing out of the surface from above. Show that the above becomes:

$$-\vec{B}^- \cdot \vec{n} + \vec{B}^+ \cdot \vec{n} = 0.$$

Thus conclude that the component of the magnetic field which is perpendicular to the current surface, $B_\perp$, is continuous across the surface:

$$B_\perp^+ = B_\perp^-.$$

- (d) Take Ampere's law and integrate it over an at the moment arbitrary area $\mathbb{A}$ to show that:

$$\int_{\partial \mathbb{A}} \vec{B} \cdot d\vec{x} = \mu_0 I[\mathbb{A}]$$

where $I[\mathbb{A}]$ is the current flowing through that area $\mathbb{A}$. Then, take the integration region to be a rectangle of length ℓ which is parallel to the charged surface and thickness w which is perpendicular to the charged surface and for which one side of the rectangle lies on each side of the charged surface. Call the side of the rectangle “below” the charged surface T_- , the side of the rectangle which crosses from below to above N_+ , the side of the rectangle “above” the charged surface T_+ , and the side of the rectangle which crosses from above to below N_- . Then, show that the above integral formula becomes:

$$\int_{T_-} \vec{B} \cdot d\vec{x} + \int_{N_+} \vec{B} \cdot d\vec{x} + \int_{T_+} \vec{B} \cdot d\vec{x} + \int_{N_-} \vec{B} \cdot d\vec{x} = \mu_0 I[\mathbb{A}].$$

- (e) Show that in the limit that the thickness of the rectangle is taken to 0, the area goes to 0 and N_+ and N_- go to 0. As well, show that T_- and T_+ both make contact with the charged surface (but one on each side of the surface). Let $\vec{T}$ be the unit tangent vector to the current surface in the direction of the side T_+ of the rectangle and $\vec{n}$ be the unit normal vector to the current surface pointing from below to above. Show taking $w \rightarrow 0$ gives:

$$\int_{T_-} \vec{B}^- \cdot d\vec{x} + \int_{T_+} \vec{B}^+ \cdot d\vec{x} = \mu_0 \int_T (\vec{K} \times \vec{n}) \cdot d\vec{x}.$$

- (f) Divide both sides of the above by ℓ and take the limit that $\ell \rightarrow 0$. Show that the above becomes:

$$-\vec{T} \cdot \vec{B}^- + \vec{T} \cdot \vec{B}^+ = \mu_0 (\vec{K} \times \vec{n}) \cdot \vec{T}.$$

Thus conclude that the part of the magnetic field which is parallel to the charged surface, $\vec{B}_{\parallel}$, is discontinuous across the surface with discontinuity given by the surface current:

$$\vec{B}_{\parallel}^+ = \vec{B}_{\parallel}^- + \mu_0 \vec{K} \times \vec{n}.$$

- (g) Combine both components of the boundary conditions to show that:

$$\vec{B}^+ - \vec{B}^- = \mu_0 \vec{K} \times \vec{n}.$$

Problem 3.76: Magnetic Multipole Expansion. We can also make a magnetostatic multipole expansion, although it is a little different from the electrostatic and gravitational cases.

- (a) Show that an arbitrary localized current distribution can be rewritten as:

$$\vec{J}(\vec{x}) = \sum_{n=0}^{\infty} \int_{\mathbb{S}} \vec{J}(\vec{x}') \frac{x'^{a_1} \dots x'^{a_n}}{n!} d^3 \vec{x}' (-1)^n \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

- (b) Define the raw magnetic multipole moments by:

$$M_n^{a_0 a_1 \dots a_n} = \int_{\mathbb{S}} J^{a_0}(\vec{x}') x'^{a_1} \dots x'^{a_n} d^3 \vec{x}'$$

Thus show that the total distribution is given by:

$$J^{a_0}(\vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} M_n^{a_0 \dots a_n} \partial_{a_1 \dots a_n}^n \delta(\vec{x}).$$

- (c) Use this series to show that the total potential is given by:

$$A^{a_0}(\vec{x}) = \sum_{n=0}^{\infty} \frac{\mu_0 (-1)^n}{n!} M_n^{a_0 \dots a_n} \partial_{a_1 \dots a_n}^n \frac{1}{4\pi |\vec{x}|}.$$

- (d) Consider the two lowest order terms in this series. Show that:

$$A^{a_0}(\vec{x}) = \frac{\mu_0 M_0^{a_0}}{4\pi r} + \frac{\mu_0 M_1^{a_0 a_1} \iota_{a_1}}{4\pi r^2} + \text{Higher Order Terms}$$

where $r = |\vec{x}|$, $\vec{\iota} = \vec{x}/r$.

- (e) Take the divergence of Ampere’s law to show that in magnetostatics:

$$\nabla \cdot \vec{J} = 0.$$

- (f) Consider a function $f(\vec{x})$ and our localized current distribution $\vec{J}$. Show using the previous part and the product rule that:

$$\nabla \cdot (f \vec{J}) = \nabla f \cdot \vec{J}.$$

Now use that our current distribution is localized (is 0 sufficiently far from the origin) and integrate

this result over all space to show by the divergence theorem that:

$$0 = \int_{\mathbb{S}} \nabla f \cdot \vec{J} d\mathbb{S}.$$

- (g) Use the result of the previous part with $f = x^a$ to show that:

$$\int_{\mathbb{S}} J^a(\vec{x}) d\mathbb{S} = 0.$$

Use this to show that in magnetostatics, the monopole moment in the multipole expansion vanishes: $M_0^{a_0} = 0$. In this way there is no magnetic term analogous to the electric monopole (point charge) in the multipole expansion.

- (h) Use the integral result from before with $f = x^a x^b$ to show that:

$$\int_{\mathbb{S}} (x^a J^b(\vec{x}) + x^b J^a(\vec{x})) d\mathbb{S} = 0.$$

Use this to show that the dipole moment in the multipole expansion, $M_1^{a_0 a_1}$ becomes:

$$M_1^{a_0 a_1} = -\epsilon^{a_0 a_1 a_2} m_{a_2}$$

where:

$$\vec{m} = \frac{1}{2} \int_{\mathbb{S}} \vec{x} \times \vec{J}(\vec{x}) d\mathbb{S}$$

is called the magnetic dipole moment. Use this to show that the dipole contribution to the potential becomes:

$$\frac{\mu_0 M_1^{a_0 a_1} \iota_{a_1}}{4\pi r^2} = \frac{\mu_0 (\vec{m} \times \vec{\iota})^{a_0}}{4\pi r^2}.$$

Thus, the vector potential for a magnetic dipole $\vec{m}$ is:

$$\vec{A}(\vec{x}) = \frac{\mu_0 \vec{m} \times \vec{\iota}_r}{4\pi r^2}.$$

A similar line of argumentation can be completed at each higher order in the multipole expansion to reduce the number of independent components in the reduced multipole expressions. As well, show that the dipole current distribution is given by:

$$\vec{J}_{\text{dip}}(\vec{x}) = -\vec{m} \times \nabla \delta(\vec{x}).$$

- (i) Consider a circular loop of radius R carrying current I counterclockwise around the loop's outward pointing normal vector $\vec{n}$ (the vector which points out of the center of circle). Show that the magnetic dipole moment of this current distribution is given by:

$$\vec{m} = I\mathbb{A}\vec{n}$$

where $\mathbb{A}$ is the area of the loop. Now consider keeping $\vec{m}$ fixed while taking $R \rightarrow 0$. Show that in this limit all of the other multipole moments of the distribution go to 0. Thus, a magnetic dipole vector potential is the potential due to a tiny loop of circulating current.

Problem 3.77: Dipole in a Magnetic Field. Consider a perfect magnetic dipole of dipole moment $\vec{m}$ located at a position $\vec{y}$ experiencing a magnetic field $\vec{B}(\vec{x})$.

- (a) Show using equation (2.9.123) and the expression for the current density of a dipole that the net force on the dipole is:

$$\vec{F} = \nabla(\vec{m} \cdot \vec{B}(\vec{x})) \Big|_{\vec{x}=\vec{y}}$$

- (b) Show using equation (2.9.124) and the expression for the current density of a dipole that the net torque on the dipole about the point $\vec{y}$ is:

$$\vec{\tau} = \vec{m} \times \vec{B}(\vec{y}).$$

- (c) Consider a uniformly massive circular loop of current I , mass m , and radius R . The current flows counterclockwise around the outward pointing normal vector $\vec{n}$ of the loop. The loop is placed in an external magnetic field $\vec{B}(\vec{x})$. Suppose that the loop can rotate so that its orientation changes with respect to the magnetic field but it is otherwise fixed. Let $\theta(t)$ be the angle between $\vec{n}$ and $\vec{B}(\vec{y})$. Show that in the limit that $R \rightarrow 0$, if the magnetic dipole moment and moment of inertia are held fixed then

the Lagrangian for its orientation becomes:

$$\mathcal{L} = \frac{1}{2}I\dot{\theta}^2 + \vec{m} \cdot \vec{B}.$$

Finally, show that the equation of motion is:

$$\ddot{\theta} + \frac{|\vec{m}||\vec{B}|}{I} \sin \theta = 0.$$

So, a magnetic dipole will oscillate around aligning with an external field just like an electric dipole will.

Problem 3.78: Interaction of Current Distributions.

- (a) Consider a current distribution $\vec{J}(\vec{x})$ in a region M . Show, using Ampere's Law and the expression for $\vec{B}$ in terms of $\vec{A}$ that the force on any such charge distribution due to any magnetostatic field is:

$$\vec{F} = \int_{\partial M} \frac{1}{\mu_0} \left(\vec{B}\vec{B} - \frac{1}{2}|\vec{B}|^2 \mathbb{1} \right) \cdot d\vec{A}$$

and thus the force on the distribution only depends on the magnetic field on its boundary. This integrand is called the magnetostatic stress tensor.

- (b) Using the result of the previous part, consider a current distribution alone in space which vanishes for distance greater than R_0 from the origin. Using a sphere of radius $R > R_0$, show that the above integrand goes to 0 as $R \rightarrow \infty$ and thus because it is independent of R , it is in fact 0. To do so, refer to the Biot-Savart law.
- (c) Show that the magnetostatic part of the Lagrangian (3.8.1), meaning:

$$\mathcal{L}_{\text{Mag}} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \frac{|\vec{B}|^2}{2\mu_0} \right) d\mathbb{S}$$

becomes:

$$\mathcal{L}_{\text{Mag}} = \frac{1}{2} \int_{\mathbb{S}} \vec{J} \cdot \vec{A} d\mathbb{S}$$

when the solution for $\vec{A}$ is inserted into it.

- (d) Consider two nonoverlapping current distributions $\vec{J}_1$ and $\vec{J}_2$. Show, using the linearity of Coulomb's law that $\mathcal{L}_{\text{Mag}}$ becomes:

$$\mathcal{L}_{\text{Mag}} = \frac{1}{2} \int_{\mathbb{S}} \left(\vec{J}_1(\vec{x}) \cdot \vec{A}_1(\vec{x}) + \vec{J}_2(\vec{x}) \cdot \vec{A}_1(\vec{x}) + \vec{J}_1(\vec{x}) \cdot \vec{A}_2(\vec{x}) + \vec{J}_2(\vec{x}) \cdot \vec{A}_2(\vec{x}) \right) d\mathbb{S}$$

where $\vec{A}_1$ and $\vec{A}_2$ are the potentials due to solely $\vec{J}_1$ or $\vec{J}_2$ respectively. Show that the $\vec{J}_1 \cdot \vec{A}_1$ integral in the Lagrangian has 0 variation under translations of the center of the distribution and rotations of its orientation. Thus, conclude that it does not contribute to the equations of motion for the center or orientation. Extend this to the $\vec{J}_2 \cdot \vec{A}_2$ term as well. Thus, conclude that for the center of mass motion we can take the effective Lagrangian to be:

$$\begin{aligned} \mathcal{L}_{\text{Mag, eff}} &\simeq \frac{1}{2} \int_{\mathbb{S}} \left(\vec{J}_2(\vec{x}) \cdot \vec{A}_1(\vec{x}) + \vec{J}_1(\vec{x}) \cdot \vec{A}_2(\vec{x}) \right) d\mathbb{S} \\ &= \int_{\mathbb{S}} \vec{J}_1(\vec{x}) \cdot \vec{A}_2(\vec{x}) d\mathbb{S} = \int_{\mathbb{S}, \mathbb{S}'} \frac{\mu_0 \vec{J}_1(\vec{x}) \cdot \vec{J}_2(\vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d\mathbb{S} d\mathbb{S}'. \end{aligned}$$

Problem 3.79: Magnetic Dipole-Dipole interaction. Consider two magnetic dipoles $\vec{m}_1$ and $\vec{m}_2$ separated by a distance r in the z direction with moments of inertia $I_1 \mathbb{1}$ and $I_2 \mathbb{1}$. Each dipole is allowed to rotate.

- (a) Show using the result of the previous question that the magnetostatic term in the Lagrangian for this system becomes:

$$\mathcal{L}_{\text{Mag}} = \mu_0 \frac{3\vec{m}_1 \cdot \vec{e}_z \vec{e}_z \cdot \vec{m}_2 - \vec{m}_1 \cdot \vec{m}_2}{4\pi r^3}.$$

- (b) Show then that the full Lagrangian for this system in spherical coordinates becomes:

$$\mathcal{L} = \frac{1}{2}I_1(\dot{\theta}_1^2 + \dot{\varphi}_1^2 \sin^2 \theta_1) + \frac{1}{2}I_2(\dot{\theta}_2^2 + \dot{\varphi}_2^2 \sin^2 \theta_2) + \frac{\mu_0 m_1 m_2}{4\pi r^3} (2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\varphi_1 - \varphi_2)).$$

- (c) Find the equilibria of this Lagrangian's equations of motion and classify their stability.

Problem 3.80: Establishing properties of Magnetostatics.

- (a) Most everyday objects do not seem to attract or repel each other in any noticeable measure. Thus, explain that this allows one to conclude that everyday objects tend not to carry any significant currents.
- (b) When a current is specifically generated in a wire (such as in an RC circuit), it is observed that it will be attracted toward another wire carrying current in the same direction and repelled from a wire carrying current in the opposite direction. Explain how this allows us to conclude that $\mu_0 > 0$.
- (c) Some everyday objects (magnets) do attract each other through a force which isn't gravity (because then they would attract other objects the same way as each other regardless of mass) or electrostatics (as they aren't attracted or repelled by charged objects). As well, everyday magnets move each other into aligning in specific orientations and strongly resist aligning in specific other orientations. Explain how all of this is perfectly consistent with everyday magnets being described as interacting current distributions via magnetostatics. Though the logic of the multipole expansion, it is often good enough to model everyday magnets as a magnetic dipole.
- (d) Everyday magnets have the interesting property that when dropped or banged on surfaces they tend to become weaker (in the sense of their effects on other magnets). Draw a picture and argue using the results of our analysis of the magnetic dipole-dipole interaction to explain how this is consistent with a model of everyday magnets consisting of several magnetic dipoles arranged throughout their volumes with the net magnetic field produced by each stronger whenever more of these dipoles are aligned and weaker when their orientations are essentially unrelated.
- (e) Consider a permanent magnet which has its internal dipoles strongly aligned with each other. Explain how the results of the dipole in a magnetic field and dipole-dipole interaction questions explain that when a material whose internal dipoles are not aligned but can be rotated is brought close to our permanent magnet, the permanent magnet will cause the dipoles in our other material to begin to align. Iron is a common choice for the "other material" here. Once the magnetic dipoles in iron are brought to alignment, they keep each other aligned by the dipole-dipole interaction even once the external permanent magnet is taken away. An easy way to do this at home is to rub paperclips on refrigerator magnets. After doing so, you will notice that the paperclips can stick to and repel each other. They have been magnetized!

Problem 3.81: ★ Measuring c .

- (a) Consider very large parallel plates prepared so that the EMF between them is $\mathcal{E}$. Assume they are large enough that it takes a very long time for the charge density on them to change and so we can approximate this EMF as constant over the time scales we are interested in. Such a scenario can be designed by the method of problem 3.64. Next, consider a known resistor R measured by that same technique which is connected in series to the parallel plates by a long length of wire which runs out far away from these two components straight for a while then makes a nearly closed circle of radius r and returns straight to the circuit components. Using the definition of the magnetic multipole moments, show that the magnetic dipole moment of the wire is given by $\vec{m}_c = \pi r^2 \frac{\mathcal{E}}{R} \vec{n}$.
- (b) Suppose we have magnetized two small needles by rubbing them on a large existing magnet in the same way so that the two needles are essentially magnetic dipoles with the same magnetic dipole moment $\vec{m}$ pointing along the axis of the needle. Let both needles have moment of inertia I about their centers of mass for rotations not along the needle axis and moment of inertia of essentially 0 about the needle axis. Suppose we fix in place our ring of current from the previous part and place at a distance d above the center of the ring one of the needles, allowing it to rotate about its center of mass in any direction. Show using the result of the dipole-dipole interaction question that the Lagrangian for the orientation of the needle is given by:

$$\mathcal{L} = \frac{1}{2}I(\dot{\theta}^2 + \dot{\varphi}^2 \sin^2 \theta) + \frac{\mu_0 m_c m}{2\pi d^3} \cos \theta.$$

As well, show that for small oscillations off of alignment of the needle axis and the normal to the ring, the needle oscillates back and forth with angular frequency ω_1 given by:

$$\omega_1^2 = \frac{\mu_0 m_c m}{2\pi d^3 I}.$$

- (c) Consider now that we replace the fixed ring of current from before with our other needle and also fix it in place to point along the line of separation between it and the other needle. Show that the freely

rotating needle now oscillates with angular frequency ω_2 given by:

$$\omega_2^2 = \frac{\mu_0 m^2}{2\pi d^3 I}.$$

- (d) Show that the magnetic dipole moment (magnitude) m for the needles is given by:

$$m = \left(\frac{\omega_2}{\omega_1} \right)^2 m_c$$

and that this provides us a way of measuring μ_0 as:

$$\mu_0 = \frac{2\pi d^3 I \omega_1^4}{m_c^2 \omega_2^2}.$$

Recall that we can measure or compute in terms of measurable quantities all of the quantities on the right hand side here using our so far developed experiments. Thus, we can measure μ_0 by this experiment. In SI units, the value of μ_0 is $\mu_0 = 1.25663706212(19) \times 10^{-6} \frac{\text{kgm}}{\text{C}^2}$. Then, using our value of ϵ_0 , whether measured by using a reference charge as in SI units or set to 1 as in natural units, we can compute the corresponding value of the parameter c . In terms of meters and seconds, the value of c is: $c = 299792458 \frac{\text{m}}{\text{s}}$. Historically, it was true that c was measured in an experiment in terms of predefined units of length and time. However, in the modern day the meter is actually defined so that c takes the value given exactly. In this way, the experiment given here to measure c in modern day language would be an experiment to calibrate the meter.

Problem 3.82: ★ Measuring Current with an Astatic Galvanometer Consider two needles magnetized as in the previous problem with the same magnetic moment magnitude m and each of moment of inertia I_{rot} and aligned opposite each other, suspended by a string passing through the center of each hanging in the z direction with some distance separating the two needles from each other on the string. The string has torsion constant κ and when it is untwisted the lower needle points in the x direction. Consider as well a solenoid of wire with turns per unit length n with its axis in the y direction and a small opening in its winding so that the string can pass through. The lower needle is inside of the solenoid and the upper needle is outside of the solenoid. Suppose that the whole system is experiencing an unknown background magnetic field $\vec{B}_0$ and that the solenoid is connected to some source which produces an unknown current I . Let θ be the angle the string has twisted.

- (a) Show that the Lagrangian for the orientation of the needles is given by:

$$\mathcal{L} = I_{\text{rot}} \dot{\theta}^2 - \frac{1}{2} \kappa \theta^2 + \mu_0 m n I \sin \theta.$$

Notice that the upper needle allows the cancellation of the background field and thus makes this device useful even when unknown background fields are present. This is important because the Earth itself has a background magnetic field and so devices which can cancel the effect of it are necessary for measuring currents.

- (b) Show that in equilibrium we can measure the current through the solenoid by the expression:

$$I = \frac{\kappa \theta_{\text{eq}}}{\mu_0 m n \cos \theta_{\text{eq}}}.$$

Thus, this device, known as an astatic galvanometer allows us to measure unknown currents by observing the deflection of the needle. This is very convenient because we can place a protractor around the upper needle which because it is outside of the solenoid will be entirely visible.

- (c) Explain how using a known resistor (which we have already established how to measure) and this astatic galvanometer, we can measure an unknown EMF $\mathcal{E}$.
 (d) Explain how using a known resistor and this astatic galvanometer we can measure an unknown capacitance C .

Problem 3.83: Integral form of Faraday's Law.

- (a) Integrate Faraday's Law over a surface $\mathbb{A}$ to show that the "electric circulation" around the boundary of a surface is related to the "magnetic flux" through the surface by:

$$\int_{\partial \mathbb{A}} \vec{E} \cdot d\vec{x} = - \frac{d}{dt} \int_{\mathbb{A}} \vec{B} \cdot d\vec{\mathbb{A}}.$$

- (b) Now consider a time dependent surface $\mathbb{A}(t)$ and let $\vec{v}(t, \vec{x})$ refer to the velocity of a point on the surface

at location $\vec{x}$ at time t . Show then that by adding the right term to each side of the above it becomes:

$$\int_{\partial\mathbb{A}} \left(\vec{E} + \vec{v} \times \vec{B} \right) \cdot d\vec{x} = -\frac{d}{dt} \int_{\mathbb{A}(t)} \vec{B} \cdot d\vec{\mathbb{A}}.$$

- (c) Finally, consider a closed wire making a loop $\gamma(t)$ and let $\mathbb{A}(t)$ be the area bounded by the loop. Show that the EMF of going around the loop 1 time $\mathcal{E}[\gamma]$ is given by:

$$\mathcal{E}[\gamma] = -\frac{d}{dt} \int_{\mathbb{A}(t)} \vec{B} \cdot d\vec{\mathbb{A}}.$$

This result is known as the integral form of Faraday's Law.

Problem 3.84: Inductors and Inductance. Consider a perfect solenoid of N total turns, length ℓ , and cross sectional area $\mathbb{A}$. Suppose that a time dependent current $I(t)$ runs through the solenoid. Show that the EMF between the two ends of the Solenoid is given by:

$$\mathcal{E} = -\frac{\mu_0 N^2 \mathbb{A}}{\ell} \frac{dI}{dt}$$

Whenever a circuit component has EMF proportional to the negative of the rate of change of current, that proportionality constant is called the inductance L of that component. That is:

$$\mathcal{E} = -L \frac{dI}{dt}$$

and $L = \frac{\mu_0 N^2 \mathbb{A}}{\ell}$ for a perfect solenoid. For less idealized coils of wire, one can compute similar but generally much nastier expressions for the inductance.

Problem 3.85: Circuit Theory and Voltage. Consider a closed loop γ in a circuit which has some magnetic components (meaning inductors).

- (a) Show that the emf through the closed loop is given by:

$$\mathcal{E} = \sum_n \mathcal{E}_n = -\sum_m L_m \frac{dI_m}{dt}$$

where $\mathcal{E}_n$ are the emfs across non-magnetic circuit components and L_m are the inductances of the inductors of the circuit (with I_m the currents across those inductors).

- (b) For non-magnetic components, define the “voltage across” or “voltage drop” V of that component as the emf across it. For inductors, define the voltage drop across the inductor by the negative of the emf across it. Show then that the sum of all voltage drops across the components in a closed loop is given by:

$$\sum_n V_n = 0.$$

This is the magnetic version of Kirchoff's loop rule. So, we can see that our previous circuit results are still applicable when inductors are involved provided we phrase our equations in terms of voltage defined here instead of emf. From now on we use that for a resistor R , capacitor C , or inductor L , the voltage drop V across that component is related to the current I across that component by:

$$V = IR, \quad \frac{dV}{dt} = \frac{I}{C}, \quad V = L \frac{dI}{dt}$$

with power $\mathcal{P}$ dissipated across any component given by:

$$\mathcal{P} = IV$$

Problem 3.86: Inductors in Circuits.

- (a) Consider two inductors (of inductances L_1 and L_2 respectively) which are connected in series experiencing a current $I(t)$ into the left terminal of the left inductor. Let V be the sum of voltage drops of across the inductors. Show using Kirchoff's laws that:

$$V = (L_1 + L_2) \frac{dI}{dt}$$

and thus justify that two inductors in series effectively act as a single inductor with equivalent inductance:

$$L = L_1 + L_2.$$

- (b) Consider two inductors which are connected in parallel with a voltage drop V across either inductor. Let $I(t)$ be the total current into the left terminals of the inductors from the junction at which they are connected. Show that:

$$V = \frac{1}{\frac{1}{L_1} + \frac{1}{L_2}} \frac{dI}{dt}$$

and thus justify that two inductors in parallel effectively act as a single inductor with equivalent inductance:

$$\frac{1}{L} = \frac{1}{L_1} + \frac{1}{L_2}.$$

Problem 3.87: Energy stored by an inductor.

- (a) Show from the Lagrangian (3.8.1) and Ampere's law that the energy stored in the magnetic field is given by:

$$E = \int_S \frac{|\vec{B}|^2}{2\mu_0} d\mathbb{S}.$$

- (b) Consider a solenoid with total turns N , length ℓ , and cross sectional area $\mathbb{A}$ carrying a current I . Show that the energy stored in this solenoid is given by:

$$E = \frac{\mu_0 N^2 \mathbb{A}}{2\ell} I^2.$$

- (c) Use the expression for the inductance of the solenoid to conclude that the energy stored in an inductor is given by:

$$E = \frac{1}{2} L I^2.$$

Problem 3.88: The RL Circuit. Consider a resistor R which is connected in series with an inductor L and a battery of voltage V_0 .

- (a) Show using Kirchoff's laws that the current I through the circuit satisfies the differential equation:

$$L \frac{dI}{dt} + IR = V_0.$$

- (b) Solve this differential equation to show that $I(t)$ is given by:

$$I(t) = \frac{V_0}{R} + \left(I_0 - \frac{V_0}{R} \right) e^{-\frac{R}{L}t}.$$

Thus, the circuit equilibrates to the current that would flow if only a resistor was placed there and it decays to this value with a characteristic time scale $\tau = \frac{L}{R}$. It is certainly a stretch of our theory to be applying our electrostatics results and magnetostatics results together like this as we found the two are not exactly compatible together with Galilean symmetry. We will return to this issue very soon.

Problem 3.89: The LC Circuit. Consider an inductor L which is connected in series with a capacitor C and a variable voltage source $V_0(t)$.

- (a) Show using Kirchoff's laws that the charge q accumulated on one plate of the capacitor satisfies the differential equation:

$$L \frac{d^2q}{dt^2} + \frac{q}{C} = V_0(t).$$

Thus, the system is a driven harmonic oscillator with angular frequency $\omega = \frac{1}{\sqrt{LC}}$. Solve this equation of motion for $V_C(t)$, the voltage across the capacitor.

- (b) Suppose $V_0(t) = 0$. Show that the resultant equation conserves the energy stored in the capacitor plus the energy stored in the inductor.
- (c) Suppose still that $V_0(t) = 0$. Consider (very recklessly) the sum of the electrostatic and magnetostatic Lagrangians. Show that if the only charges present are those on the capacitor and flowing through the inductor then applying the solutions of Gauss' law and Ampere's law to the Lagrangian gives (by the holonomic constraint theorem):

$$\mathcal{L} = \frac{1}{2} L \dot{q}^2 - \frac{q^2}{2C}.$$

As well, show that the Euler-Lagrange equation of motion implied by this Lagrangian is the correct one for $V_0(t) = 0$.

- (d) Show that using a known capacitor and an astatic galvanometer we can measure an unknown inductance L .

Problem 3.90: The LRC circuit. Consider an inductor L which is connected in series with a resistor R , a capacitor C , and a voltage source $V_0(t)$.

- (a) Show using Kirchoff's laws that the charge q accumulated on one plate of the capacitor satisfies the differential equation:

$$L \frac{d^2 q}{dt^2} + R \frac{dq}{dt} + \frac{q}{C} = V_0(t).$$

Thus, the system is a driven damped harmonic oscillator. Solve this equation of motion for $V_C(t)$, the voltage across the capacitor. As well, find the resonant frequency of the circuit and the full width at half maximum of its frequency response.

- (b) Suppose $V_0(t) = 0$. Show that the rate at which the energy of the capacitor and inductor together fail to be conserved is exactly matched by the rate at which the resistor dissipates energy. The inclusion of the resistor causes the energy of the circuit to not be conserved as the resistor (by our original Ohmic model) exchanges energy with the material of the resistor (the various internal scattering targets i.e. atoms within it).

Problem 3.91: Mutual Inductance and Transformers. For finite solenoids the magnetic field outside is non-zero. This causes the magnetic field of one solenoid to contribute to the magnetic flux in Faraday's law of another solenoid. This produces the phenomenon of mutual inductance. Consider a system of closed current carrying wires with currents I_n . Let the path of each wire be given by γ_n .

- (a) Use the linearity of Ampere's law to show that the total vector potential in the Coulomb gauge is given by:

$$\vec{A}(t, \vec{x}) = \sum_n \vec{A}_n(t, \vec{x})$$

where $\vec{A}_n(t, \vec{x})$ is the vector potential due to just wire n and show that it is given by:

$$\vec{A}_n(t, \vec{x}) = I_n \int_{\gamma_n} \frac{\mu_0 d\vec{x}'}{4\pi |\vec{x} - \vec{x}'|}.$$

- (b) Let the magnetic flux Φ through a loop of wire be defined by:

$$\Phi = \int_{\mathbb{A}} \vec{B} \cdot d\vec{\mathbb{A}}$$

where $\mathbb{A}$ is the area enclosed by the wire. Show that it is equivalently given by:

$$\Phi = \int_{\gamma} \vec{A} \cdot d\vec{x}.$$

- (c) Let the magnetic flux through wire n due to wire m be defined by:

$$\Phi_{nm} = \int_{\mathbb{A}_n} \vec{B}_m \cdot d\vec{\mathbb{A}}.$$

Show that it is given by:

$$\Phi_{nm} = I_n \int_{\gamma_n} \int_{\gamma_m} \frac{\mu_0 d\vec{x} \cdot d\vec{x}'}{4\pi |\vec{x} - \vec{x}'|}$$

- (d) The mutual inductance L_{nm} between two wires n and m is defined as the flux through n due to m per unit current through I_m :

$$L_{nm} = \frac{\Phi_{nm}}{I_m}.$$

Show that $L_{nm} = L_{mn}$ and by using Faraday's law that the emf through loop γ_n is given by:

$$\mathcal{E}_n = - \sum_m L_{nm} \frac{dI_m}{dt}.$$

- (e) Consider now only two wires in this manner. Suppose they are solenoidal coils having N_1 and N_2 total turns respectively. Let Φ_{nm} refer to only the flux through one turn of wire n due to wire m . Show that because not all of the magnetic field of wire 2 will pass through the coil of 1 and vice versa:

$$\frac{L_{21}}{N_2} \leq \frac{L_{11}}{N_1}, \quad \frac{L_{12}}{N_1} \leq \frac{L_{22}}{N_2}.$$

In the approximation that all of the magnetic field of one wire does pass through the other, these inequalities become equalities and the system is said to be ideally coupled.

- (f) Consider the above two coils to be ideally coupled (real wires could only ever be strongly coupled, meaning that the inequalities are near enough to be equalities for equality to be a reasonable approximation). Show that under this condition $L_{12} = \sqrt{L_1 L_2}$. As well, show that the voltage drops across the inductors are related by:

$$\frac{V_1}{\sqrt{L_1}} = \frac{V_2}{\sqrt{L_2}}.$$

A pair of ideally coupled inductors is called a transformer and as you can see it provides a way to multiply a voltage by an arbitrary factor (if you can produce inductors of desired inductances) and thus is very useful for electronic components which need a higher or lower voltage to operate than the voltage which is provided by standard wall outlets.

Problem 3.92: Impedance.

- (a) For each of the basic components of a resistor, capacitor, and inductor show that $\tilde{V}(\omega)$, the Fourier transform of the voltage across that component, is linearly related to $\tilde{I}(\omega)$, the Fourier transform of the current through that component as:

$$\tilde{V}(\omega) = Z(\omega)\tilde{I}(\omega)$$

for some function $Z(\omega)$ which depends on the circuit component. As well, show that for a resistor $Z(\omega) = R$, for a capacitor $Z(\omega) = \frac{i}{C\omega}$, and that for an inductor $Z(\omega) = -i\omega L$. This function exists for any linear circuit component and it is called the impedance of that component.

- (b) Show using Kirchoff's laws that impedances combine among components in series or in parallel with exactly the same combination rules as ordinary resistors.
 (c) Show, using that $I(t)$ and $V(t)$ are real valued, that the impedance of any circuit component must satisfy:

$$Z^*(\omega) = Z(-\omega).$$

- (d) Show by integrating the power with respect to time that the total energy dissipated across a circuit component is given by:

$$E = \int_0^\infty 2\text{Re}(Z(\omega))|\tilde{I}(\omega)|^2 d\omega.$$

Thus, just as the total energy can be written as the integral of power with respect to time, it can be written as the integral of the "power spectral density" (PSD) defined by:

$$\tilde{\mathcal{P}}(\omega) = 2\text{Re}(Z(\omega))|\tilde{I}(\omega)|^2$$

with respect to angular frequency.

- (e) Suppose we consider two points on a circuit and attach a device between them. These two points are called terminals and to understand what will happen when we plug our device into them, we would like to understand the relationship between the voltage between those two points and the current flowing between those two points. Assume that in the rest of the circuit there are linear circuit components (resistors, capacitors, inductors) and voltage sources. Let $V_{th}(t)$ be the "open-circuit voltage" between the terminals. That is, the voltage between the terminals when no device is attached. As well, let $I_N(t)$ be the "short-circuit current". That is, the current which would flow between the terminals if they were directly connected to each other. Define $Z_{th} = \frac{\tilde{V}_{th}}{\tilde{I}_N}$. Show that device behaves equivalently when connected to our original circuit as it would if it were connected to a voltage source with voltage V_{th} in series with a component of impedance Z_{th} . This equivalent circuit is called the Thévenin equivalent circuit for our 2 terminals. Importantly, the Thévenin equivalent circuit is completely different for each pair of terminals you may select in a circuit.
 (f) Very commonly, a circuit will have 4 terminals grouped in two pairs called the input terminals and the

output terminals. The expectation is that some source will be connected across the input terminals which will produce some output to be measured by a measurement device connected across the output terminals. For this circuit, it is assumed that if no input is connected, the voltage between both the input and the output terminals is 0. Then, explain that the Thévenin equivalent circuit for the input terminals consists of an equivalent voltage of 0 and some impedance Z_{in} . This impedance is called the input impedance of the device. As well, the impedance of the Thévenin equivalent circuit for the output terminals is called the output impedance Z_{out} . Finally, the ratio of the output voltage Fourier transform to the input voltage Fourier transform of such a device is called the transfer function $\tilde{G}(\omega)$. Show that for the purposes of calculations, such a device is completely characterized by its input and output impedances and transfer function. As such, these devices are often called “black-boxes” because it is not important to see what is inside them once you know these three functions.

- (g) Suppose that we connect the output terminals (of output impedance Z_{out} and Thévenin equivalent voltage V_{th}) of one blackbox to the input terminals of another blackbox (of input impedance Z_{in}). Show that the Fourier transform of the voltage across the input terminals of the input device is given by:

$$\tilde{V} = \frac{Z_{\text{in}}}{Z_{\text{in}} + Z_{\text{out}}} \tilde{V}_{\text{th}}.$$

Often, one designs the first box intending for V_{th} to be the voltage it “delivers” to the second box, meaning that $\tilde{V}$ is intended to be (at least approximately) equal to $\tilde{V}_{\text{th}}$. Show that this requires that the input impedance of the “driven” box be much greater in magnitude than the output impedance of the “driving” box. Using this technique is called impedance bridging.

- (h) Show alternatively that for the previous part the power spectral density delivered to the second box is:

$$\tilde{\mathcal{P}}(\omega) = \frac{2\text{Re}(Z_{\text{in}}(\omega))}{|Z_{\text{in}} + Z_{\text{out}}|^2} |\tilde{V}_{\text{th}}|^2.$$

In contrast to the previous part, sometimes one instead wants to transfer as much energy as power to the second box. Show that in order to maximize the transferred energy (equivalently, maximize the PSD), one should design the second box so that $Z_{\text{in}}(\omega) = Z_{\text{out}}^*(\omega)$. This is known as “maximizing power transfer” and is often called “impedance matching”¹¹.

Problem 3.93: Penning trap. Consider a charge q to be surrounded by a solenoid producing a background magnetic field $\vec{B} = B\vec{e}_z$ and a charge distribution so that the interior multipole expansion for the scalar potential can be used. The charge distribution has no net charge or interior dipole moment so we will approximate it only by the interior quadrupole moment. Suppose further that the charge distribution has rotational symmetry about the z axis.

- (a) Show that the $\hat{M}$ matrix defined in problem 3.71 can be written in the form:

$$\hat{M} = Q \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

for some constant Q by using that that matrix is symmetric and traceless and that the given charge distribution has rotational symmetry about the z axis.

- (b) Show then that in cylindrical coordinates the Lagrangian for the charge in this background becomes:

$$\mathcal{L} = \frac{1}{2}m\dot{\mathbf{r}}^2 + \frac{1}{2}m\mathbf{r}^2\dot{\varphi}^2 + \frac{1}{2}m\dot{z}^2 + \frac{qB}{2}\mathbf{r}^2\dot{\varphi} + \frac{qQ}{8\pi\epsilon_0}\mathbf{r}^2 - \frac{qQ}{4\pi\epsilon_0}z^2.$$

- (c) Show that the charge oscillates stably around the origin in the z direction if $qQ > 0$ and find the angular frequency of oscillation. As well, let L be the angular momentum of the charge about the z axis and show that it is conserved. Using this, show that the $\mathbf{r}$ equation of motion for the charge becomes:

$$\ddot{\mathbf{r}} + \left(\frac{q^2 B^2}{4m^2} - \frac{qQ}{4\pi\epsilon_0} \right) \mathbf{r} - \frac{L^2}{m^2 \mathbf{r}^3} = 0.$$

- (d) Show that there is a radius $\mathbf{r}_0$ for fixed L at which the charge persists in a circle around the z axis. Consider then the charge to be perturbed off of this orbit by a perturbation $\delta\mathbf{r}(t)$. Show that the charge oscillates around $\mathbf{r}_0$ stably and identify the angular frequency of oscillations for small oscillations of the charge. Thus, identify that this device, known as the Penning trap, allows one to stably contain a charge in all directions.

¹¹Although, there are other techniques which are also called impedance matching in the context of wave propagation.

Problem 3.94: ★ The Hall Effect. Consider a conducting box of length L in the x direction, width w in the y direction, and height h in the z direction with current I running through it by a wire straight through its center down the x direction provided by some source. As well, an external magnetic field of magnitude B is present in the z direction.

- (a) Show using the Lorentz force that the external magnetic field causes charges flowing in the conductor to accumulate on the walls of the box which have normal vectors in the y direction.
- (b) The charges accumulating on the walls as the current flows cause an additional contribution to the electric field (by summing the fields due to those charges). Eventually, enough charges accumulate so that charges are no longer pulled toward the walls. Show using the Lorentz force that once charges are no longer pulled toward the walls the y component of the electric field is given by:

$$E_y = v_x B$$

where v_x is the velocity at which charges are flowing down the wire in the x direction.

- (c) Show that the emf between the walls of the conductor which are normal to the y direction is given by:

$$\mathcal{E} = v_x B w$$

- (d) Assuming the current is carried by charges each with the same charge q and that there are n charges per unit volume (called the number density), show that the current through the conductor is given by:

$$I = q n v_x w h.$$

- (e) Thus, show that the voltage drop of the conductor across the box in the y direction is given by:

$$V = \frac{IB}{qn h}.$$

This is known as the Hall effect. Notice that we can determine I by using a galvanometer and we can determine B by placing a dipole (such as a magnetic needle) with known dipole moment (which can be measured in the question on measuring c) and using our known results on the dynamics of a dipole placed in an external magnetic field. We can then measure this voltage drop by placing in parallel to the walls of the conductor a large known resistor R (so that it draws little current as to not affect the result much) and measuring the current it draws with our galvanometer. After measuring the voltage drop then, if it is positive we see that q must be positive and if it is negative (meaning it drops in the other direction) then q must be negative. Hence, this device gives a way of determining the sign of the charges which are actually carrying the current in our conductor. It is found by experiment that the charge carriers in conducting metals are negative (recall that which charge is positive and which is negative is a convention. Based on the convention established historically, the carriers of current are negative). This is one early hint that there is a single species of charge doing most of the activity in the world (called the electron, which we will discuss later). Unfortunately, the Hall effect gives us no way of measuring q if we do not already know the number density n of charge carriers in our material.

3.9 Electromagnetic Coexistence and Causality

Now we return to the very disturbing tension between our vector and scalar theories. Electrostatics works very well as a steady state theory of charges and magnetostatics works very well as a theory of steadily flowing current. However, electrostatics is a scalar theory of electric charge and magnetostatics is a vector theory of electric charge. As we found in section 3.3, there is no way to have both while preserving Galilean symmetry. However, they are both experimentally successful theories. We call this problem the problem of electromagnetic coexistence. Because this conflict only depends on the Taylor series expansion of the Lagrangian density to quadratic order, it is not resolved by either higher order terms in the fields or higher derivatives. Higher order terms will not explain why these two different inconsistent expansions are both successful at low field strengths. So, what gives? The terms in the Lagrangian density for both of these theories were perfectly allowed right up until we enforced Galilean boost symmetry in section 3.3. Because experiment always supersedes theory, the success of electrostatics and magnetostatics in contradiction with Galilean symmetry is experimental proof that **Galilean symmetry is not fundamental**. The boost symmetry we believed in must not quite be right (the observed terms are consistent with all of our other symmetries but this one). We need to go beyond Galilean boost symmetry.

3.9.1 A Big Bold Leap

For electrostatics, the Lagrangian was:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho\phi + \frac{\epsilon_0}{2} |\vec{E}|^2 \right) d\mathbb{S}. \quad (3.9.1)$$

For magnetostatics, the Lagrangian was:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho\phi - \frac{|\vec{B}|^2}{2\mu_0} \right) d\mathbb{S}. \quad (3.9.2)$$

Because the two are simultaneously successful, we make the big bold leap to consider the two theories at the same time:

$$\boxed{\mathcal{L} = \int_{\mathbb{S}} \left(\vec{J} \cdot \vec{A} - \rho\phi + \frac{\epsilon_0}{2} |\vec{E}|^2 - \frac{|\vec{B}|^2}{2\mu_0} \right) d\mathbb{S}.} \quad (3.9.3)$$

We know ahead of time that this big leap is not Galilean invariant. We are now in new territory. Let's compute the equations of motion:

$$\frac{\delta S}{\delta \phi} = \frac{\partial \mathcal{L}}{\partial \phi} + \nabla \cdot \frac{\partial \mathcal{L}}{\partial \vec{E}} \stackrel{!}{=} 0 \implies \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}. \quad (3.9.4)$$

$$\frac{\delta S}{\delta \vec{A}} = \frac{\partial \mathcal{L}}{\partial \vec{A}} + \nabla \times \frac{\partial \mathcal{L}}{\partial \vec{B}} + \partial_t \frac{\partial \mathcal{L}}{\partial \vec{E}} \stackrel{!}{=} 0 \implies \nabla \times \vec{B} = \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}. \quad (3.9.5)$$

Recalling Theorem 2.9, which gives the interdependence between $\vec{E}$ and $\vec{B}$, we are left with the equations:

$$\boxed{\begin{aligned} \nabla \cdot \vec{E} &= \frac{\rho}{\epsilon_0}, & \nabla \cdot \vec{B} &= 0, \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t}, & \nabla \times \vec{B} &= \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}. \end{aligned}} \quad (3.9.6)$$

These are called **Maxwell's equations** and they give an extremely experimentally consistent description of electromagnetism. Notice that the only difference between these equations and the combination of the equations of motion for the vector and scalar Galilean theories is the singular $\epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}$ term in the final equation. The modified equation in (3.9.6) is known as the **Ampere-Maxwell law**. Whenever this new term is 0 or negligibly small, the theory will look like the Galilean theory, which explains the success of the Galilean theory under certain conditions even though it violates Galilean symmetry overall.

3.9.2 Electromagnetic Waves

Now that we have some equations of motion, let's see what they do and what their solutions look like. Take the curl of Faraday's Law and use our favorite cross product identity:

$$\nabla \times (\nabla \times \vec{E}) = \nabla \times \left(-\frac{\partial \vec{B}}{\partial t} \right) \quad (3.9.7)$$

$$\implies \nabla \nabla \cdot \vec{E} - \nabla \cdot \nabla \vec{E} = -\frac{\partial}{\partial t} \nabla \times \vec{B} \quad (3.9.8)$$

$$\implies \frac{1}{\epsilon_0} \nabla \rho - \nabla^2 \vec{E} = -\frac{\partial}{\partial t} \left(\mu_0 \vec{J} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} \right) \quad (3.9.9)$$

$$\implies \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} - \nabla^2 \vec{E} = -\frac{1}{\epsilon_0} \nabla \rho - \mu_0 \frac{\partial \vec{J}}{\partial t}. \quad (3.9.10)$$

This equation is of the form:

$$\frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \eta(t, \vec{x}) \quad (3.9.11)$$

by identifying $\vec{E} = \phi$ (this ϕ is not the same ϕ as the scalar potential, it is simply whatever function appears here in this differential equation) and η as the expression on the right hand side in equation (3.9.10). Equation (3.9.11) is called the **d'Alembert wave equation**. Now take the curl of the Ampere-Maxwell law:

$$\nabla \times (\nabla \times \vec{B}) = \nabla \times \left(\mu_0 \vec{J} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} \right) \quad (3.9.12)$$

$$\implies \nabla \nabla \cdot \vec{B} - \nabla^2 \vec{B} = \mu_0 \nabla \times \vec{J} + \frac{1}{c^2} \frac{\partial}{\partial t} \nabla \times \vec{E} \quad (3.9.13)$$

$$\implies 0 - \nabla^2 \vec{B} = \mu_0 \nabla \times \vec{J} - \frac{1}{c^2} \frac{\partial^2 \vec{B}}{\partial t^2} \quad (3.9.14)$$

$$\implies \frac{1}{c^2} \frac{\partial^2 \vec{B}}{\partial t^2} - \nabla^2 \vec{B} = \mu_0 \nabla \times \vec{J}. \quad (3.9.15)$$

Hence not only does the electric field satisfy the wave equation, but the magnetic field does as well. We can manually solve the d'Alembert wave equation by taking the spatial Fourier transform:

$$\tilde{\phi}(t, \vec{k}) \stackrel{\text{def}}{=} \int_{\mathbb{S}} \frac{e^{-i\vec{k} \cdot \vec{x}}}{\sqrt{8\pi^3}} \phi(t, \vec{x}) d^3 \vec{x}, \quad \tilde{\eta}(t, \vec{k}) \stackrel{\text{def}}{=} \int_{\mathbb{S}} \frac{e^{-i\vec{k} \cdot \vec{x}}}{\sqrt{8\pi^3}} \eta(t, \vec{x}) d^3 \vec{x} \quad (3.9.16)$$

$$\implies \frac{1}{c^2} \frac{\partial^2 \tilde{\phi}(t, \vec{k})}{\partial t^2} + |\vec{k}|^2 \tilde{\phi}(t, \vec{k}) = \tilde{\eta}(t, \vec{k}). \quad (3.9.17)$$

Equation (3.9.17) is a second order inhomogeneous linear ordinary differential equation and at fixed $\vec{k}$ can be written in the form:

$$\ddot{y} + \omega_0^2 y = \omega_0^2 x(t). \quad (3.9.18)$$

This is precisely the driven harmonic oscillator! Hence, the d'Alembert wave equation is equivalent to an infinite number of independent driven harmonic oscillators, 1 for each wavenumber $\vec{k}$. Using problem 2.29 we can solve the driven harmonic oscillator exactly:

$$y(t) = \int_{-\infty}^t x(t') \sin(\omega_0(t-t')) \omega_0 dt'. \quad (3.9.19)$$

This is the solution for $y(t)$ which limits to 0 as $t \rightarrow -\infty$. Identifying $\omega_0 \rightarrow c|\vec{k}|$, $\omega_0^2 x(t) \rightarrow c^2 \tilde{\eta}(t, \vec{k})$, $y(t) \rightarrow \tilde{\phi}(t, \vec{k})$ in (3.9.17), we have the solution:

$$\tilde{\phi}(t, \vec{k}) = \int_{-\infty}^t \frac{c}{|\vec{k}|} \sin(c|\vec{k}|(t-t')) \tilde{\eta}(t', \vec{k}) dt'. \quad (3.9.20)$$

Now to recover the solution $\phi(t, \vec{x})$, we just need to take the inverse Fourier transform:

$$\phi(t, \vec{x}) = \int_{\mathbb{K}} \frac{e^{i\vec{k} \cdot \vec{x}}}{\sqrt{8\pi^3}} \tilde{\phi}(t, \vec{k}) d^3 \vec{k} \quad (3.9.21)$$

$$= \int_{-\infty}^t \int_{\mathbb{S}} \eta(t', \vec{x}') \int_{\mathbb{K}} \frac{ce^{i\vec{k} \cdot (\vec{x} - \vec{x}')} \sin(c|\vec{k}|(t - t'))}{8\pi^3 |\vec{k}|} d^3 \vec{k} d^3 \vec{x}' dt'. \quad (3.9.22)$$

We see the solution for ϕ is given by integrating η against some function. That function is called the delayed Green's function (for the wave equation):

$$G(t, \vec{x}) \stackrel{\text{def}}{=} \int_{\mathbb{K}} \frac{ce^{i\vec{k} \cdot \vec{x}} \sin(c|\vec{k}|t)}{8\pi^3 |\vec{k}|} \vartheta(t) d^3 \vec{k} \quad (3.9.23)$$

$$\implies \phi(t, \vec{x}) = \int_{-\infty}^{\infty} \int_{\mathbb{S}} G(t - t', \vec{x} - \vec{x}') \eta(t', \vec{x}') d^3 \vec{x}' dt'. \quad (3.9.24)$$

By switching to spherical coordinates, we can perform the integral:

$$G(t, \vec{x}) = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} \frac{ce^{ik|\vec{x}| \cos \theta} \sin(ckt)}{8\pi^3 k} \vartheta(t) k^2 \sin \theta d\varphi d\theta dk \quad (3.9.25)$$

$$= \frac{c\vartheta(t)}{8\pi^3} \int_0^{2\pi} d\varphi \int_0^{\infty} k \sin(ckt) \int_0^{\pi} e^{ik|\vec{x}| \cos \theta} \sin \theta d\theta dk \quad (3.9.26)$$

$$= \frac{c\vartheta(t)}{8\pi^3} 2\pi \int_0^{\infty} k \sin(ckt) \left. \frac{-e^{ik|\vec{x}| \cos \theta}}{ik|\vec{x}|} \right|_0^{\pi} dk \quad (3.9.27)$$

$$= \frac{c\vartheta(t)}{4\pi^2 |\vec{x}|} \int_0^{\infty} \sin(ckt) \frac{e^{ik|\vec{x}|} - e^{-ik|\vec{x}|}}{i} dk \quad (3.9.28)$$

$$= \frac{c\vartheta(t)}{4\pi^2 |\vec{x}|} \int_0^{\infty} \frac{e^{ickt} - e^{-ickt}}{2i} \frac{e^{ik|\vec{x}|} - e^{-ik|\vec{x}|}}{i} dk \quad (3.9.29)$$

$$= -\frac{c\vartheta(t)}{8\pi^2 |\vec{x}|} \int_0^{\infty} \left(e^{i(|\vec{x}|+ct)k} + e^{-i(|\vec{x}|+ct)k} - e^{i(|\vec{x}|-ct)k} - e^{-i(|\vec{x}|-ct)k} \right) dk \quad (3.9.30)$$

$$= -\frac{c\vartheta(t)}{8\pi^2 |\vec{x}|} \int_{-\infty}^{\infty} \left(e^{i(|\vec{x}|+ct)k} - e^{i(|\vec{x}|-ct)k} \right) dk. \quad (3.9.31)$$

Using the fundamental Fourier integral:

$$\int_{-\infty}^{\infty} e^{ikx} dk = 2\pi \delta(x) \quad (3.9.32)$$

where $\delta(x)$ is the Dirac delta distribution, we are left with:

$$G(t, \vec{x}) = \frac{c\vartheta(t)}{4\pi |\vec{x}|} (\delta(|\vec{x}| - ct) - \delta(|\vec{x}| + ct)). \quad (3.9.33)$$

By using the rescaling property of the Dirac delta:

$$\delta(ax) = \frac{\delta(x)}{|a|} \quad (3.9.34)$$

$$\implies G(t, \vec{x}) = \frac{\delta(t - \frac{|\vec{x}|}{c})\vartheta(t)}{4\pi |\vec{x}|} - \frac{\delta(t + \frac{|\vec{x}|}{c})\vartheta(t)}{4\pi |\vec{x}|}. \quad (3.9.35)$$

The second delta never contributes because the Heaviside step function is only nonzero for $t > 0$ and the peak of the delta is at $t = -\frac{|\vec{x}|}{c}$ which is guaranteed to be negative. Thus, the delayed Green's function for the wave equation is:

$$G(t, \vec{x}) = \frac{\delta(t - \frac{|\vec{x}|}{c})\vartheta(t)}{4\pi |\vec{x}|}. \quad (3.9.36)$$

Putting the Green's function into the integral relating ϕ and η , we finally have the solution to the wave equation:

$$\phi(t, \vec{x}) = \int_{-\infty}^{\infty} \int_{\mathbb{S}} \eta(t', \vec{x}') \frac{\delta(t - t' - \frac{|\vec{x} - \vec{x}'|}{c})\vartheta(t - t')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}' dt' \quad (3.9.37)$$

$$\implies \phi(t, \vec{x}) = \int_{\mathbb{S}} \frac{\eta(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.9.38)$$

Notice how similar the solution to the wave equation, equation (3.9.38), is to the solution to the Poisson

equation in Theorem 3.2. In fact, the only difference is that instead of evaluating η at time t (as is done in the solution to the Poisson equation), η is evaluated at time $t - \frac{|\vec{x} - \vec{x}'|}{c}$. This has a very nice interpretation. The time difference between the time at which the source (η) is evaluated and the time at which the signal (ϕ) is detected is $t - (t - \frac{|\vec{x} - \vec{x}'|}{c}) = \frac{|\vec{x} - \vec{x}'|}{c}$. That is, a signal produced at a point $\vec{x}'$ at a time $t - \frac{|\vec{x} - \vec{x}'|}{c}$ will reach a second point $\vec{x}$ a distance $l = |\vec{x} - \vec{x}'|$ away at time t . The distance traveled by the signal per unit time is $\frac{\Delta x}{\Delta t} = \frac{l}{l/c} = c$, meaning c is precisely the speed at which the wave in the wave equation propagates across space. Thus:

Theorem 3.4: Solution to the Wave Equation

The solution for $\phi(t, \vec{x})$ which limits to 0 as $t \rightarrow -\infty$ to the inhomogeneous wave equation:

$$\frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \eta(t, \vec{x}) \quad (3.9.39)$$

with source $\eta(t, \vec{x})$ and propagation speed c on all space is:

$$\phi(t, \vec{x}) = \int_{\mathbb{S}} \frac{\eta(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (3.9.40)$$

Matching the terms in the wave equations for the electric (3.9.10) and magnetic (3.9.15) fields with the general wave equation (3.9.11), we find that both of them propagate with the same speed c which appeared in the Lagrangian. This speed at which electromagnetism propagates is called the **speed of light**. Having the effects of the sources (charges and currents) propagate at a finite speed removes a subtle curiosity of the Galilean theory. In the solution to the Poisson equation solution, the field arbitrarily far away from a source is affected instantaneously by that source; effects happen at the same time as their causes (because $\phi(t, \vec{x})$ is written as an integral over $\rho(t, \vec{x}')$ over all $\vec{x}'$, arbitrarily far away, at the present time t). However, in the wave equation the effect of a source takes non-zero time to propagate across space and so effects happen after their causes. This property is called **causality**.

3.9.3 Much Ado About Boosting

We broke our Galilean boost symmetry by hand. What does this mean? Well, it is actually pretty straightforward to see why Maxwell's equations don't have Galilean boost symmetry. As we found in solving the wave equation, Maxwell's equations have a special speed c encoded in them. That speed is a constant parameter in the Lagrangian which defines the theory and so it takes the same value under any symmetry transformations of the theory. However, a Galilean boost shifts all velocities equally and so cannot possibly leave any special speed unchanged. As such, no theory with a special speed can have Galilean boost symmetry. What is the resolution? There are two options available to us: we could say that perhaps boost symmetry just isn't real and there was no symmetry to actually be found or we can say that we were getting at a true symmetry but we only found what that symmetry was approximately; perhaps by modifying the symmetry slightly we can make a consistent theory.

Let us start by supposing that boost symmetry is not real. Then, we could have Maxwell's Lagrangian (3.9.3) together with our particle Lagrangian (2.5.5) with no issue. However, to derive that particle Lagrangian we used Galilean boost symmetry and so once we throw out that symmetry we in principle have more terms which are allowed in it we would need to consider. As well, because that Lagrangian gives so many good predictions, we would need to explain why there is an apparent approximate boost symmetry under many every day circumstances and why so often those possible additional terms are apparently irrelevant. It could just happen that the universe is that way but a system very nearly having a symmetry with no explanation is reasonably considered suspicious. On more concrete grounds, if there is no boost symmetry, then the coordinates in which the Lagrangian for ϕ and $\vec{A}$ takes the form of (3.9.3) define a special set of coordinates (called a reference frame) and in no other reference frame (boosted coordinate system) will the Lagrangian be of the same form (because the Lagrangian doesn't have Galilean boost symmetry). So, the absence of Galilean boost symmetry implies one can define "absolute motion" with respect to these special coordinates. This is in direct contrast to the core assumption of boost symmetry which was that only relative motion mattered. The reference frame against which absolute motion would be defined is called the Aether. Then, for any frame other than the Aether's, the relative motion between that frame and the Aether's would mean

that in the frame the speed of light appears to be $c - v$ when looking in the direction of relative motion, $c + v$ when looking away, and continuously interpolates between the two values for intermediate directions. As well, because the Earth is whirling around the Sun and so has its velocity constantly changing in space, the speed of light in different directions on Earth should not only be different at any given time but also vary throughout the year. However, experimental searches for variation in the speed of light with direction and time have completely failed to detect any such effect. So, the belief in an Aether is plagued not only by the burden of needing to explain why so often boost symmetry seems to hold but also its experimental predictions are not observed. Therefore, it is wrong.

The alternative is that there is some generalized notion of boost symmetry. Because the speed of light is predicted straight from Maxwell's Lagrangian, it must be the same under any transformation for which this Lagrangian has symmetry. If we are to have some generalized notion of boost symmetry then, it must leave the speed of light unchanged. Such a generalized boost would need to approximately reduce to our Galilean boost under the circumstances in which our Galilean theory has been successful. If we can find such a thing, it may resolve the discrepancy between Maxwell's theory and Galileo's. This is the approach we will take next chapter.

Exercises

Problem 3.95: Variation of the Speed of Light with direction in an Aether. Suppose that the Aether theory was correct and there was a preferred frame in which electromagnetic waves propagate with speed c in all directions. Suppose that an observer is in a coordinate system moving at velocity $\vec{v}$ relative to the Aether and that there is an electromagnetic wave moving in the Aether at an angle θ relative to $\vec{v}$. Show that the observer sees the electromagnetic wave moving with speed:

$$c' = \sqrt{c^2 - 2cv \cos \theta + v^2}$$

where $v = |\vec{v}|$. Famously the Michelson-Morley experiment tried to detect this effect by using two orthogonal beams of light and a system of mirrors to see if they arrived onto a screen together or with some separation. Due to the way the experiment is setup, they would arrive always together if there was no effect. In the many repeated trials of this experiment there is never any significant beam separation (within the experimental precision, which has been tuned over the years to be plenty good enough to detect an effect for the observed speed of light c). For this reason, we see that Aether theory fails.

Problem 3.96: The Nonrelativistic Doppler Effect. Consider waves which propagate with speed c in a medium (such as sound in air, where c would be the speed of sound, or light in a Aether theory) in 1 spatial dimension. Consider a wave source which is moving relative to the medium at velocity v_s and produces waves of frequency f_s . Consider a wave detector which is on the right of the source and which is moving relative to the medium at velocity v_d . Assume that $|v_s|$ and $|v_d|$ are both less than c . Show that the frequency of waves observed by the detector, f_d , is given by:

$$f_d = \frac{c - v_d}{c - v_s} f_s.$$

Problem 3.97: Integral form of the Ampere-Maxwell Law. Using the Ampere-Maxwell Law, show that the current through a surface $\mathbb{A}$, $I[\mathbb{A}]$, is related to the integral of the $\vec{B}$ field around the boundary of that surface and the electric flux through that surface by:

$$\int_{\partial \mathbb{A}} \vec{B} \cdot d\vec{x} = \mu_0 I[\mathbb{A}] + \frac{1}{c^2} \frac{d}{dt} \int_{\mathbb{A}} \vec{E} \cdot d\vec{\mathbb{A}}.$$

Problem 3.98: The wave-equation in spatial 2 dimensions. Instead of 3 spatial dimensions, consider the d'Alembert wave equation in 2 spatial dimensions.

- (a) Starting from (3.9.11) follow through equations (3.9.16) to (3.9.24) to show that the delayed Green's function in 2 spatial dimensions is given by:

$$G(t, \vec{x}) = \int_{\mathbb{K}} \frac{ce^{i\vec{k} \cdot \vec{x}} \sin(c|\vec{k}|t)}{4\pi^2|\vec{k}|} \vartheta(t) d^2 \vec{k}.$$

- (b) Then, switch to polar coordinates for the integral and recall that the Fourier transform is truly defined with an exponential damping which is relaxed to 0 at the end to show that the Green's function can be

rewritten:

$$G(t, \vec{x}) = \frac{c\vartheta(t)}{8\pi^2 i} \lim_{\varepsilon \rightarrow 0^+} \int_0^{2\pi} \int_0^\infty \left(e^{-(\varepsilon - i|\vec{x}| \cos \theta - i c t)k} - e^{-(\varepsilon - i|\vec{x}| \cos \theta + i c t)k} \right) dk d\theta.$$

- (c) Perform the k integration and rewrite the $\cos(\theta)$ in the result in terms of complex exponentials. Transform the θ integral to a complex contour integral using the variable substitution $z = e^{i\theta}$ and apply the residue theorem to show that the Green's function in 2 dimensions is given by:

$$G(t, \vec{x}) = \frac{c\vartheta(ct - |\vec{x}|)}{2\pi \sqrt{c^2 t^2 - |\vec{x}|^2}}.$$

Thus, notice that unlike in the 3 dimensional case, the Green's function in 2D is nonzero on the interior of the ball $|\vec{x}| \leq ct$. In 3D, the Green's function is only non-zero on the sphere $|\vec{x}| = ct$. This is a general phenomenon that in even spatial dimensions the wave equation has non-zero ripples inside the ball of its propagation (think of the ripping rings of a drop of water hitting a still pond) while in odd spatial dimension the wave equation is only non-zero on the sphere bounding that ball (and so there are no echoing ripples of soundwaves or lightwaves when there is nothing for the waves to reflect off of). Speech would be much harder to understand in a two spatial dimension universe; there would be way too many echoes.

Problem 3.99: Magnetic Monopoles. Over the years and having various different motivations, theorists have hypothesized “magnetic monopoles” in some way analogous to the electric monopole (the point charge). As we found, there is automatically no monopole term in the magnetic multipole expansion. However, the language here is a bit misleading. When a physicist says magnetic monopole they usually do not mean the first term in the magnetic multipole expansion we performed but simply not set to 0 in the way that would be directly analogous with the monopole term appearing in the scalar potential. Instead of thinking about an analogous term to appear in $\vec{A}$ as one does in ϕ , the magnetic monopole physicists have often meant is intended to make a magnetic field $\vec{B}$ analogous to the electric field $\vec{E}$ of a point charge. That is, a magnetic monopole of “magnetic charge” g at the origin would produce a magnetic field by a sort of “magnetic Gauss’ law”:

$$\nabla \cdot \vec{B} = \mu_0 g \delta(\vec{x}).$$

This should be alarming as we know that by the definition of $\vec{B} = \nabla \times \vec{A}$, its divergence is automatically 0. Let us explore this for a moment and see what happens.

- (a) Consider a modified version of Maxwell’s equations in which the Ampere-Maxwell law still holds and instead of the solenoid law we have a magnetic monopole at the origin. Assuming there are no other charges and everything is static, show that the Maxwell’s equations for $\vec{B}$ become:

$$\nabla \times \vec{B} = 0 \quad \nabla \cdot \vec{B} = \mu_0 g \delta(\vec{x}).$$

As well, from these solve for the magnetic field and show that:

$$\vec{B} = \frac{\mu_0 g \vec{r}}{4\pi r^2}.$$

- (b) Using the magnetic field found in the previous part and the expression for the curl in spherical coordinates, show that the magnetic field for a monopole can be produced by the vector potential:

$$\vec{A} = \frac{\mu_0 g}{4\pi r} \frac{a - \cos \theta}{\sin \theta} \vec{r}_\varphi$$

if one ignores issues of what happens when θ goes to 0 or π . Here a is an arbitrary constant. Show that there is no value of a so that this vector potential has bounded magnitude for both $\theta = 0$ and $\theta = \pi$. Show that for any a there is a line extending out of the origin to spatial infinity along which $\vec{A}$ is divergent. Notice that changing the value of a appears to be a gauge transformation but that the “gauge function” is discontinuous when winding about the z axis and thus cannot be made to be differentiable when enclosing the z axis. So, it is impossible to have any everywhere defined continuously differentiable function $\vec{A}(t, \vec{x})$ which produces a magnetic monopole, as predicted by basic vector calculus (even if one smears it out to make it not a “point charge”). The reason it naively appears to work if one ignores the bad behavior at the poles of spherical coordinates is that locally, everywhere away from the origin $\nabla \cdot \vec{B} = 0$ and so in any open ball not crossing the origin we can make a vector potential so that $\vec{B} = \nabla \times \vec{A}$. Unlike the usual case, because the magnetic field has non-zero divergence at the origin,

we have $\nabla \cdot \vec{B} = 0$ on all of space except a point, which makes the domain on which the Solenoid law applies non-contractible and so the Poincare lemma does not hold.

We can make the magnetic monopole a more reasonable idea if we allow space to be non-contractible and allow the vector potential to be such that instead of being specified by a function $\vec{A}(t, \vec{x})$ on all of space it is specified by a list of functions $\vec{A}_s(t, \vec{x})$ so that each particular entry in the list is taken as the vector potential on a particular open region of space D_s , those open regions cover all of space, and on any volume where two regions D_s and $D_{s'}$ overlap the vector potentials $\vec{A}_s$ and $\vec{A}_{s'}$ are related by a gauge transformation. With these weaker relaxed conditions we can resolve the above magnetic monopole issue by taking space to have a hole at the origin so that $\nabla \cdot \vec{B} = 0$ everywhere on space, taking $\vec{A}_1$ as above with $a = 1$ on all of space except the half line $x = y = 0, z < 0$, and taking $\vec{A}_2$ as above with $a = -1$ on all of space except the half line $x = y = 0, z > 0$. These weaker conditions then give a continuously differentiable vector potential in open regions of space and satisfy the Solenoid law everywhere. So, magnetic monopoles are an entirely reasonable idea on a space with holes in it. It turns out anyway that magnetic monopoles have never been observed in experiment. There is remaining theoretical interest in magnetic monopoles today which are not exactly of the type discussed here. Instead there is a sort of “effective magnetic field” (which is not the curl of some vector potential) in how it appears in some equations of motion and in which that effective magnetic field does not satisfy the solenoid law¹². Thus, while there is no experimental reason to believe in “basic” magnetic monopoles in the sense discussed in this problem there can still theoretically be in some sense effective magnetic monopoles which we will look at briefly in chapter 12. However, at this time even these effective magnetic monopoles have not been seen in experiment.

- (c) Assuming the weaker conditions mentioned before, consider a point electric charge q which is allowed to move around a fixed magnetic monopole g at the origin by taking the vector potential found in the previous part. Show that the Lagrangian for the charge q becomes:

$$\mathcal{L} = \frac{1}{2} m |\dot{\vec{x}}|^2 - \frac{\mu_0 q g}{4\pi} \cos \theta \dot{\varphi}.$$

Thus, while the vector potential has divergent behavior at the poles it seems that the Lagrangian for a charge experiencing a monopole is fine. This allows us to study the hypothetical dynamics we would expect from one. (This is part of the motivation for these weaker conditions; the motion they predict is still reasonable.)

- (d) We would expect this Lagrangian to have rotational symmetry about the origin. To confirm this, we will need to show that the Lagrangian under rotations satisfies equation (1.10.34) for some function $\mathcal{D}f$. In order to prepare for this, let $\mathcal{D}_x$, $\mathcal{D}_y$, and $\mathcal{D}_z$ be the derivatives with respect to rotation angle at rotation angle equal to 0 about the x , y , and z axes respectively. Show by using the definition of spherical coordinates and rotations about each axis that:

$\mathcal{D}_x r = 0$	$\mathcal{D}_x \theta = -\sin \varphi$	$\mathcal{D}_x \varphi = -\frac{\cos \theta \cos \varphi}{\sin \theta}$
$\mathcal{D}_y r = 0$	$\mathcal{D}_y \theta = \cos \varphi$	$\mathcal{D}_y \varphi = -\frac{\cos \theta \sin \varphi}{\sin \theta}$
$\mathcal{D}_z r = 0$	$\mathcal{D}_z \theta = 0$	$\mathcal{D}_z \varphi = 1$
$\mathcal{D}_x \dot{r} = 0$	$\mathcal{D}_x \dot{\theta} = -\dot{\varphi} \cos \varphi$	$\mathcal{D}_x \dot{\varphi} = \dot{\theta} \frac{\cos \varphi}{\sin^2 \theta} + \dot{\varphi} \frac{\sin \varphi \cos \theta}{\sin \theta}$
$\mathcal{D}_y \dot{r} = 0$	$\mathcal{D}_y \dot{\theta} = -\dot{\varphi} \sin \varphi$	$\mathcal{D}_y \dot{\varphi} = \dot{\theta} \frac{\sin \varphi}{\sin^2 \theta} - \dot{\varphi} \frac{\cos \varphi \cos \theta}{\sin \theta}$
$\mathcal{D}_z \dot{r} = 0$	$\mathcal{D}_z \dot{\theta} = 0$	$\mathcal{D}_z \dot{\varphi} = 0$

- (e) Using the formulas from the previous part, show that under rotations the Lagrangian for our system changes by:

$$\begin{aligned} \mathcal{D}_x \mathcal{L} &= \frac{d}{dt} \left(\frac{\mu_0 q g}{4\pi} \frac{\cos \varphi}{\sin \theta} \right) \\ \mathcal{D}_y \mathcal{L} &= \frac{d}{dt} \left(\frac{\mu_0 q g}{4\pi} \frac{\sin \varphi}{\sin \theta} \right) \\ \mathcal{D}_z \mathcal{L} &= 0. \end{aligned}$$

¹²This kind of effective monopole is called a 't Hooft–Polyakov monopole.

Thus identify that this Lagrangian does in fact have rotational symmetry.

- (f) Use these results to show from Noether's theorem that the system has conserved angular momentum:

$$\vec{L} = m\vec{x} \times \dot{\vec{x}} - \frac{\mu_0 qg}{4\pi} \frac{\vec{x}}{|\vec{x}|}.$$

Verify by explicitly computing the equations of motion of the given Lagrangian that this angular momentum is in fact conserved.

- (g) Define the z axis as the axis along which the angular momentum points so that $\vec{L} = L\vec{e}_z$. Show using the conservation of energy and angular momentum that the equations of motion require:

$$\cos \theta = -\frac{\mu_0 qg}{4\pi L}, \quad \dot{\varphi} = \frac{L}{mr^2},$$

$$E = \frac{1}{2}m\dot{r}^2 + \frac{L^2 - \left(\frac{\mu_0 qg}{4\pi}\right)^2}{2mr^2}$$

and use our previous results about the $1/r^2$ potential to solve the system. Thus, one can solve for how an electric charge would react to a magnetic charge, if such a thing were real.

Problem 3.100: Wave equation with initial conditions.

- (a) Split the integral in (3.9.20) into a piece from $-\infty$ to 0 and a piece from 0 to t . Use a trigonometric identity to expand further and show that (3.9.20) can equivalently be rewritten:

$$\tilde{\phi}(t, \vec{k}) = a(\vec{k}) \cos(c|\vec{k}|t) + b(\vec{k}) \sin(c|\vec{k}|t) + \int_0^t \frac{c}{|\vec{k}|} \sin(c|\vec{k}|(t-t')) \tilde{\eta}(t', \vec{k}) dt'$$

for appropriately chosen definitions of the functions $a(\vec{k})$ and $b(\vec{k})$. As well, determine expressions for $a(\vec{k})$ and $b(\vec{k})$ in terms of $\tilde{\phi}(0, \vec{k}) = \tilde{\phi}_0(\vec{k})$ and $\dot{\tilde{\phi}}(0, \vec{k}) = \dot{\tilde{\phi}}_0(\vec{k})$.

- (b) Take the inverse Fourier transform of the above expression and recall the derived formula for the Green's function of the wave equation to show that $\phi(t, \vec{x})$ can be rewritten for $t > 0$ as:

$$\phi(t, \vec{x}) = \int_{S'} \left(\phi_0(\vec{x}') \frac{1}{c^2} \frac{\partial G}{\partial t}(t, \vec{x} - \vec{x}') + \dot{\phi}_0(\vec{x}') \frac{1}{c^2} G(t, \vec{x} - \vec{x}') + \int_0^t \eta(t', \vec{x}') G(t - t', \vec{x} - \vec{x}') dt' \right) d^3 \vec{x}'.$$

This shows us that even though in solving the wave equation we assumed the initial conditions $\phi \rightarrow 0$ as $t \rightarrow -\infty$, we can generate whatever initial conditions we like from that solution.

- (c) Use the expression for the Green's function and change the integrals over $\vec{x}'$ to spherical coordinates with the origin placed at $\vec{x}$ to show that the wave equation solution can be further simplified to:

$$\phi(t, \vec{x}) = \int_{\Omega} \left(\phi_0(\vec{x} + ct\vec{n}) + ct\nabla\phi_0(\vec{x} + ct\vec{n}) \cdot \vec{n} + t\dot{\phi}_0(\vec{x} + ct\vec{n}) + \int_0^{ct} \eta\left(t - \frac{r}{c}, \vec{x} + r\vec{n}\right) r dr \right) \frac{d\Omega}{4\pi}$$

where $d\Omega$ is the differential solid angle of the unit sphere, Ω is the unit sphere, and $\vec{n}(\theta, \varphi)$ is the unit vector pointing from the center of the sphere in the direction of the point on the sphere given in spherical coordinates by θ and φ .

- (d) Show using the above that the value for the wave equation solution ϕ at a point $\vec{x}$ at time t is determined only by the values of its source and initial conditions and their derivatives at times t' and locations $\vec{x}'$ satisfying:

$$c = \frac{|\vec{x} - \vec{x}'|}{t - t'}$$

and thus all of the "information" in the initial conditions and source propagates under the wave equation exactly at the speed c .

Problem 3.101: Drag on a Falling Wire. Consider a rectangular loop of wire with length l in the x direction and height w in the y direction which is falling the y direction. The wire has resistance R and is experiencing a background magnetic field $\vec{B} = B\vec{e}_z$ (but no electric field) which is initially below the wire but as the wire falls, eventually the bottom side of the field crosses into the region of space in which this magnetic field is present. Define $-y(t)$ as the amount the wire has fallen by time t past the point where its bottom entered the magnetic field.

- (a) Show that the magnetic flux Φ through the wire is given by:

$$\Phi(t) = -Bly(t)$$

assuming the top of the wire has not yet entered the magnetic field. As well, show from the integral form of Faraday's law that the emf through one loop of the wire is given by:

$$\mathcal{E} = Bl\dot{y}.$$

- (b) Let $\vec{E}'$ be the electric field in the instantaneous rest frame of the wire. Show using the boost transformation properties of the electric and magnetic fields that the emf through one loop of the wire is given by:

$$\mathcal{E} = \int_{\text{1 loop}} \vec{E}' \cdot d\vec{x}.$$

As well, use the macroscopic version of Ohm's law (and recall that it is valid only in the rest frame of the Ohmic material) to show that this emf is also given by:

$$\mathcal{E} = IR$$

where I is the current counterclockwise through the wire. Thus, find the induced current in the wire due to falling in the background magnetic field.

- (c) Use the Lorentz force to compute that the electromagnetic force on the wire is:

$$\vec{F} = -\frac{l^2 B^2 \dot{y}}{R} \vec{e}_y.$$

Thus, identify that the wire experiences a sort of "linear drag" in the way it would due to air resistance at low speeds due to the magnetic field.

Problem 3.102: ★ Measuring the Electron charge-to-mass ratio. Consider a metal plate connected in series first to a battery with voltage V and then to a cylindrical tube (on the higher voltage side of the battery) so that charges moving down the wire enter the tube (assume the wire is normal to the tube at the entrance) and then are allowed to freely move within the tube. In the tube there is a uniform constant electric field $\vec{E}$ orthogonal to the direction of the incoming wire and a uniform constant magnetic field $\vec{B}$ orthogonal to both the incoming wire and $\vec{E}$. At the other end of the tube there is a screen so that when a charge is incident on the screen its position is registered by the screen.

- (a) Explain how using the devices so far established in this chapter one could physically prepare such electric and magnetic fields.
- (b) Suppose that the charges coming from the metal plate enter the tube with speed v . Show that the charges will shoot straight through the tube if and only if $E = vB$ where $E = |\vec{E}|$ and $B = |\vec{B}|$.
- (c) Suppose that the charges moving through the wire each have charge q and mass m . Explain that if $q > 0$ and the lower voltage side of the battery is attached to the metal plate, no charges will flow into the tube. Thus, the fact that charges do move through the tube is proof $q < 0$. Explain that with $q < 0$, v is related to the voltage of the battery by:

$$\frac{1}{2}mv^2 = |q|V.$$

- (d) Show that if $\vec{E}$ and $\vec{B}$ are adjusted by the experimenter so as to ensure the charges beam straight through the tube with minimal deflection one can measure the charge-to-mass ratio r of the charge carriers by:

$$r \stackrel{\text{def}}{=} \frac{|q|}{m} = \frac{E^2}{2VB^2}.$$

This technique, used by J. J. Thomson, established that the electron charge is negative and was the first to measure the charge-to-mass ratio of the electron. As well, Thomson found that the result of the measurement was the same across charges from plates and wires of different metals so established that particles of the same charge-to-mass ratio are present in many materials. This "species" of charge which is so ever-present is precisely what is meant by the electron.

Problem 3.103: ★ Measuring the electron mass and electron charge. Suppose we have a proton (essentially at rest, trapped using an ion-trap like a Penning trap for example) and we fire a electron beam at it (where the beam is produced as in the previous question, by accelerating the electrons from a metal plate through a battery of voltage V). Further, suppose that we have a detector all around the apparatus so that we can detect the locations at which charges are scattered off of the protons.

- (a) Using the analysis of Rutherford scattering and recalling that the electron and proton of equal magnitudes of charge while the proton has a much greater mass, show that the charge-square-to-mass ratio $\mathfrak{r}' \stackrel{\text{def}}{=} \frac{q^2}{m}$ for the electron can be determined from the scattering cross section. (For higher precision, the m here should be the reduced mass of the electron-proton system.)
- (b) Using the charge-to-mass ratio $\mathfrak{r}$ (which can be measured as in the Thomson experiment) and the charge-square-to-mass ratio $\mathfrak{r}'$ show that the electron's charge and mass can be determined to be:

$$q = -\frac{\mathfrak{r}'}{\mathfrak{r}}, \quad m = \frac{\mathfrak{r}'}{\mathfrak{r}^2}.$$

Going forward we will use the symbol q_e to mean the magnitude of the electron charge and m_e to mean the electron mass. In SI units the unit of charge was historically set by arbitrary reference value to a particular given amount of charge called the Coulomb. In those units, the experimental value of the electron charge is found to be:

$$q = -1.602176634 \times 10^{-19} \text{C}.$$

In modern SI units the value of the electron charge is defined to be this exactly and the Coulomb is defined from this value. In Galilean Natural Units (units in which $\epsilon_0 = 1$) the corresponding value of the electron charge is:

$$q = -5.3843840463 \times 10^{-12} \frac{\text{kg}^{\frac{1}{2}} \text{m}^{\frac{3}{2}}}{\text{s}}.$$

In either case, in terms of the arbitrary reference value of the kilogram, the mass of the electron is experimentally found to be:

$$m = 9.1093837015(28) \times 10^{-31} \text{kg}.$$

3.10 Problems with Point Matter

Before we try to solve the conflict between the existence of a special speed and boost symmetry, we will explore another challenge with the Galilean theory: the infinite energy of point particles. The only fully self-contained case in the Galilean theory was the Scalar theory. Then, the Lagrangian for N particles before dropping the self-field contribution is as we found in (3.4.82):

$$\mathcal{L} = \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - \lim_{\text{point}} \sum_{n=1}^N E_n(t) - \sum_{n=1}^{N-1} \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|} \quad (3.10.1)$$

The corresponding Energy is given by the Legendre transform:

$$E = \sum_{n=1}^N \frac{1}{2} m_n |\dot{\vec{x}}_n|^2 + \lim_{\text{point}} \sum_{n=1}^N E_n(t) + \sum_{n=1}^{N-1} \sum_{k=n+1}^N \frac{q_n q_k}{4\pi\epsilon |\vec{x}_n - \vec{x}_k|} \quad (3.10.2)$$

In the point limit, each $E_n(t)$ diverges to positive ∞ . This is not an issue if the number of charges and value of charge is fixed. Then, the apparently divergent term is just a constant and is removable by gauge transformation, with no effect on the equations of motion. However, if the number of charges or values of charges are dynamical (meaning there exist processes in which charges combine or break apart), then we have to include these diverging terms (because they are dynamical and would affect the equations of motion) which simply makes no sense in the point limit. Experimentally, there do exist processes in which charges combine or break apart or in which two charges of opposite values of charge are produced from something charge neutral. These processes are impossible in our scalar theory of point particles due to this need of infinite energy to do it, and so something is wrong. This theory simply cannot handle a variable number of particles. This should not be surprising as there is ultimately something logically missing in the theory to even discuss particles breaking apart and combining. By setting out with point particles we took by definition there to be no “internal degrees of freedom”, meaning no variables other than position. However, then there are no variables in the Hamiltonian which govern the dynamics of splitting apart and combining together. There is no way (without adding more variables) to fully incorporate these processes into the Hamiltonian/Lagrangian/Action. So, independently of how the particles are interacting, the fact that splitting and combining are observed tells us that a point theory of matter just isn't quite right.

There is another massive failure of the point-particle worldview. If the matter of the world is made out of separated points, then around any point of matter $\vec{x}_n$ there is some neighborhood (a ball of radius r) in which there are no other points of matter (if this were false, then the matter would be continuous, not separated). Then, take the equation of motion for such a matter element in the Galilean scalar theory:

$$m\ddot{\vec{x}}_n = -\frac{\partial U}{\partial \vec{x}_n}. \quad (3.10.3)$$

There is no appearance of $\vec{K}$ because in the scalar theory $\vec{K}$ is 0 ($\vec{K}$ is given by (2.5.4) in terms of the vector potentials and all the vector potentials are 0 in the scalar theory, which is the only self-consistent and self-contained Galilean theory we found). Everyday matter is observed to be able to be stably at rest. Thus, for a successful theory of matter, we would need this mass element to be able to be in a stable equilibrium. Let $\vec{x}_0$ be the equilibrium position. By definition when placed at that location at rest the matter stays there and so:

$$m\ddot{\vec{x}}_n \Big|_{\vec{x}_n=\vec{x}_0} = 0 \implies \nabla U(t, \vec{x}) \Big|_{\vec{x}=\vec{x}_0} = 0. \quad (3.10.4)$$

In order for the equilibrium to be stable, when the point is near the equilibrium value, it must accelerate toward the equilibrium. The acceleration is opposite the direction of the gradient of U and so therefore the gradient of U in the neighborhood of $\vec{x}_0$ must always point out of $\vec{x}_0$. The gradient gives the direction of fastest increase and so therefore because it always points out of $\vec{x}_0$, $\vec{x}_0$ must be a local minimum of U (as U increases in all directions when displaced from $\vec{x}_0$). Thus, for stable Galilean matter to exist, we need $U(t, \vec{x})$ to have a local minimum. Now recall the relationship between U and the scalar potentials (equation (2.5.3), here we allow there to be multiple potentials to show that doing so will not fix our issue) and take the Laplacian:

$$U(t, \vec{x}) = \sum_s q_s \phi_s(t, \vec{x}) \implies \nabla^2 U(t, \vec{x}) = \sum_s q_s \nabla^2 \phi_s(t, \vec{x}). \quad (3.10.5)$$

By the Poisson equation then:

$$\nabla^2 U(t, \vec{x}) = - \sum_s \frac{q_s}{\epsilon_s} \rho_s(t, \vec{x}). \quad (3.10.6)$$

Then, because the matter particle $\vec{x}_n$ exists in a region with some separation between it and any other matter elements, there is no charge density in that region: $\rho_s = 0$ (we exclude the charge's own contribution because there is no effect due to $\vec{x}_n$'s own charge on itself as found in section 3.4). So:

$$\nabla^2 U(t, \vec{x}) = 0 \quad (3.10.7)$$

in a neighborhood of the location of $\vec{x}_n(t)$. This is Poisson's equation with the inhomogeneous term equal to 0. This special case of the Poisson equation is called the **Laplace equation**. Using 3.2, we can solve U on the ball of radius R centered at $\vec{x}_0$, $\mathbb{B}(\vec{x}_0, R)$:

$$U(t, \vec{x}) = \int_{\partial \mathbb{B}(\vec{x}_0, R)} (G(\vec{x}, \vec{x}') \nabla' U(t, \vec{x}') - U(t, \vec{x}') \nabla' G(\vec{x}, \vec{x}')) \cdot d\vec{\mathbb{A}} \quad (3.10.8)$$

where we have used a general Green's function G . Evaluate this at the center of the ball:

$$U(t, \vec{x}_0) = \int_{\partial \mathbb{B}(\vec{x}_0, R)} (G(\vec{x}_0, \vec{x}') \nabla' U(t, \vec{x}') - U(t, \vec{x}') \nabla' G(\vec{x}_0, \vec{x}')) \cdot d\vec{\mathbb{A}}. \quad (3.10.9)$$

Recall that the Green's function is not quite uniquely defined (up to adding a function with vanishing Laplacian). So, choose:

$$G(\vec{x}, \vec{x}') = \frac{1}{4\pi|\vec{x} - \vec{x}'|} - \frac{1}{4\pi R}. \quad (3.10.10)$$

This addition is just a constant and so it is certainly allowed. On the surface of the ball we have:

$$G(\vec{x}_0, \vec{x}')|_{\partial \mathbb{B}(\vec{x}_0, R)} = \frac{1}{4\pi R} - \frac{1}{4\pi R} = 0. \quad (3.10.11)$$

With this (3.10.9) becomes:

$$U(t, \vec{x}_0) = - \int_{\partial \mathbb{B}(\vec{x}_0, R)} U(t, \vec{x}') \nabla' G(\vec{x}_0, \vec{x}') \cdot d\vec{\mathbb{A}}. \quad (3.10.12)$$

As well, we can evaluate the gradient of G :

$$\nabla' G(\vec{x}, \vec{x}') = \frac{\vec{x} - \vec{x}'}{4\pi|\vec{x} - \vec{x}'|^3} \implies \nabla' G(\vec{x}, \vec{x}')|_{\partial \mathbb{B}(\vec{x}_0, R)} = -\frac{\vec{n}}{4\pi R^2} \quad (3.10.13)$$

where $\vec{n}$ is the outward pointing unit vector on the surface of the ball. Then, we have:

$$U(t, \vec{x}_0) = \int_{\partial \mathbb{B}(\vec{x}_0, R)} U(t, \vec{x}') \frac{\vec{n}}{4\pi R^2} \cdot d\vec{\mathbb{A}} = \frac{\int_{\partial \mathbb{B}(\vec{x}_0, R)} U(t, \vec{x}') d\mathbb{A}}{\int_{\partial \mathbb{B}(\vec{x}_0, R)} d\mathbb{A}}. \quad (3.10.14)$$

This is precisely the average value of U on the boundary of the ball. Hence, the value of U at the center of the ball of radius R is given by its average over the boundary of that ball. This is known as the mean-value property of the Laplace equation. The average value over the sphere is bounded below by the minimum value on the sphere and above by the maximum value. Because the value at the center is precisely that average, it can neither be lower than the minimum on the boundary nor larger than the maximum. Because this is true no matter how small we consider the ball to be, it will never be the case that there exists a neighborhood around $\vec{x}_0$ such that $U(\vec{x}_0)$ is the maximum or minimum in that neighborhood. $U(\vec{x}_0)$ cannot be a local minimum nor a local maximum if U satisfies the Laplace equation around $\vec{x}_0$. This gives us:

Theorem 3.5: Mean-value property of the Laplace equation

If $\phi(\vec{x})$ satisfies the Laplace equation $\nabla^2 \phi = 0$ in a region $\mathbb{V}$ and $\mathbb{B}(\vec{x}_0, R)$ is a ball contained in that region with radius R and center $\vec{x}_0$ then the $\phi(\vec{x}_0)$ is given by the average value of $\phi(\vec{x})$ over the sphere $\partial \mathbb{B}(\vec{x}_0, R)$. As such, no point in the interior of the region $\mathbb{V}$ can be a local minimum or maximum of ϕ .

Because a local minimum of U is required for matter to be in stable equilibrium and no local minimum of U can exist in a region in which that matter is separated from other matter, there cannot be a stable configuration of discrete, separated matter in the Galilean theory. This result is known as **Earnshaw's theorem**. There are potential loopholes to Earnshaw's theorem (perhaps higher derivative or higher order

terms become important with matter) but they don't do much to resolve the tension. At least at the level of the scalar theory Lagrangian, it proves such a theory with point particles cannot produce the stable matter we see in our world. This proof crucially required that the matter was comprised of separated points. If we dropped our model of point particles and went to continuous matter, then the problem would be solved immediately. Certainly, something must be changed to escape this issue and the repeated issues with point particles suggest that they are it.

3.11 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 3.2: Change of Variables in the Dirac Delta** and
- **Problem 3.3: Multidimensional Dirac Delta** and
- **Problem 3.4: Derivatives of the Dirac Delta** introduce important mathematical properties of the Dirac delta which we will use often.
- **Problem 3.7: The Diffusion Equation** establishes how to solve the diffusion equation and how to do Gaussian integrals.
- **Problem 3.31: The Cavendish Experiment** establishes how to experimentally measure the gravitational constant G .
- **Problem 3.46: Measuring Charge with a Coulomb Balance** establishes how to measure unknown charges.
- **Problem 3.55: Classical Scattering** introduces the formalism of scattering which will be useful across many disciplines of physics.
- **Problem 3.57: Rutherford Scattering** computes the scattering cross section for the Coulomb potential which we will reference when studying the structure of the atom.
- **Problem 3.81: Measuring c** establishes how to experimentally measure the speed of light c .
- **Problem 3.82: Measuring Current with an Astatic Galvanometer** establishes how to measure current experimentally.
- **Problem 3.94: The Hall Effect** establishes that the moving charges in conducting metals are negatively charged.
- **Problem 3.102: Measuring the electron charge-to-mass ratio** and
- **Problem 3.103: Measuring the electron mass and electron charge** establish the basic notion of what an electron is and how to measure its mass and charge.

In this chapter we developed the full theory of Galilean particles interacting with the potentials thus arriving at the theory of **Galilean Classical Mechanics** (or nonrelativistic classical mechanics). To do so, we made the following experimentally motivated assumptions:

Assumptions generally made in Physics:

- PHSXI: Smoothness of Time and Time Evolution.**
- PHSXII: Smoothness of 3-dimensional Space.**
- PHSXIII: Time Translational Symmetry.**
- PHSXIV: Space Translational Symmetry.**
- PHSXV: Rotational Symmetry.**
- PHSXVI: Locality.**

Assumptions specific to Galilean Classical Mechanics:

- GCM I: Matter consists of moving points.**
- GCM II: Galilean Boost Symmetry.**
- GCM III: Space is static and Euclidean.**
- GCM IV: Parity Symmetry.**

In making these assumptions in chapter 2 we found the Lagrangian for particles was determined up to some unknown potentials. In section 3.1, we developed how to think of those potentials, the scalar potential ϕ and vector potential $\vec{A}$, as the new variables for which we need to find a Lagrangian to complete the theory. As well, we found that the charge density naturally satisfies the continuity equation which has the interpretation of local charge conservation. In section 3.2, we developed the basic structure of classical field theory, the formalism necessary to find equations of motion in analytical mechanics when our variables are fields. In section 3.3, we used classical field theory and our assumptions to derive what Lagrangians were possible for our potentials. In section 3.4, we analyzed the first of these two Lagrangians and developed the Galilean scalar theory, our only self-contained and self-consistent theory at this point. In section 3.5, we analyzed the second of these two Lagrangians and developed the Galilean vector theory, which we found is certainly not fundamental and is only a tenable effective theory when there is no appreciable charge density in the region to which we apply it. In section 3.6, we applied the Galilean scalar theory to derive the Newtonian

theory of gravity and explored its experimental consequences. In section 3.7, we did the same to derive electrostatics. In section 3.8, we applied the Galilean vector theory to derive magnetostatics. In section 3.9, we faced the mutual inconsistency of the Galilean scalar and vector theories even though electrostatics and magnetostatics are found to coexist in experiment. In doing so, we found a new idea of boost is necessary to reconcile the inconsistency. In section 3.10, we found that the Galilean scalar theory cannot explain the dynamical stability of matter (Earnshaw's theorem) and that it cannot explain the experimentally found processes of particles decaying into other particles or combining to make new ones.

In addition to the development of theory in this chapter, we also further developed our set of physical quantities which we can measure. In particular, we developed the unit of charge and found that in the convention in which the unit of charge is chosen so that $\epsilon_0 = 1$, the unit of charge $[q]$ is expressible in terms of one's choices of unit of length L , time T , and mass M by:

$$[q] = \frac{\sqrt{ML^3}}{T}. \quad (3.11.1)$$

Historically, an arbitrary reference value was chosen for the units of charge and doing so induces a dimensionful value of $\epsilon_0 \neq 1$.

As well, we found how to measure charge using a Coulomb Balance. We then found how to design other devices to measure current, the strength of the electric field, the strength of the magnetic field, and various material properties such as capacitance, inductance, and resistance. Using the Cavendish experiment, we found how to measure G , the parameter appearing in the gravitational Lagrangian. As well, we found how to measure the speed of light c , even though that concept itself is in tension with Galilean mechanics.

So, the culmination of Galilean Classical Mechanics is that in such a theory the general consistent Lagrangian for a system of particles is given by:

$$\mathcal{L} = \sum_{n=1}^N \left(\frac{1}{2} m_n |\dot{\vec{x}}_n|^2 - m_n \phi_g(t, \vec{x}_n) - q_n \phi(t, \vec{x}_n) \right) + \int_{\mathbb{S}} \left(\frac{\epsilon_0}{2} |\nabla \phi|^2 - \frac{|\nabla \phi_g|^2}{8\pi G} \right) d\mathbb{S} \quad (3.11.2)$$

where ϕ is the electric scalar potential and ϕ_g is the gravitational scalar potential. We have our first complete (meaning self-consistent and self-contained) theory of physics, it just happens that this theory has several flaws revealed by experiment. By sections 3.8, 3.9, 3.10, such a Lagrangian cannot fundamentally describe our world. However, it is a very successfully model under many circumstances. It is a very good effective theory. The various applications of this Lagrangian are sufficient for understanding much (but not all) of the physics of every-day life. It can be used, among other things, to (mostly) successfully model:

- The motion of (most) celestial bodies in our solar system.
- The motion of (most) nonmagnetic objects on Earth which are not too fast or too small.
- The behavior of gases and fluids under every-day conditions.

We know that this theory has two fundamental problems: it cannot explain electromagnetic coexistence and point-particles are inconsistent with the experimental facts of stable matter and the existence of decay/combination processes. Thus, we have two directions to explore with improving our theory: modifying the boost symmetry to fix the electromagnetic problem and modifying our model of particles to fix the point-particle problem. At this point our view of physics is then summarized by Figure 3.1.

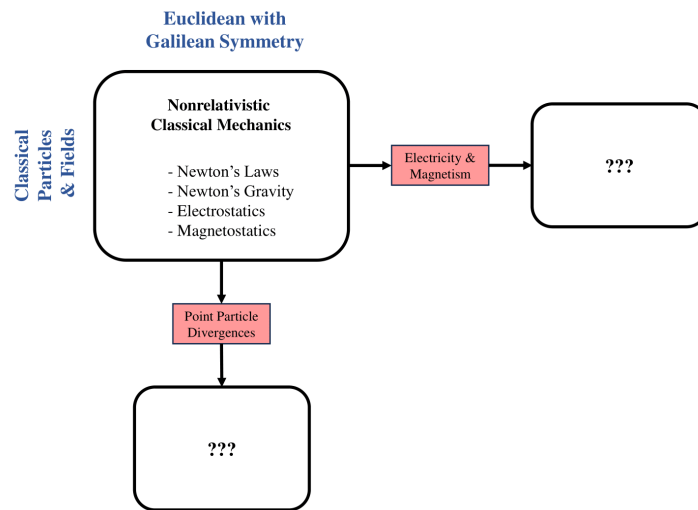


Figure 3.1: Our perspective on physics as of the end of this chapter. We have many successes and two major problems. Those two problems will be our guides for what to try next.

This and the previous chapter are by no means a complete treatment of essential topics in Galilean Mechanics. For completeness sake, refer to the list at the end of Chapter 2; as well, any standard work on electromagnetism such as [121], [89], [128], [52] will cover electrostatics and magnetostatics in great detail in the first few chapters and any standard work in circuits such as [70] will cover all of the circuit theory we discussed and much more.

Chapter 4

Relativistic Classical Mechanics

If I pursue a beam of light with the velocity c , I should observe such a beam of light as an electromagnetic field at rest though spatially oscillating. There seems to be no such thing, however, neither on the basis of experience nor according to Maxwell's equations. From the very beginning it appeared to me intuitively clear that, judged from the standpoint of such an observer, everything would have to happen according to the same laws as for an observer who, relative to the earth, was at rest. For how should the first observer know or be able to determine, that he is in a state of fast uniform motion? One sees in this paradox the germ of the special relativity theory is already contained.

– Albert Einstein [102]

Meep, meep. Nyooooom!!!

– Roadrunner [55]

4.1 Lorentz Boost Symmetry

We need to resolve the dissonance between the observation of boost symmetry and the derivation of a fundamental speed in electromagnetism. Galilean boost symmetry is inconsistent with the coexistence of electricity and magnetism. To reconcile, we need a new kind of boost. When we defined Galilean boosts we took the old time t and old position $\vec{x}$ to a new time and new position $t' = t$ and $\vec{x}' = \vec{x} + \vec{v}(t - t_b)$. That is, we assumed time stayed the same and shifted the velocity by $\vec{v}$. We will now consider a completely general idea of a boost and see what else is possible. We call a point in space at a particular time an event X . Events are labeled by coordinates, a coordinate for the time t and a vector for position $\vec{x} = (x, y, z)$. The same event may be expressed with different coordinates if two parties use different coordinates (if they choose different origins and axes or different objects to measure relative motion against). Consider a continuous family of events $X(\alpha)$ labeled by a real parameter α and let dX be the derivative:

$$dX \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{X(\alpha + \varepsilon) - X(\alpha)}{\varepsilon}. \quad (4.1.1)$$

dX is just the displacement between nearby events. The continuous family of events $X(\alpha)$ is arbitrary. It could be the positions of all of the bits of an object at a particular time, the positions through which any particle passes with time, or anything else really. One ought to be careful and understand that by subtracting two events we mean that in coordinates (t, x, y, z) we subtract their coordinates so that the result is a vector in 4 dimensions (time gives 1, space gives the other 3) which points from the initial event to the final event. Under a boost by velocity $\vec{v}$ the coordinates before $(t, \vec{x})$ and after $(t', \vec{x}')$ will be related somehow: $t' = t'(t, \vec{x})$, $\vec{x}' = \vec{x}'(t, \vec{x})$ where this map depends on $\vec{v}$. Then, by the chain rule, the coordinate displacements between events become:

$$\begin{pmatrix} dt' \\ dx' \\ dy' \\ dz' \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix} \quad (4.1.2)$$

Here all of the components $a_{\mu\nu}$ are the partial derivatives of the event $(t'(t, \vec{x}), \vec{x}'(t, \vec{x}))$ with respect to t and $\vec{x}$ and are functions of the boost velocity. In principle they could depend on $(t, \vec{x})$ but if that were the case we would have a spatially or temporally varying boost (that is, the relative velocity of the primed coordinates with respect to the unprimed coordinates would depend on time and position). Because by boost symmetry we mean symmetry under a boost of the whole space by a uniform amount, we will take the components $a_{\mu\nu}$ to not be functions of t or $\vec{x}$. A spatially or temporally varying boost symmetry would be incompatible space and time translational symmetries anyway. We can also write (4.1.2) as:

$$\begin{pmatrix} dt' \\ d\vec{x}' \end{pmatrix} = \hat{L} \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} \quad (4.1.3)$$

where $\hat{L}$ is the 4x4 matrix of a coefficients.

Now let us consider such a coordinate transformation which is supposed to represent a boost of the system by velocity v in the x direction. The velocity of an object in the y direction after the boost is then:

$$\dot{y}' = \frac{dy'}{dt'} = \frac{a_{20}dt + a_{21}dx + a_{22}dy + a_{23}dz}{a_{00}dt + a_{01}dx + a_{02}dy + a_{03}dz} = \frac{a_{20} + a_{21}\dot{x} + a_{22}\dot{y} + a_{23}\dot{z}}{a_{00} + a_{01}\dot{x} + a_{02}\dot{y} + a_{03}\dot{z}}. \quad (4.1.4)$$

If the initial velocity in the y direction is 0 then after a boost in the x direction, the velocity in the y direction must still be 0 (if not, we would not say the boost is in the x direction). Hence:

$$\dot{y} = 0 \implies \dot{y}' = \frac{a_{20} + a_{21}\dot{x} + a_{23}\dot{z}}{a_{00} + a_{01}\dot{x} + a_{03}\dot{z}} = 0 \quad \forall \dot{x}, \dot{z} \implies a_{20} = a_{21} = a_{23} \stackrel{!}{=} 0. \quad (4.1.5)$$

All three coefficients must vanish because the equation must hold regardless of what the x and z velocities are before the boost. Applying the exact same argument to the z direction gives $a_{30} = a_{31} = a_{32} = 0$.

To keep rotational symmetry, a boost about the x axis is unchanged by a rotation about the x axis (because rotations about any axis leave that axis unchanged). Hence rotating about an axis and then boosting along that axis is the same as boosting along that axis and then rotating about it as the two do not affect each other:

$$\hat{R}_x(\theta) \begin{pmatrix} dt' \\ d\vec{x}' \end{pmatrix} \stackrel{!}{=} \hat{L}_x(v) \hat{R}_x(\theta) \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} \quad (4.1.6)$$

$$\implies \hat{R}_x(\theta) \hat{L}_x(v) \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} = \hat{L}_x(v) \hat{R}_x(\theta) \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} \quad \forall dt, d\vec{x} \quad (4.1.7)$$

$$\implies \hat{R}_x(\theta) \hat{L}_x(v) = \hat{L}_x(v) \hat{R}_x(\theta) \quad (4.1.8)$$

Now calculate this explicitly for a rotation by 90° about the x axis using our formula for the rotation matrices (2.4.5):

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ 0 & 0 & a_{22} & 0 \\ 0 & 0 & 0 & a_{33} \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ 0 & 0 & a_{22} & 0 \\ 0 & 0 & 0 & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (4.1.9)$$

$$\implies \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ 0 & 0 & 0 & -a_{33} \\ 0 & 0 & a_{22} & 0 \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & a_{03} & -a_{02} \\ a_{10} & a_{11} & a_{13} & -a_{12} \\ 0 & 0 & 0 & -a_{22} \\ 0 & 0 & a_{33} & 0 \end{pmatrix} \quad (4.1.10)$$

$$\implies a_{22} = a_{33}, \quad a_{02} = a_{03} = a_{12} = a_{13} = 0. \quad (4.1.11)$$

At this point the transformation is simplified to:

$$\begin{pmatrix} dt' \\ dx' \\ dy' \\ dz' \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & 0 & 0 \\ a_{10} & a_{11} & 0 & 0 \\ 0 & 0 & a_{22} & 0 \\ 0 & 0 & 0 & a_{22} \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix} \quad (4.1.12)$$

The velocity in the x direction is thus transformed as:

$$\dot{x}' = \frac{dx'}{dt'} = \frac{a_{10}dt + a_{11}dx}{a_{00}dt + a_{01}dx} = \frac{a_{10} + a_{11}\dot{x}}{a_{00} + a_{01}\dot{x}}. \quad (4.1.13)$$

When the unboosted system is at velocity 0, the boosted system has velocity:

$$\dot{x}' = \frac{a_{10}}{a_{00}}. \quad (4.1.14)$$

The velocity the system has when it is boosted from rest is exactly what we mean by the boost velocity v :

$$v \stackrel{\text{def}}{=} \frac{a_{10}}{a_{00}} \implies a_{10} = a_{00}v. \quad (4.1.15)$$

Now consider a rotation about the y axis by 180° . This inverts x and z and thus turns our boost along the x axis to a boost by the same amount in the $-x$ direction. To keep notation condensed, write $a_{\mu\nu}$ for $a_{\mu\nu}(v)$ and $a_{\mu\nu}^-$ for $a_{\mu\nu}(-v)$. Hence:

$$\hat{R}_y(\pi)\hat{L}_x(v) = \hat{L}_x(-v)\hat{R}_y(\pi) \quad (4.1.16)$$

$$\implies \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & 0 & 0 \\ va_{00} & a_{11} & 0 & 0 \\ 0 & 0 & a_{22} & 0 \\ 0 & 0 & 0 & a_{22} \end{pmatrix} = \begin{pmatrix} a_{00}^- & a_{01}^- & 0 & 0 \\ -va_{00}^- & a_{11}^- & 0 & 0 \\ 0 & 0 & a_{22}^- & 0 \\ 0 & 0 & 0 & a_{22}^- \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (4.1.17)$$

$$\implies a_{00}(v) = a_{00}(-v), \quad a_{11}(v) = a_{11}(-v), \quad a_{22}(v) = a_{22}(-v). \quad (4.1.18)$$

Boosting by $-v$ in a given direction is the inverse of boosting by v in that direction. So, the composition of these must give the identity matrix:

$$\begin{pmatrix} dt'' \\ d\vec{x}'' \end{pmatrix} = \hat{L}_x(-v) \begin{pmatrix} dt' \\ d\vec{x}' \end{pmatrix} = \hat{L}_x(-v)\hat{L}_x(v) \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} dt \\ d\vec{x} \end{pmatrix} \quad \forall dt, d\vec{x} \quad (4.1.19)$$

$$\implies \hat{L}_x(-v)\hat{L}_x(v) = 1 \quad (4.1.20)$$

$$\begin{pmatrix} a_{00}^- & a_{01}^- & 0 & 0 \\ -va_{00}^- & a_{11}^- & 0 & 0 \\ 0 & 0 & a_{22}^- & 0 \\ 0 & 0 & 0 & a_{22}^- \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & 0 & 0 \\ va_{00} & a_{11} & 0 & 0 \\ 0 & 0 & a_{22} & 0 \\ 0 & 0 & 0 & a_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4.1.21)$$

$$\begin{pmatrix} a_{00}^-a_{00} + va_{01}^-a_{00} & a_{00}^-a_{01} + a_{01}^-a_{11} & 0 & 0 \\ -va_{00}^-a_{00} + va_{11}^-a_{00} & -va_{00}^-a_{01} + a_{11}^-a_{11} & 0 & 0 \\ 0 & 0 & a_{22}^-a_{22} & 0 \\ 0 & 0 & 0 & a_{22}^-a_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4.1.22)$$

This requires that $a_{22}(-v)a_{22}(v) = 1$. We found in (4.1.18), $a_{22}(-v) = a_{22}(v)$. Hence:

$$a_{22}^2(v) = 1 \implies a_{22}(v) = \pm 1. \quad (4.1.23)$$

Because $v = 0$ is the identity transformation, $a_{22}(0) = 1$. For the $a_{\mu\nu}$ coefficients to be continuous functions of v we must have $a_{22}(v) = 1$ for all v . From (4.1.22) we also have:

$$-va_{00}(-v)a_{00}(v) + va_{11}(-v)a_{00}(v) = 0 \implies a_{11}(-v) = a_{00}(-v) \implies a_{11}(v) = a_{00}(v). \quad (4.1.24)$$

We now put in the requirement that there be an invariant speed. That is, a speed which is left unchanged by any boost (so that the speed of light in electromagnetism is protected under boost symmetry). We call this speed c :

$$\dot{x}' = \frac{dx'}{dt'} = \frac{va_{00}(v) + a_{00}(v)\dot{x}}{a_{00}(v) + a_{01}(v)\dot{x}}, \quad \dot{x} = c \implies \dot{x}' = c \quad (4.1.25)$$

$$\implies c = \frac{va_{00}(v) + a_{00}(v)c}{a_{00}(v) + a_{01}(v)c} \quad (4.1.26)$$

$$\implies ca_{00}(v) + c^2a_{01}(v) = va_{00}(v) + a_{00}(v)c \quad (4.1.27)$$

$$\implies a_{01}(v) = \frac{v}{c^2}a_{00}(v). \quad (4.1.28)$$

Now we only have one free coefficient:

$$\begin{pmatrix} dt' \\ dx' \\ dy' \\ dz' \end{pmatrix} = \begin{pmatrix} a_{00} & \frac{v}{c^2}a_{00} & 0 & 0 \\ va_{00} & a_{00} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix} \quad (4.1.29)$$

Finally pulling the last condition from (4.1.22):

$$a_{00}(-v)a_{00} + va_{01}(-v)a_{00} = 1 \quad (4.1.30)$$

$$\implies a_{00}^2 + v \left(-\frac{v}{c^2} a_{00} \right) a_{00} = 1 \quad (4.1.31)$$

$$\implies a_{00}^2 = \frac{1}{1 - \frac{v^2}{c^2}} \implies a_{00}(v) = \frac{\pm 1}{\sqrt{1 - \frac{v^2}{c^2}}}. \quad (4.1.32)$$

$a_{00}(0) = 1$ because $v = 0$ is the identity transformation and so by continuity we must take the positive root for all v . This expression for a_{00} will show up often and so has a special name, the Lorentz factor:

$$\gamma(\vec{v}) \stackrel{\text{def}}{=} \frac{1}{\sqrt{1 - \frac{|\vec{v}|^2}{c^2}}}. \quad (4.1.33)$$

Then we arrive at the unique form for our boost in the x direction:

$$\hat{L}_x(v) = \begin{pmatrix} \gamma & \frac{v}{c^2}\gamma & 0 & 0 \\ v\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (4.1.34)$$

Written in differentials we have:

$$dt' = \gamma \left(dt + \frac{v}{c^2} dx \right), \quad dx' = \gamma (dx + v dt), \quad dy' = dy, \quad dz' = dz. \quad (4.1.35)$$

Importantly, this new boost, called the Lorentz boost, does reduce to the Galilean boost when the boost velocity is much less than c (equivalently c is taken extremely large compared to all velocities and thus we can take $c \rightarrow \infty$). Taking this limit of equation (4.1.35), we recover the Galilean boost:

$$\lim_{c \rightarrow \infty} dt' = \lim_{c \rightarrow \infty} \frac{dt + \frac{v}{c^2} dx}{\sqrt{1 - \frac{v^2}{c^2}}} = dt, \quad \lim_{c \rightarrow \infty} dx' = \lim_{c \rightarrow \infty} \frac{dx + v dt}{\sqrt{1 - \frac{v^2}{c^2}}} = dx + v dt. \quad (4.1.36)$$

Hence, if the boost velocity is so much smaller than c that c can be treated as effectively infinite, we recover the Galilean boost. Because the experimental value of the speed of light is much much larger than every day velocities, we see that the Galilean theory is an effective good description of objects at every day velocities. However, if they are sufficiently fast or if we would like to explain electromagnetism, we have to use Lorentz boost symmetry.

To this point we have only considered boosts along the x axis but by rotational symmetry we can directly generalize this to an arbitrary direction. We can rewrite our boost from equation (4.1.35) in a more geometric way by rewriting dx as the position element parallel to the boost $dx_{\parallel}$ and dy and dz as the position elements perpendicular to the boost $d\vec{x}_{\perp}$:

$$dt' = \gamma \left(dt + \frac{v}{c^2} dx_{\parallel} \right), \quad dx'_{\parallel} = \gamma (dx_{\parallel} + v dt), \quad d\vec{x}'_{\perp} = d\vec{x}_{\perp}. \quad (4.1.37)$$

It is useful to define $\vec{t}_v$ as the unit vector in the direction of the boost:

$$\vec{t}_v \stackrel{\text{def}}{=} \frac{\vec{v}}{|\vec{v}|}. \quad (4.1.38)$$

Then, any vector can be written as a part parallel to the boost and a part perpendicular:

$$d\vec{x} = dx_{\parallel} \vec{t}_v + d\vec{x}_{\perp} \quad (4.1.39)$$

$$\implies d\vec{x} \cdot \vec{t}_v = dx_{\parallel} \quad (4.1.40)$$

$$\implies d\vec{x}_{\perp} = d\vec{x} - \vec{t}_v \vec{t}_v \cdot d\vec{x}. \quad (4.1.41)$$

Finally then, in terms of the boost:

$$d\vec{x}' = dx'_{\parallel} \vec{t}_v + d\vec{x}'_{\perp} = \gamma (dx_{\parallel} + v dt) \vec{t}_v + d\vec{x}_{\perp} \quad (4.1.42)$$

$$= \gamma d\vec{x} \cdot \vec{t}_v \vec{t}_v + \gamma v dt + d\vec{x} - \vec{t}_v \vec{t}_v \cdot d\vec{x} = (\mathbb{1} + (\gamma - 1) \vec{t}_v \vec{t}_v) \cdot d\vec{x} + \gamma v dt. \quad (4.1.43)$$

So the fully generalized Lorentz boost in an arbitrary direction is:

$$dt' = \gamma \left(dt + \frac{\vec{v} \cdot d\vec{x}}{c^2} \right) \quad (4.1.44)$$

$$d\vec{x}' = (\mathbb{1} + (\gamma - 1) \vec{t}_v \vec{t}_v) \cdot d\vec{x} + \gamma \vec{v} dt. \quad (4.1.45)$$

By integrating the boost in differential form, we can find the boost effect on the coordinates. Let t_b be

the time at which the boost is applied and $\vec{x}_b$ be the position of the point we are looking at time t_b :

$$t' - t_b = \gamma(t - t_b + \frac{\vec{v}}{c^2} \cdot (\vec{x} - \vec{x}_b)), \quad \vec{x}' - \vec{x}_b = (\mathbb{1} + (\gamma - 1)\vec{v}_v\vec{v}_v) \cdot (\vec{x} - \vec{x}_b) + \gamma\vec{v}(t - t_b). \quad (4.1.46)$$

The Lorentz theory is a little quirky because unlike in the Galilean theory, different frames measure time differently as $t' \neq t$. Our naive assumption when we did Galilean theory that every clock passes time the same way isn't possible once we require that there be an invariant speed. If we consider our family of events $X(\alpha)$ to be the events actually passed through by an object, the proper time τ is defined as the time the object experiences when traveling through that sequence of events. The proper time between two events depends on the path one takes between them. In an object's own frame, by definition, it does not move relative to itself. So, if primed coordinates indicate the instantaneous coordinates of the object at a particular moment, then $dt' = d\tau$ is the rate at which time is passing and $d\vec{x}' = 0$ because the object is stationary relative to itself. Considering transforming from an arbitrary frame $t, \vec{x}$ to the object's coordinates $t', \vec{x}'$ and using that the Lorentz boost in equations (4.1.44) and (4.1.45) can be inverted by replacing primed with unprimed and $\vec{v}$ with $-\vec{v}$, we have:

$$d\vec{x} = (\mathbb{1} + (\gamma - 1)\vec{v}_v\vec{v}_v) \cdot d\vec{x}' - \gamma\vec{v}dt' = -\gamma\vec{v}d\tau. \quad (4.1.47)$$

$$dt = \gamma \left(dt' - \frac{\vec{v} \cdot d\vec{x}'}{c^2} \right) = \gamma d\tau. \quad (4.1.48)$$

$$\implies \dot{\vec{x}} = \frac{d\vec{x}}{dt} = -\vec{v}. \quad (4.1.49)$$

Hence in order to boost to the instantaneous rest frame of the object (the primed coordinates) from coordinates $(t, \vec{x})$, the necessary boost velocity is $-\dot{\vec{x}}$ where $\dot{\vec{x}}$ is the velocity of the object as seen in the unprimed coordinates. Then, we can see that the proper time is given in the general unprimed coordinates by:

$$d\tau = dt' = \gamma \left(dt + \frac{\vec{v} \cdot d\vec{x}}{c^2} \right) = \frac{dt - \frac{\dot{\vec{x}} \cdot d\vec{x}}{c^2}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} \quad (4.1.50)$$

$$= \frac{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} dt = \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} dt = \sqrt{dt^2 - \frac{|d\vec{x}|^2}{c^2}} \quad (4.1.51)$$

$$\implies d\tau^2 = dt^2 - \frac{|d\vec{x}|^2}{c^2}. \quad (4.1.52)$$

Because $d\vec{x}' = 0$ when $dt' = d\tau$, the proper time is also equivalent to the time between two events in the frame in which those events happen at the same location. If t is the time coordinate in one frame and $\vec{x}$ is the position of an object as a function of time measured in the frame, then the time which is experienced by the object τ along some path can be calculated by integrating equation (4.1.51) along that path. Because the interpretation of the proper time is independent of frame, we should expect that it is invariant under boosts. Consider now primed coordinates which are arbitrarily boosted relative to the unprimed coordinates and recall the decomposition into parallel and perpendicular components to the boost velocity:

$$d\tau'^2 = dt'^2 - \frac{|d\vec{x}'|^2}{c^2} = dt'^2 - \frac{|dx'_{\parallel}\vec{v} + d\vec{x}'_{\perp}|^2}{c^2} = dt'^2 - \frac{dx'^2_{\parallel} + 2\vec{v} \cdot d\vec{x}'_{\perp} + |d\vec{x}'_{\perp}|^2}{c^2} \quad (4.1.53)$$

$$= \left(\gamma \left(dt + \frac{v}{c^2} dx_{\parallel} \right) \right)^2 - \frac{1}{c^2} (\gamma (dx_{\parallel} + vdt))^2 - \frac{|d\vec{x}'_{\perp}|^2}{c^2} \quad (4.1.54)$$

$$= dt^2 - \frac{|d\vec{x}|^2}{c^2} \quad (4.1.55)$$

$$= d\tau^2. \quad (4.1.56)$$

And so we see that in fact the proper time is left invariant under the Lorentz boost as expected. We also define the proper distance s as the distance between events in the frame in which they happen at the same time. That is, the proper distance element $ds = |d\vec{x}'|$ between two nearby events whenever $dt' = 0$ between those events. Using that we just computed that (4.1.55) is Lorentz invariant:

$$dt'^2 - \frac{|d\vec{x}'|^2}{c^2} = dt^2 - \frac{|d\vec{x}|^2}{c^2} \quad (4.1.57)$$

$$\implies -\frac{ds^2}{c^2} = dt^2 - \frac{|d\vec{x}|^2}{c^2} \quad (4.1.58)$$

$$\implies ds^2 = |d\vec{x}|^2 - c^2 dt^2. \quad (4.1.59)$$

Hence the proper time and the proper distance are related by:

$$ds^2 = -c^2 d\tau^2. \quad (4.1.60)$$

Automatically, the proper distance is also invariant. If $d\tau^2 > 0$, meaning the right hand side of (4.1.52), is positive, then $d\tau$ between the events is a real number and we see:

$$d\tau^2 = \frac{dt^2}{c^2} (c^2 - |\dot{\vec{x}}|^2) > 0 \implies |\dot{\vec{x}}| < c. \quad (4.1.61)$$

So, an object passing between the events in question would move at a speed less than c in any coordinates. As such, any displacement between events for which $d\tau^2 > 0$ is called **timelike** and one can travel between the events at less than the speed of light. If two events are separated by a timelike interval then there exists a frame in which they happen at the same location $\vec{x}' = \vec{x}$. The difference in the times at which the events occur in this frame is then the proper time between those events. If instead $d\tau$ is exactly 0 we have what is called a **lightlike** interval. Then:

$$d\tau^2 = \frac{dt^2}{c^2} (c^2 - |\dot{\vec{x}}|^2) = 0 \implies |\dot{\vec{x}}| = c. \quad (4.1.62)$$

If two events have lightlike separation, one has to move at precisely the speed of light to get from one to the other. Finally, if instead $d\tau^2$ is negative so that ds^2 is positive, then ds is a real number and the distance between the events at fixed time exists and is non-zero (by boosting to the frame in which dt vanishes). This is called a **spacelike** interval. If two events are separated by a spacelike interval then there exists a frame in which they happen at the same time $t' = t$. The distance between the events in this frame is then the proper distance between them. By the same reasoning, we see:

$$ds^2 = dt^2 (|\dot{\vec{x}}|^2 - c^2) > 0 \implies |\dot{\vec{x}}| > c. \quad (4.1.63)$$

If two events have spacelike separation, one has to move faster than light to get from one event to the other. As well, suppose that in one frame $dt > 0$ between two events which are spacelike separated (thus the second event happens after the first in this frame). Consider a boost by velocity $\vec{v}$ in the opposition direction of $d\vec{x}$ and with magnitude $v > c^2 \frac{dt}{|d\vec{x}|}$:

$$dt = \gamma \left(dt + \frac{\vec{v} \cdot d\vec{x}}{c^2} \right) = \gamma \left(dt - \frac{v|d\vec{x}|}{c^2} \right) < \gamma \left(dt - c^2 \frac{dt}{|d\vec{x}|} \frac{|d\vec{x}|}{c^2} \right) = \gamma (dt - dt) = 0 \quad (4.1.64)$$

$$\implies dt' < 0. \quad (4.1.65)$$

Hence, an observer moving with speed v in the opposite direction of $d\vec{x}$ would see the events in the opposite order in time as for them dt' has the opposite sign of dt . This is one of the funny things about the Lorentz transformation. The order in time of events which are spacelike separated depends on your reference frame! Because $ds^2 = |d\vec{x}|^2 - c^2 dt^2 > 0$ we have that $|d\vec{x}| > cdt$ and so the boost speed used to change the sign of the time displacement is less than c : $c^2 \frac{dt}{|d\vec{x}|} < c$. This raises an interesting question of causality. If we are to believe that effects happen after their causes and our theory is to work at speeds less than light (as it must, since that is the regime in which we already observe daily life), we have to impose some conditions. For effects to happen after their causes in all frames which are related by boosts at less than the speed of light, it must be impossible for spacelike separated events to affect each other because at these speeds it is possible to reverse the order of events in time by going to a different frame. This means that causality requires the outcome of any experiment at time t and location $\vec{x}$ to be able to be determined from data at time 0 and at locations which are less than distance ct away from $\vec{x}$. No data about any events with spacelike separation from $(t, \vec{x})$ should be necessary. From a given event, the set of all other events which are timelike or lightlike separated from that event defines a (higher dimensional) cone called the lightcone of that event. The lightcone contains a half-cone of events “before” the event around which the cone is built, called the past lightcone and it contains a half-cone of events “after” the event called the future lightcone. Thus, **causality requires that everything that happens at an event can be computed only from data in its past lightcone.**

There is a bit of subtlety in the causality requirement as many of our variables, such as the potentials, carry some arbitrariness due to gauge transformation or redefining coordinates by translations, rotations, et cetera. So when we say that we must be able to predict the outcomes of any experiments from data in the past lightcone, we really mean that all quantities which are invariant under all the symmetries of our theory have to be able to be computed from data in the past lightcone. It is important we only place this

condition on the invariant quantities of our theory because we can make whatever pointlessly complicated gauge transformation we want which depends on whatever we feel like but gauge transformations do not affect the outcome of any experiments. From our causality condition, it further must be the case that **nothing in our theory moves faster than light**. If something did move faster than light, it could carry data between spacelike separated points, between which we already know there is not an invariant notion of before or after. This would violate that effects must only happen after their causes. Or, more mathematically, making it so we would need data from outside of the light cone of an event to calculate what happens at that event.

Now that we have space and time intermixing when we change coordinates, it is more appropriate to speak of them together as one thing called **spacetime**. Due to their mixing, there is no way which is preserved by our symmetry to separate the two, and so thinking of space and time as completely distinct is artificial within the Lorentz theory. When we have a flat Euclidean space with this boost relationship with time, the result is known as Minkowski spacetime. The volume element of spacetime is unchanged by Lorentz transformations:

$$d\mathbb{T} \stackrel{\text{def}}{=} dt d\mathbb{S} = dt d^3\vec{x} \quad (4.1.66)$$

$$\implies d\mathbb{T}' = dt' d^3\vec{x}' = \det \left(\frac{\partial(t', \vec{x}')}{\partial(t, \vec{x})} \right) dt d^3\vec{x} = \det \begin{pmatrix} \gamma & \gamma \frac{v}{c^2} & 0 & 0 \\ \gamma v & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} d\mathbb{T} \quad (4.1.67)$$

$$\implies d\mathbb{T}' = \gamma^2 \left(1 - \frac{v^2}{c^2} \right) d\mathbb{T} = d\mathbb{T}. \quad (4.1.68)$$

All of this gives us:

Theorem 4.1: Lorentz Transformation Theorem

The general continuous boost transformation with invariant speed c is given by the Lorentz boost:

$$dt' = \gamma \left(dt + \frac{\vec{v} \cdot d\vec{x}}{c^2} \right) \quad (4.1.69)$$

$$d\vec{x}' = (\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot d\vec{x} + \gamma \vec{v} dt \quad (4.1.70)$$

where:

$$\gamma = \frac{1}{\sqrt{1 - \frac{|\vec{v}|^2}{c^2}}}, \quad \vec{v}_v = \frac{\vec{v}}{|\vec{v}|}. \quad (4.1.71)$$

All Lorentz boosts do not change the proper time $d\tau$ or proper distance ds between events defined by:

$$d\tau^2 = -\frac{ds^2}{c^2} = dt^2 - \frac{|d\vec{x}|^2}{c^2} \quad (4.1.72)$$

or the spacetime volume element $d\mathbb{T} = dt dx dy dz$.

Exercises

Problem 4.1: Time Dilation. Consider an object which is ejected from a source and then moves at constant velocity $\vec{v}$ with respect to an observer who is not accelerating¹. Suppose that it takes a time t in the frame of the object to strike a wall by which the observer is standing once it leaves the source. Show that in this same interval, a time t' passes for the observer where:

$$t' = \gamma t$$

and γ is the usual Lorentz factor in terms of the object's velocity. This effect is known as “time dilation” as the apparent time it takes for something to happen to an object in any frame other than that object's rest frame is longer than it would have been in that object's rest frame.

¹It is important to make the condition that the observer is not accelerating so that we can treat the observer's rest frame as one which we could always go to by a Lorentz boost. If the observer was accelerating, we would need to constantly be boosting to its rest frame. This is entirely mathematically possible to calculate, just more complicated. Some (especially lower level) books misunderstand and believe that acceleration is for some reason not allowed in special relativity and must be saved for general relativity. This is entirely and wholly wrong, misguided, and empirically denied but it is an occasionally repeated error.

Problem 4.2: Length Contraction. Suppose an object of length l is moving at speed v along the axis of its length with respect to an observer who is not accelerating. The observer, in order to measure the object's length, marks both endpoints of the object at the same time². The observer measures a distance l' between the two endpoints. Show that the measured length l' of the object is related to the proper length of the object l by:

$$l' = \frac{l}{\gamma}.$$

This effect is known as “Length Contraction” as the apparent length of the object is shorter than the actual length of the object in its own rest frame³.

Problem 4.3: ★ Calibrating relative motion. We will see soon that a freely moving object in the Lorentz theory does not accelerate, just like in the Galilean theory. So, suppose we have two free observers (and thus they are not accelerating). Let us go to the rest frame of observer A and let $\vec{v}$ be the velocity of observer B in this frame. Observer B emits flashes of light with a time τ in their frame between each flash. Let $\vec{r}$ be the difference in positions between the two observers when observer A 's clock reads 0. Observer A does not know ahead of time the values of $\vec{r}$, $\vec{v}$, or τ .

- (a) Show that for some constant δ , the time at which pulse n is emitted by B in A 's coordinates is given by:

$$t_{n,\text{emit}} = n\gamma\tau + \delta.$$

- (b) Show that the time t_n at which pulse n is detected by A is given by:

$$t_n = t_{n,\text{emit}} + \frac{1}{c} \sqrt{|\vec{r}|^2 + 2\vec{r} \cdot \vec{v}t_{n,\text{emit}} + |\vec{v}|^2 t_{n,\text{emit}}^2}.$$

- (c) Show then that after observing 5 pulses, A has enough data to determine $|\vec{v}|$, τ , $\vec{v} \cdot \vec{r}$, $|\vec{r}|$, and δ . Thus, A can measure the speed $|\vec{v}|$ at which B is moving relative to it. Do not struggle to find explicit expressions for these quantities; in practice one would do so numerically on a computer. If A in addition was able to resolve the direction from which the emitted light came (by having a spherical detector), they could also determine the direction of $\vec{v}$ as the points would impinge on a circular arc of the detector. The plane of that arc gives the plane which contains both A and the line of motion of B and thus is spanned by $\vec{r}$ and $\vec{v}$. Because knowing $\vec{r} \cdot \vec{v}$, $|\vec{r}|$, and $|\vec{v}|$ allows one to determine the cosine of the angle between $\vec{r}$ and $\vec{v}$, all that is left to determine to determine the direction of $\vec{v}$ is which solution to the cosine for the angle. This is determined by the direction the arc is developing on the detector. Thus, from light signals alone A can measure the velocity of B . A could then send a signal to B (they now can determine the future position of B by extrapolating the line) and inform it of its relative velocity. B can then use some fuel to accelerate and cancel that velocity so that it is stationary with respect to A . In this way, two observers can bring themselves into a state of no relative motion by sending light signals.

Problem 4.4: ★ Clock Synchronization. Suppose two free observers have brought themselves into a state of no relative motion between each other by the method of the previous problem. They would now like to synchronize their clocks. That is, they want to adjust their clocks so that they both read the same number.

- (a) Show that for some number δ , the time t_A on A 's clock is always related to the time t_B on B 's clock by:

$$t_A = t_B + \delta.$$

- (b) Suppose the observers are an unknown distance l away from each other and that B points a mirror directly at A . A emits a light pulse when their clock reads t_{A1} . B observes that light pulse when their clock reads t_{B1} which is then reflected by the mirror back to A . A receives the reflected signal when their clock reads t_{A2} . Show that:

$$\begin{aligned} t_{A2} - t_{A1} &= \frac{2l}{c} \\ t_{A2} &= t_{B1} + \delta + \frac{l}{c}. \end{aligned}$$

²There are some subtleties here on how to actually pull this off. One could have two observers who are not moving relative to each other and have clocks which are synchronized to read the same number agree ahead of time at what time to each measure an endpoint. Then, they can make their measurements and compare afterward. How the observers can establish that they are not moving relative to each other and that their clocks are synchronized are covered in other questions this section.

³One may be concerned that in the object's rest frame, the endpoints are apparently marked at different times. This does not matter because in that frame the object isn't moving and so whenever its endpoints are marked they will be marked in the same location.

- (c) The observers want to each adjust their clocks using their locally measured information so that they will read the same values afterward. That is, they seek functions $T_A(t_{A1}, t_{A2})$ and $T_B(t_{B1})$ so that their adjusted times t'_A and t'_B satisfy:

$$t'_A = t_A - T_A, \quad t'_B = t_B - T_B, \quad t'_A = t'_B.$$

Show that this requires δ can be written as:

$$\delta = T_A(t_{A1}, t_{A2}) - T_B(t_{B1}).$$

- (d) Show that one convention for how to synchronize the clocks is to take:

$$T_B = t_{B1}, \quad T_A = \frac{t_{A1} + t_{A2}}{2}.$$

Thus, through the exchange of light signals two observers can synchronize their clocks to read the same values. As well, this provides a way to measure the speed of light very directly by placing two mirrors a distance l apart (which you measure by sticks) and detectors which record the times at which a light signal is detected. By having a light pulse bounce back and forth between the mirrors, one can collect many data points and the difference between the recorded times on each mirror should be $\frac{2l}{c}$, thus allowing one to find c using data from each mirror (the more data the better!).

Problem 4.5: The Twin “Paradox”. Consider two identical twins. One of them stays put and does not accelerate while the other one is launched at velocity $\vec{v}$ away. The moving twin travels for what to them feels like a time $t/2$ and then returns home at velocity $-\vec{v}$. Show that the time which passed for the moving twin is t and that the time which passed for the stationary twin is: $t' = \gamma t$. As well, consider the speed at which the moving twin was launched at to be 99% the speed of light and that they were traveling for what to them was 1 year. Show that the stationary twin in that same time aged by just over 7 years. This is the twin “paradox”; they won’t be the same age anymore! One should remember that all “paradoxes” are fake. When someone says paradox, what they really mean is unexpected conclusion. Certainly this conclusion is not what one might naively expect from daily life but it is completely logically and experimentally consistent (this effect is noticed and adjusted for by clocks on GPS satellites) and so it isn’t any sort of contradiction. The only reason this is typically called the twin paradox is by the prejudice of the one who conceived of the name, not anything intrinsic to the phenomenon. There is another layer to this “paradox” in which one asks how the universe knew which twin to age more as isn’t there a symmetry to interchanging the twins? But, there is no such symmetry because one twin has to be accelerated to turn around and return while the other did not.

4.2 The Free Lagrangian of a Relativistic Particle

Now that we have successfully reformulated boost symmetry in a way which is consistent with the existence of an invariant speed, we need to define the assumptions of our new theory, Lorentz Classical Mechanics (LCM) with this boost symmetry. We are still working with point particles and so we still have:

Assumption :: LCM I - Matter is point-like

Matter consists of moving points. The points have no internal structure and so the state of each point is given by its position in space at the present time.

Now that we have dispensed of Galilean boost symmetry, we have our new boost symmetry:

Assumption :: LCM II - Lorentz Boost Symmetry

The Universe has symmetry under applying a Lorentz boost.

Any theory with Lorentz Boost Symmetry is called a (special) relativistic theory. Now that we are going to consider space and time as part of one thing (because they mix under boosts), we have 3 space and 1 time dimension to make 4 dimensions total and still believe the geometry to be static and the space to be flat. Thus,

Assumption :: LCM III - Spacetime is static and Minkowskian

The background spacetime in which objects move is not itself dynamical and is instead fixed without any curvature or punctures.

The group of time translations, space translations, rotations, and Galilean boosts was called the connected Galilean group. Now we have replaced that group of transformations with a new group of interest, that of time translations, space translations, rotations, and Lorentz boosts, which is called the **connected Poincare group**. The subgroup of transformations of just rotations and Lorentz boosts is called the **connected Lorentz group**.

Finally, our last assumption is that of causality:

Assumption :: PHSXVII - Causality

The results of any experiment can be determined from data only in the past light cone of that experiment.

Taking these assumptions, let us find the Lagrangian $\mathcal{L}$ for a particle which is consistent with them. To do this, we have essentially the opposite situation of section 3.3. There we wanted to find the Lagrangian for the potentials given the charge and current densities, now we want to find the Lagrangian for the charges given the potentials. We know the interaction terms already. Then, we need $\mathcal{L}_0(t, \vec{x}, \dot{\vec{x}})$, the Lagrangian for a single charge when it is isolated. Just like section 3.3, we just have to directly apply each of our symmetries. Fortunately, we already did almost all the work in chapter 2 when we found that the most general possible Lagrangian for a point particle with time translational symmetry, space translational symmetry, and rotational symmetry is just a function of the speed (up to adding total time derivatives). That is, by (2.4.82) for some function $L(|\dot{\vec{x}}|)$:

$$\mathcal{L}_0(t, \vec{x}, \dot{\vec{x}}) = L(|\dot{\vec{x}}|). \quad (4.2.1)$$

All we need to do now is require symmetry under Lorentz boost. Because time changes with the Lorentz boost, we need to account for this in the transformation of the Lagrangian when we apply (1.10.34). That is, Lorentz boost symmetry will imply that there exist functions $\vec{g}(t, \vec{x})$ so that:

$$\vec{\mathcal{D}} \left(\mathcal{L}_0(t', \vec{x}', \dot{\vec{x}}') \frac{dt'}{dt} \right) = \frac{d\vec{g}}{dt} \quad (4.2.2)$$

$$\implies \left. \frac{dt'}{dt} \right|_{\varepsilon=0} \vec{\mathcal{D}} \mathcal{L}_0 + \mathcal{L}_0 \vec{\mathcal{D}} \left(\frac{dt'}{dt} \right) = \frac{\partial \vec{g}}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g} \quad (4.2.3)$$

$$\implies \vec{\mathcal{D}} \dot{\vec{x}} \cdot \frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} + \mathcal{L}_0 \vec{\mathcal{D}} \left(\frac{dt'}{dt} \right) = \frac{\partial \vec{g}}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}. \quad (4.2.4)$$

Here the $\vec{\mathcal{D}}$ is the derivative with respect to the boost velocity $\vec{v}$. Then:

$$\frac{dt'}{dt} = \frac{\gamma (dt + \frac{\vec{v} \cdot d\vec{x}}{c^2})}{dt} = \gamma \left(1 + \frac{\vec{v} \cdot \dot{\vec{x}}}{c^2} \right) = 1 + \frac{\vec{v} \cdot \dot{\vec{x}}}{c^2} + \mathcal{O}(v^2) \quad (4.2.5)$$

$$\implies \vec{\mathcal{D}} \frac{dt'}{dt} = \frac{\dot{\vec{x}}}{c^2}. \quad (4.2.6)$$

$$\dot{\vec{x}}' = \frac{d\vec{x}'}{dt'} = \frac{(\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot d\vec{x} + \gamma d\vec{t}}{\gamma (dt + \frac{\vec{v} \cdot d\vec{x}}{c^2})} = \frac{(\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \dot{\vec{x}} + \gamma \vec{v}}{\gamma \left(1 + \frac{\vec{v} \cdot \dot{\vec{x}}}{c^2} \right)} = \dot{\vec{x}} + \left(\mathbb{1} - \frac{\dot{\vec{x}} \dot{\vec{x}}}{c^2} \right) \cdot \vec{v} + \mathcal{O}(v^2) \quad (4.2.7)$$

$$\implies \vec{\mathcal{D}} \dot{\vec{x}} = \mathbb{1} - \frac{\dot{\vec{x}} \dot{\vec{x}}}{c^2}. \quad (4.2.8)$$

So, (4.2.4) becomes:

$$\frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} - \frac{\dot{\vec{x}}}{c^2} \dot{\vec{x}} \cdot \frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} + \frac{\dot{\vec{x}}}{c^2} \mathcal{L}_0 = \frac{\partial \vec{g}}{\partial t} + (\dot{\vec{x}} \cdot \nabla) \vec{g}. \quad (4.2.9)$$

The left hand side is not an explicit function of t . As such, the partial t derivative of this equation vanishes:

$$0 = \frac{\partial^2 \vec{g}}{\partial t^2} + (\dot{\vec{x}} \cdot \nabla) \frac{\partial \vec{g}}{\partial t}. \quad (4.2.10)$$

At $\dot{\vec{x}} = 0$:

$$\frac{\partial^2 \vec{g}}{\partial t^2} = 0 \implies \vec{g}(t, \vec{x}) = \vec{h}(\vec{x}) + t \vec{i}(\vec{x}) \quad (4.2.11)$$

for some functions $\vec{h}(\vec{x})$ and $\vec{i}(\vec{x})$. Then, for $\dot{\vec{x}} \neq 0$:

$$(\dot{\vec{x}} \cdot \nabla) \frac{\partial \vec{g}}{\partial t} = 0 \implies \frac{\partial^2 \vec{i}^a}{\partial x^b} = 0 \implies \vec{i}(\vec{x}) = \vec{C} \quad (4.2.12)$$

for a constant vector $\vec{C}$. Then:

$$\frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} - \frac{\dot{\vec{x}}}{c^2} \dot{\vec{x}} \cdot \frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} + \frac{\dot{\vec{x}}}{c^2} \mathcal{L}_0 = \vec{C} + (\dot{\vec{x}} \cdot \nabla) \vec{h}(\vec{x}). \quad (4.2.13)$$

The left hand side is not an explicit function of $\vec{x}$. As such, its partial $\vec{x}$ derivative vanishes:

$$0 = \dot{x}^b \frac{\partial^2 h_a}{\partial x^b \partial x^c} \implies h_a(\vec{x}) = M_{ab} x^b + N_a \quad (4.2.14)$$

for some constant matrix $\hat{M}$ and constant vector $\vec{N}$. Then, (4.2.13) becomes:

$$\frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} - \frac{\dot{\vec{x}}}{c^2} \dot{\vec{x}} \cdot \frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} + \frac{\dot{\vec{x}}}{c^2} \mathcal{L}_0 = \vec{C} + \hat{M} \dot{\vec{x}}. \quad (4.2.15)$$

Using (4.2.1), we have:

$$\frac{\partial \mathcal{L}_0}{\partial \dot{\vec{x}}} = \frac{\partial L(|\dot{\vec{x}}|)}{\partial |\dot{\vec{x}}|} \frac{\partial |\dot{\vec{x}}|}{\partial \dot{\vec{x}}} = \frac{\dot{\vec{x}}}{|\dot{\vec{x}}|} L'(|\dot{\vec{x}}|) \quad (4.2.16)$$

(here L' indicates the derivative of L with respect to its parameter $|\dot{\vec{x}}|$) and with this (4.2.15) becomes:

$$\dot{\vec{x}} \left(\left(1 - \frac{|\dot{\vec{x}}|^2}{c^2} \right) \frac{L'}{|\dot{\vec{x}}|} + \frac{L}{c^2} \right) = \vec{K} + \hat{N} \dot{\vec{x}}. \quad (4.2.17)$$

Let $v = |\dot{\vec{x}}|$ and $\vec{n}$ be the unit vector in the direction of $\dot{\vec{x}}$. Then:

$$\vec{n} \left(\left(1 - \frac{v^2}{c^2} \right) L'(v) + v \frac{L(v)}{c^2} \right) = \vec{K} + v \hat{N} \vec{n}. \quad (4.2.18)$$

Taking the limit $v \rightarrow 0$ of both sides:

$$L'(0)\vec{n} = \vec{K}. \quad (4.2.19)$$

The right hand side is independent of $\vec{n}$ but the left hand side is not. This is only possible if both are 0. Therefore:

$$L'(0) = 0, \quad \vec{K} = 0 \quad (4.2.20)$$

$$\vec{n} \left(\left(1 - \frac{v^2}{c^2} \right) L'(v) + v \frac{L(v)}{c^2} \right) = v \hat{N} \vec{n}. \quad (4.2.21)$$

The left hand side points in the $\dot{\vec{x}}$ direction and so the right hand side must as well. Therefore, for some function $\lambda(\dot{\vec{x}})$:

$$\hat{N} \dot{\vec{x}} = \lambda(\dot{\vec{x}}) \dot{\vec{x}}. \quad (4.2.22)$$

The left hand side is linear in $\dot{\vec{x}}$ and so the right hand side must be as well. Consequently, λ must be independent of $\dot{\vec{x}}$, giving:

$$\vec{n} \left(\left(1 - \frac{v^2}{c^2} \right) L'(v) + v \frac{L(v)}{c^2} \right) = \lambda v \vec{n} \quad (4.2.23)$$

$$\implies \left(1 - \frac{v^2}{c^2} \right) L'(v) + v \frac{L(v)}{c^2} = v \lambda \quad (4.2.24)$$

for a constant λ .

Equation (4.2.24) is a first order differential equation for L which we can solve using an integrating factor. In particular, we can rewrite it as:

$$\frac{d}{dv} \left(\frac{L(v) - \lambda c^2}{\sqrt{1 - \frac{v^2}{c^2}}} \right) = 0 \quad (4.2.25)$$

$$\implies L(v) = \lambda c^2 + a \sqrt{1 - \frac{v^2}{c^2}} \quad (4.2.26)$$

for some constant a . Therefore, the Lagrangian for a single isolated particle with all of our required symmetries is:

$$\mathcal{L}_0(t, \vec{x}, \dot{\vec{x}}) = a \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} + \frac{d}{dt}(\lambda c^2) \quad (4.2.27)$$

$$\simeq a \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}. \quad (4.2.28)$$

All that is left is to determine this parameter a . However, we know that for speeds very low compared to light this must reduce to the Galilean theory as in that regime that theory was already successful. Taylor expanding for small $|\dot{\vec{x}}|/c$, we have:

$$\mathcal{L}_0 = a \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} = a \left(1 - \frac{|\dot{\vec{x}}|^2}{2c^2} + \mathcal{O}\left(\frac{|\dot{\vec{x}}|^4}{c^4}\right) \right) = a - \frac{1}{2} \frac{a}{c^2} |\dot{\vec{x}}|^2 + \text{Higher Order Terms} \quad (4.2.29)$$

$$= \frac{d}{dt}(at) - \frac{1}{2} \frac{a}{c^2} |\dot{\vec{x}}|^2 + \text{H.O.T.} \simeq -\frac{1}{2} \frac{a}{c^2} |\dot{\vec{x}}|^2 + \text{H.O.T.} \quad (4.2.30)$$

This must match equation (2.5.2) to lowest order:

$$\mathcal{L}_{\text{Galileo}} = \frac{1}{2} m |\dot{\vec{x}}|^2. \quad (4.2.31)$$

Hence, we see that to match, $a = -mc^2$. Finally then, the Lagrangian for an isolated relativistic particle is:

$$\boxed{\mathcal{L}_0 = -mc^2 \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}}. \quad (4.2.32)$$

In the nonrelativistic case our free Lagrangian was 0 when the particle was stationary. This one is nonzero when the particle is stationary (it takes the value $-mc^2$). One can shift the value of the Lagrangian

by a constant (as a constant is a total time derivative of that constant times t) without affecting the dynamics and so the value of the Lagrangian when the particle is stationary can be set to whatever you like. However, the choice given above has a special uniqueness to it. Notice that in terms of the proper time, $\mathcal{L}_0$ can be written:

$$\mathcal{L}_0 = -mc^2 \frac{d\tau}{dt}. \quad (4.2.33)$$

Therefore, the action can be written:

$$S_0 = -mc^2 \int_{t_0}^{t_f} d\tau(t). \quad (4.2.34)$$

So, the action is Lorentz *invariant* meaning no surface term is added to it at all under any of our symmetries (if there was a surface term we would just say it is Lorentz symmetric). Nicely, in this form it is *manifestly* Lorentz invariant, meaning you can just look at it and see that it is Lorentz invariant because every piece of notation in how it is written is. There is no way to add a total time derivative of a function $f(t, \vec{x})$ to $\mathcal{L}_0$ so that the new action has this property. Therefore, (4.2.32) is a uniquely natural gauge choice; it is the only one where the Lorentz symmetry is completely manifest.

Exercises

Problem 4.6: Behavior of a relativistic free particle. Taking Lagrangian (4.2.32), find the equations of motion and solve them to show that a relativistic free particle behaves exactly like a Galilean free particle.

4.3 The Interacting Hamiltonian of a Relativistic Particle

Now that we have the free Lagrangian, we can use theorem 2.11 to write that the Lagrangian for our relativistic particle of charge q when experiencing background potentials is given by the addition of the free Lagrangian and the known interaction terms:

$$\mathcal{L} = -mc^2 \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} + q\dot{\vec{x}} \cdot \vec{A}(t, \vec{x}) - q\phi(t, \vec{x}). \quad (4.3.1)$$

This gives us the action:

$$S = \int_{t_0}^{t_f} \mathcal{L} dt = \int_{t_0}^{t_f} \left(-mc^2 \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} + q\dot{\vec{x}} \cdot \vec{A} - q\phi \right) dt. \quad (4.3.2)$$

Notice again that the first term of the action, the one corresponding to the free Lagrangian, is just $-mc^2$ times the proper time which the particle experiences along the path that it takes! Thus, not only is the proper time conceptually meaningful, it is in fact the free part of the action (up to a constant multiplier).

From here, we can now perform the Legendre transformation and compute the associated Hamiltonian. First, eliminate the velocity in favor of the momentum:

$$\vec{p} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{m\dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} + q\vec{A} \quad (4.3.3)$$

$$\implies |\vec{p} - q\vec{A}|^2 = \frac{m^2 |\dot{\vec{x}}|^2}{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} \quad (4.3.4)$$

$$\implies |\dot{\vec{x}}|^2 = \frac{c^4 |\vec{p} - q\vec{A}|^2}{c^2 |\vec{p} - q\vec{A}|^2 + m^2 c^4} \quad (4.3.5)$$

$$\implies \dot{\vec{x}} = \frac{c^2 (\vec{p} - q\vec{A})}{\sqrt{c^2 |\vec{p} - q\vec{A}|^2 + m^2 c^4}}. \quad (4.3.6)$$

Then, the Hamiltonian is given as always:

$$\mathcal{H} = \dot{\vec{x}} \cdot \vec{p} - \mathcal{L} \quad (4.3.7)$$

$$= \dot{\vec{x}} \cdot \left(\frac{m\dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} + q\vec{A} \right) + mc^2 \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} - q\dot{\vec{x}} \cdot \vec{A}(t, \vec{x}) + q\phi(t, \vec{x}) \quad (4.3.8)$$

$$= \frac{mc^2}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} + q\phi(t, \vec{x}) \quad (4.3.9)$$

$$= \sqrt{c^2 |\vec{p} - q\vec{A}(t, \vec{x})|^2 + m^2 c^4} + q\phi(t, \vec{x}). \quad (4.3.10)$$

Using that the Hamiltonian is also the energy, we can notice from the second to last line that as the speed of a massive particle approaches c , the energy diverges. That is, it takes an infinite amount of energy to get an object with non-zero mass up to the speed of light. This explains how the need to keep speeds below c for causality is enforced mechanically; because energy is conserved one would need some term in the Hamiltonian which could be made arbitrarily negative in order to push even a single mass toward the speed of light. Interestingly, unlike the Galilean theory, one can meaningfully take this Hamiltonian and consider it for $m = 0$:

$$\mathcal{H} = c|\vec{p} - q\vec{A}| + q\phi \implies \dot{\vec{x}} = \frac{\partial \mathcal{H}}{\partial \vec{p}} = c \frac{\vec{p} - q\vec{A}}{|\vec{p} - q\vec{A}|} \implies |\dot{\vec{x}}| = c. \quad (4.3.11)$$

Hence a massless particle always moves at the speed of light. Something interesting about this special case is that the Legendre transformation cannot be completed and so the Hamiltonian exists but the Lagrangian does not. Together we have:

Theorem 4.2: Lorentz particle Hamiltonian and Lagrangian

The Lagrangian and Hamiltonian of an LCM particle in background potentials $\phi, \vec{A}$ are:

$$\mathcal{L} = -mc^2 \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}} + q\dot{\vec{x}} \cdot \vec{A} - q\phi \quad (4.3.12)$$

$$\mathcal{H} = \sqrt{c^2|\vec{p} - q\vec{A}|^2 + m^2c^4} + q\phi. \quad (4.3.13)$$

Just like with the Galilean theory, it is worth studying the algebra of the boost. To do so first we should note an important difference between Galilean boosts and Lorentz boosts. For the purposes of this discussion we will restriction attention to boosts along a single axis. Notice that for Galilean boosts, consecutive boosts are equivalent to a single boost where the boost velocities add:

$$B_{\text{Gal}}(v_2)B_{\text{Gal}}(v_1) \begin{pmatrix} dt \\ dx \end{pmatrix} = B_{\text{Gal}}(v_2) \begin{pmatrix} dt \\ dx + v_1 dt \end{pmatrix} = \begin{pmatrix} dt \\ dx + v_2 dt + v_1 dt \end{pmatrix} = B_{\text{Gal}}(v_1 + v_2) \begin{pmatrix} dt \\ dx \end{pmatrix}. \quad (4.3.14)$$

The story is not so simple for the Lorentz boost:

$$B(v_2)B(v_1) \begin{pmatrix} dt \\ dx \end{pmatrix} = B(v_2) \begin{pmatrix} \gamma_1(dt + \frac{v_1 dx}{c^2}) \\ \gamma_1(dx + v_1 dt) \end{pmatrix} = \begin{pmatrix} \gamma_2\gamma_1(dt + \frac{v_1 dx}{c^2}) + \frac{\gamma_2 v_2}{c^2}\gamma_1(dx + v_1 dt) \\ \gamma_2\gamma_1(dx + v_1 dt) + \gamma_2 v_2\gamma_1(dt + \frac{v_1 dx}{c^2}) \end{pmatrix} \quad (4.3.15)$$

$$= \begin{pmatrix} \gamma_2\gamma_1(1 + \frac{v_1 v_2}{c^2})dt + \gamma_1\gamma_2\frac{v_1 + v_2}{c^2}dx \\ \gamma_1\gamma_2(v_1 + v_2)dt + \gamma_1\gamma_2(1 + \frac{v_1 v_2}{c^2})dx \end{pmatrix}. \quad (4.3.16)$$

This actually is equivalent to a single Lorentz boost but instead of the velocities simply adding, the total boost velocity of the combined transformation is:

$$v = \frac{v_1 + v_2}{1 + \frac{v_1 v_2}{c^2}}. \quad (4.3.17)$$

The easiest way to get this is to notice by the definition of the Lorentz boost that the boost velocity is the ratio of the coefficient on the dt term to the coefficient on the dx in the final expression for dx' and then check that all of the other components are matched using this velocity. So, the combined transformation does not simply add the velocities of the individual transformations. This isn't an issue, but note from Theorem 1.10 that Lie group parameters do add when composing transformations of the same generator:

$$T(\theta) = e^{\theta(\cdot\mathcal{L}\tau)} \implies T(\theta_1)T(\theta_2) = e^{\theta_1(\cdot\mathcal{L}\tau)}e^{\theta_2(\cdot\mathcal{L}\tau)} = e^{(\theta_1+\theta_2)(\cdot\mathcal{L}\tau)} = T(\theta_1 + \theta_2). \quad (4.3.18)$$

Hence while the velocity does not add, there must a group parameter which does. Given that this additive property comes from the properties of the operator exponential, we can find it simply by computing the exponential of the generator. The expression for the Lorentz boost is plainly a linear extended point transformation. It is convenient to scale everything so that the parameter we are working with is unitless. So, differentiate with respect to $\beta = v/c$ and use cdt as the time coordinate so it has the same units as dx . Further, let φ be the additive group parameter for the boost, whatever it is. Then:

$$\begin{pmatrix} cdt' \\ dx' \end{pmatrix} = \begin{pmatrix} \gamma(cdt + \frac{v dx}{c}) \\ \gamma(dx + \frac{v}{c}cdt) \end{pmatrix} = \begin{pmatrix} \gamma & \gamma\beta \\ \gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} cdt \\ dx \end{pmatrix} \implies \hat{B}(v) = \begin{pmatrix} \gamma & \gamma\beta \\ \gamma\beta & \gamma \end{pmatrix}. \quad (4.3.19)$$

$$\implies \hat{B}'(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (4.3.20)$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (4.3.21)$$

$$\implies \hat{B}(v) = e^{\varphi \hat{B}'(0)} = \sum_{n=0}^{\infty} \frac{\varphi^n \hat{B}'(0)^n}{n!} = \sum_{n=0}^{\infty} \frac{\varphi^{2n} \hat{B}'(0)^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{\varphi^{2n+1} \hat{B}'(0)^{2n+1}}{(2n+1)!} \quad (4.3.22)$$

$$\implies \hat{B}(v) = e^{\varphi \hat{B}'(0)} = \sum_{n=0}^{\infty} \frac{\varphi^{2n}}{(2n)!} \mathbb{1} + \sum_{n=0}^{\infty} \frac{\varphi^{2n+1}}{(2n+1)!} \hat{B}'(0). \quad (4.3.23)$$

This first series is the Taylor expansion for hyperbolic cosine and the second is the Taylor expansion for

hyperbolic sine. And so, we arrive at our final representation:

$$B(v) = e^{\varphi \hat{B}'(0)} = \cosh(\varphi) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sinh(\varphi) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \cosh(\varphi) & \sinh(\varphi) \\ \sinh(\varphi) & \cosh(\varphi) \end{pmatrix}. \quad (4.3.24)$$

Matching between equations (4.3.19) and (4.3.24) we find that:

$$v = c\beta = c \frac{\gamma\beta}{\gamma} = c \frac{\sinh(\varphi)}{\cosh(\varphi)} = c \tanh(\varphi). \quad (4.3.25)$$

This gives the relationship between the additive group parameter φ (called the rapidity) and the boost velocity v . For boosts along the x , y , or z axes then we have the matrix representations:

$$\begin{aligned} \hat{B}_x(\varphi) &= \begin{pmatrix} \cosh \varphi & \sinh \varphi & 0 & 0 \\ \sinh \varphi & \cosh \varphi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, & \hat{B}_y(\varphi) &= \begin{pmatrix} \cosh \varphi & 0 & \sinh \varphi & 0 \\ 0 & 1 & 0 & 0 \\ \sinh \varphi & 0 & \cosh \varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \\ \hat{B}_z(\varphi) &= \begin{pmatrix} \cosh \varphi & 0 & 0 & \sinh \varphi \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh \varphi & 0 & 0 & \cosh \varphi \end{pmatrix}. \end{aligned} \quad (4.3.26)$$

We call the generators of Lorentz boosts $\vec{K}$. From equation (4.3.25), the derivatives at the identity can be calculated:

$$\left. \frac{d}{d\vec{\varphi}} \right|_0 = \left. \frac{d\vec{v}}{d\vec{\varphi}} \right|_0 \cdot \left. \frac{d}{d\vec{v}} \right|_0 = c \left. \frac{d}{d\vec{v}} \right|_0. \quad (4.3.27)$$

Therefore, for computing brackets:

$$\left. \frac{du}{d\vec{\varphi}} \right|_0 = \{u, \vec{K}\} = c \left. \frac{du}{d\vec{v}} \right|_0. \quad (4.3.28)$$

We can compute the transformation of the Hamiltonian and momentum under the boost directly and then this will tell us their bracket with the boost generators. Considering that the action is required to have symmetry under Lorentz boosts, we can equivalently use S evaluated at the boosted coordinates or S evaluated at the unboosted coordinates but with those unboosted coordinates rewritten in terms of the boosted ones. Using the second automatically makes S' , the action which gives the equations of motion for the boosted coordinates, equal to S . Then, using equations (1.9.100) and (1.9.101) together with the fact that the action is Lorentz invariant we have:

$$\mathcal{H}' = \frac{\partial t}{\partial t'} \mathcal{H} - \frac{\partial \vec{x}}{\partial t'} \cdot \vec{p}, \quad \vec{p}' = -\frac{\partial t}{\partial \vec{x}'} \mathcal{H} + \frac{\partial \vec{x}}{\partial \vec{x}'} \cdot \vec{p} \quad (4.3.29)$$

We know how the boosted coordinates depend on the unboosted coordinates. Conveniently, the inverse of a boost by $\vec{v}$ is a boost by $-\vec{v}$. So, we have from Theorem 4.1 that:

$$\frac{\partial t'}{\partial t} = \gamma \implies \frac{\partial t}{\partial t'} = \gamma, \quad \frac{\partial \vec{x}'}{\partial t} = \gamma \vec{v} \implies \frac{\partial \vec{x}}{\partial t} = -\gamma \vec{v}, \quad (4.3.30)$$

$$\frac{\partial t'}{\partial \vec{x}} = \gamma \frac{\vec{v}}{c^2} \implies \frac{\partial t}{\partial \vec{x}'} = -\gamma \frac{\vec{v}}{c^2}, \quad \frac{\partial \vec{x}'}{\partial \vec{x}} = \mathbb{1} + (\gamma - 1) \vec{v}_v \vec{v}_v \implies \frac{\partial \vec{x}}{\partial \vec{x}'} = \mathbb{1} + (\gamma - 1) \vec{v}_v \vec{v}_v. \quad (4.3.31)$$

Inserting these, the Hamiltonian and momentum transform as:

$$\mathcal{H}' = \gamma(\mathcal{H} + \vec{v} \cdot \vec{p}), \quad \vec{p}' = (\mathbb{1} + (\gamma - 1) \vec{v}_v \vec{v}_v) \cdot \vec{p} + \gamma \frac{\mathcal{H}}{c^2} \vec{v}. \quad (4.3.32)$$

Now we can calculate the brackets of the momentum and Hamiltonian with the boost generators:

$$\left. \frac{d\mathcal{H}}{d\vec{v}} \right|_0 = \vec{p} \implies \{\mathcal{H}, \vec{K}\} = c\vec{p} \quad (4.3.33)$$

$$\left. \frac{d\vec{p}}{d\vec{v}} \right|_0 = \frac{\mathcal{H}}{c^2} \mathbb{1} \implies \{\vec{p}, \vec{K}\} = \frac{\mathcal{H}}{c} \mathbb{1}. \quad (4.3.34)$$

Perhaps surprisingly, at least for now, the Hamiltonian (technically $\mathcal{H}/c$) and momentum transform into each other in the exact same way the coordinate displacements do by comparing equation (4.3.32) with theorem 4.1. Consequently, just like the proper time $d\tau^2 = dt^2 - \frac{|d\vec{x}|^2}{c^2}$ is Lorentz invariant, the combination $\mathcal{H}^2/c^2 - |\vec{p}|^2$ is also Lorentz invariant. For the case of the free particle, this combination just gives $m^2 c^2$ and

so just tells us the mass of the particle.

Now that we have the Hamiltonian/Lagrangian we can compute the Lorentz equations of motion. From theorem 4.2:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} = q \nabla (\dot{\vec{x}} \cdot \vec{A}) - q \nabla \phi, \quad \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} = \frac{m \dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} + q \vec{A} \quad (4.3.35)$$

$$\Rightarrow \boxed{\frac{d}{dt} \left(\frac{m \dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} \right) = q (\vec{E} + \dot{\vec{x}} \times \vec{B})}. \quad (4.3.36)$$

By comparing the Galilean equation of motion (equation (2.6.12)) to the Lorentz equation of motion (equation (4.3.36)) we see that apparently the only effect of Lorentz symmetry over Galilean symmetry on the dynamics is a factor of γ on the inside of the time derivative. All this accomplishes is to keep the particle moving slower than c as the factor on the acceleration gets very large for speeds approaching c and thus causes ever reducing acceleration. However, we have yet to see if we can remove the effect of the field a particle produces on itself in the Lorentz theory like we did in the Galilean theory; that analysis is coming later this chapter.

I should warn you against a bad habit that has mostly fallen out of fashion but you will occasionally hear out in the wild. Some sources will call the mass m of the particle the “rest mass” and define the “relativistic mass” m_{rel} as γm where γ is the Lorentz factor exactly as it appears inside the time derivative in (4.3.36). Of course you can make up whatever words you want, the question is whether the definition is useful. The intent behind defining the “relativistic mass” m_{rel} is to hope that one can just recycle the results of nonrelativistic calculations by taking the final answer and replacing all m 's appearing in them with γm . This is motivated by the fact that this works for the linear momentum as $\vec{p}_{\text{Gal}} = m \dot{\vec{x}}$ and $\vec{p}_{\text{rel}} = \gamma m \dot{\vec{x}}$ for a free particle. However, this trick almost never works and often doesn't even make sense because γ is not constant for most systems. In this way the relativistic mass is not a useful construction or a good way to think about the relativistic theory. The mass m of a particle is just a constant parameter of that particle in relativity, exactly the way it is in the nonrelativistic theory. The reasons behind why some sources introduce the notion of relativistic mass are mostly sociological and have nothing to do with clean efficient physics⁴. Don't waste your time with “relativistic mass”.

Exercises

Problem 4.7: I mean it; relativistic mass is stupid. Consider a Lorentz point particle of mass m moving under the influence of an external force $\vec{F}$.

- (a) Show, using the Lorentz particle Lagrangian and the definition of external force, that the relativistic version of Newton's second law is:

$$\frac{d}{dt} \left(\frac{m \dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}} \right) = \vec{F}$$

or equivalently:

$$\gamma m \ddot{\vec{x}} + \frac{\gamma^3}{c^2} m \dot{\vec{x}} \dot{\vec{x}} \cdot \ddot{\vec{x}} = \vec{F}$$

where γ be the usual Lorentz factor in terms of the particle's velocity $\dot{\vec{x}}$.

- (b) Let $F_{\parallel}$ be the component of $\vec{F}$ in the direction of $\dot{\vec{x}}$ and $\vec{F}_{\perp}$ be the part of $\vec{F}$ orthogonal to $\dot{\vec{x}}$. Let $a_{\parallel}$ and $\vec{a}_{\perp}$ be the similarly decomposed parts of the particle's acceleration vector $\ddot{\vec{x}}$. Show that the parallel and perpendicular components of the relativistic version of Newton's second law give:

$$\gamma^3 m a_{\parallel} = F_{\parallel}, \quad \gamma m \vec{a}_{\perp} = \vec{F}_{\perp}.$$

⁴Because of the sociological adoration of Einstein's $E = mc^2$, which one can see from our Hamiltonian is the energy of a free particle at rest, there are some who like to elevate this formula to higher generality by changing the definition of mass so that it is true for a moving particle as well. We can see from our Hamiltonian that for a free particle $E = \gamma mc^2$, which motivates the definition of the relativistic mass as γm . However, this is silly. Mass is a Lorentz invariant parameter of a particle that gets fit to data. All electrons have the same mass. Energy is not Lorentz invariant and the energy of any individual particle is not constant. It is profoundly unhelpful to take something constant and Lorentz invariant and make it more unmanageable by always writing it in terms of nonconstant and non-Lorentz invariant stuff.

- (c) If relativistic mass $m_{\text{rel}}(t) = \gamma(t)m$ were a useful concept (it isn't), one would want it to be true that where mass m appears in nonrelativistic equations, m_{rel} should appear in the relativistic equation and capture the relativistic corrections. By looking at the relativistic version of Newton's second law, explain how this fails for literally the first example one is liable to try. If you just go around replacing m by γm and pretend you are doing relativity, you will be disastrously wrong dangerously often. One could go really crazy and say well relativistic mass makes sense, it is just different in different directions, $\gamma^3 m$ is the "parallel relativistic mass" and γm is the "perpendicular relativistic mass". Of course, if you go do some other calculation involving mass, it is generally untrue that the final answer will be able to be expressed in any simple way in terms of these replacements, and the final answer may "suggest" an equally convoluted mass redefinition in order to make it look like the nonrelativistic answer. It is true that you can redefine words to mean whatever you want, but if you want to save yourself a headache you should keep your definitions simple and consistent. Mass is an invariant property of an object. Don't break your new discoveries (Lorentz boost symmetry) out of allegiance to a dead theory (Galilean boost symmetry).

Problem 4.8: Relativistic particle in uniform electric field. Consider the Lagrangian or Hamiltonian in theorem 4.2 with the potentials given so that there is a uniform electric field and no magnetic field.

- (a) Let $\vec{v}_0$ be the velocity at $t = 0$ and $\gamma_0 = \gamma(\vec{v}_0)$. Show that the velocity of the charge is given as a function of time by:

$$\dot{\vec{x}} = c \frac{q\vec{E}t + \gamma_0 m \vec{v}_0}{\sqrt{q^2 |\vec{E}|^2 t^2 + 2q\gamma_0 m \vec{v}_0 \cdot \vec{E}t + m^2 c^2 \gamma_0^2}}.$$

- (b) Show that in the limit $t \rightarrow \infty$ the charge's velocity approaches c .
(c) Show that to the lowest order in powers of $\dot{\vec{x}}/c$, the velocity matches the Galilean result.
(d) Show that there exists a time t_0 so that the velocity of the charge in the direction of $\vec{E}$ vanishes. For the rest of this question, define the time $t = 0$ to be this t_0 . Show that after doing so, $\vec{v}_0 \cdot \vec{E} = 0$.
(e) Let the direction in which $q\vec{E}$ points be the y direction and let the direction in which $\vec{v}_0$ points be the x direction (without loss of generality, by the previous part). As well, let $v_0 = |\vec{v}_0|$ and $E = |\vec{E}|$. Show that the velocity equations become:

$$\frac{dx}{dt} = \frac{\gamma_0 m c v_0}{\sqrt{m^2 c^2 \gamma_0^2 + q^2 E^2 t^2}}, \quad \frac{dy}{dt} = \frac{c q E t}{\sqrt{m^2 c^2 \gamma_0^2 + q^2 E^2 t^2}}, \quad \frac{dz}{dt} = 0.$$

- (f) Let the origin of our coordinate system be the position of the charge at $t = 0$. Integrate the velocity equations to show that the position of the charge is given as a function of time by:

$$\begin{aligned} x(t) &= \frac{m c \gamma_0 v_0}{q E} \ln \left(\frac{q E t}{m c \gamma_0} + \sqrt{1 + \frac{q^2 E^2 t^2}{m^2 c^2 \gamma_0^2}} \right) \\ y(t) &= \frac{c}{q E} \left(\sqrt{q^2 E^2 t^2 + m^2 c^2 \gamma_0^2} - m c \gamma_0 \right) \\ z(t) &= 0. \end{aligned}$$

- (g) Show that the path the charge makes in space is described by the equation:

$$y = \frac{m c^2 \gamma_0}{q E} \left(\cosh \left(\frac{q E x}{m c \gamma_0 v_0} \right) - 1 \right).$$

Thus instead of a parabolic solution in a uniform field as in the Galilean case, the charge moves in the shape of a catenary in the Lorentz theory.

Problem 4.9: Relativistic particle in uniform magnetic field. Consider the Lagrangian or Hamiltonian in theorem 4.2 with the potentials given so that there is a uniform magnetic field and no electric field.

- (a) Show either directly from the equation of motion or from time translational symmetry and the corresponding conservation of energy that the speed of the charge does not change with time (and thus that γ does not change with time either). Notice in fact that this result is insensitive to our restriction that the field be uniform.
(b) Show that the component of the velocity of the charge in the direction of the magnetic field is constant.
(c) Let the direction in which the magnetic field points be the z direction and define the origin of our

coordinate system as the location of the charge at $t = 0$. Let v_{x0}, v_{y0}, v_{z0} be the components of the initial velocity of the charge and let $\omega = \sqrt{\frac{qB}{\gamma m}}$. Show that the position of the charge as a function of time is given by:

$$\begin{aligned} x(t) &= \frac{v_{x0}}{\omega} \sin(\omega t) + \frac{v_{y0}}{\omega} (1 - \cos \omega t) \\ y(t) &= \frac{v_{y0}}{\omega} \sin(\omega t) - \frac{v_{x0}}{\omega} (1 - \cos \omega t) \\ z(t) &= v_{z0} t. \end{aligned}$$

Thus, exactly like in the Galilean case, in the Lorentz theory a charge in a uniform magnetic field moves in the shape of a helix.

Problem 4.10: ★ Poincare Algebra. Consider a free Lorentz particle.

- (a) Using Noether's theorem, show that the energy is given by the Hamiltonian and that the linear momentum is given simply by its conjugate momentum.
 (b) Using Noether's theorem, show that its angular momentum is given by:

$$\vec{L} = \vec{x} \times \vec{p}$$

and that the vector which generates Lorentz boosts $\vec{K}$ is given by

$$\vec{K} = c\vec{p}t - \frac{\mathcal{H}}{c}\vec{x}.$$

- (c) Using these expressions for $\mathcal{H}$, $\vec{p}$, $\vec{L}$, and $\vec{K}$, show that for our free Lorentz invariant particle the full system of Poisson brackets for our symmetry generators is:

$$\begin{array}{lll} \{\mathcal{H}, \vec{p}\} = 0 & \{p_a, p_b\} = 0 & \{L_a, L_b\} = \epsilon_{ab}^c L_c \\ \{\mathcal{H}, \vec{L}\} = 0 & \{p_a, L_b\} = \epsilon_{ab}^c p_c & \{L_a, K_b\} = \epsilon_{ab}^c K_c \\ \{\mathcal{H}, \vec{K}\} = c\vec{p} & \{p_a, K_b\} = \frac{\mathcal{H}}{c} \delta_{ab} & \{K_a, K_b\} = -\epsilon_{ab}^c L_c. \end{array}$$

This system of brackets is called the Poincare algebra and it will be of great interest to us in our later studies.

Problem 4.11: Conservation law of Lorentz Boost Symmetry. By Noether's theorem, the generator of any continuous symmetry of our theory is conserved. We have already found the conservation laws corresponding to time translation (Energy), space translation (Linear Momentum), and rotation (Angular Momentum) but there is one more continuous symmetry we have: Lorentz Boost Symmetry. In this problem we will explore its conservation law. Consider a theory of N free Lorentz particles:

$$\mathcal{L} = \sum_{n=1}^N \left(-m_n c^2 \sqrt{1 - \frac{|\dot{\vec{x}}_n|^2}{c^2}} \right)$$

so that the total theory has Lorentz boost symmetry.

- (a) Show by direct calculation that under a Lorentz boost applied at time t_b the derivative of the Action under the transformation is:

$$\vec{\partial} S = c \frac{dS}{d\vec{v}} \Big|_{\vec{v}=0} = c \frac{d}{d\vec{v}} \int_{t_b}^t \mathcal{L} dt \Big|_{\vec{v}=0} = 0.$$

- (b) Show using Noether's theorem that the generator of the symmetry is given by:

$$\vec{K} = \sum_{n=1}^N \left(c\vec{p}_n t - \frac{E_n}{c} \vec{x}_n \right)$$

where E_n is the energy of just particle n (its free Hamiltonian). This $\vec{K}$ is called the “dynamic energy moment” of the system.

- (c) Using the conservation laws established, show that the center of momentum velocity:

$$\vec{v}_{\text{COM}} \stackrel{\text{def}}{=} \frac{\sum_{n=1}^N E_n \dot{\vec{x}}_n}{\sum_{n=1}^N E_n} = \frac{c^2 \vec{P}}{E}$$

is conserved (where $\vec{P}$ is the total linear momentum of the system and E is the total energy). Thus, Lorentz Boost Symmetry ultimately implies (together with our other conservation laws) that the center of momentum of the system will move at constant velocity. This is called the center of momentum velocity because as one can see it vanishes in the reference frame in which the total linear momentum is 0. So, it is the velocity at which the system is moving with respect to the total linear momentum = 0 frame.

Problem 4.12: Relativistic Central Motion. Consider the Lagrangian or Hamiltonian in theorem 4.2 with spherically constant spherically symmetric potentials.

- (a) Show that spherical symmetry requires that there exists a gauge so that:

$$\vec{A} = 0, \quad \phi(t, \vec{x}) = \frac{U(r)}{q}$$

for some function $U(r)$ (the factor of q is simply a nice choice for this question). We will work in this gauge for the rest of the question.

- (b) Show that the angular momentum of the particle is conserved and that this implies that the plane spanned by the position and velocity of remains constant in time and so that the motion of the particle lies in a plane for all time.
- (c) Parameterize the plane of motion of the particle by polar coordinates $\vec{x} = (r \cos \varphi, r \sin \varphi)$. Show that in these coordinates the Lagrangian becomes:

$$\mathcal{L} = -mc^2 \sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}} - U(r).$$

Show then that the equations of motion are:

$$\frac{d}{dt} \left(\frac{m\dot{r}}{\sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}}} \right) = -\frac{\partial U}{\partial r} + \frac{mr\dot{\varphi}^2}{\sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}}}, \quad \frac{d}{dt} \left(\frac{mr^2\dot{\varphi}}{\sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}}} \right) = 0.$$

- (d) Let E be the conserved energy of the particle and L be the conserved angular momentum of the particle. Show that:

$$E = \frac{mc^2}{\sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}}} + U(r), \quad L = \frac{mr^2\dot{\varphi}}{\sqrt{1 - \frac{\dot{r}^2 + r^2 \dot{\varphi}^2}{c^2}}}$$

$$\frac{d}{dt} \left(\frac{E - U}{c^2} \dot{r} \right) = \frac{c^2 L^2}{(E - U)r^3} - \frac{\partial U}{\partial r}, \quad \dot{\varphi} = \frac{c^2 L}{(E - U)r^2}.$$

These are the equations of motion for a relativistic particle in a central potential.

Problem 4.13: Relativistic Binet Equation. Consider the equations of motion for a relativistic particle in a central potential. Define $s = \frac{1}{r}$ and rewrite the equation of motion for $r(t)$ as an equation for $s(\varphi)$ by using the equation of motion for $\varphi(t)$. Show that it gives:

$$\frac{d^2 s}{d\varphi^2} + s + \frac{E - U}{c^2 L^2} \frac{\partial U}{\partial s} = 0.$$

This is the relativistic generalization of the Binet equation.

Problem 4.14: Relativistic Kepler Problem. Consider a particle moving under the influence of the Keplerian potential $U(r) = -\frac{\alpha}{r}$ for a constant α .

- (a) Show using energy conservation that at the turning points (times at which $\dot{r} = 0$) of the trajectory:

$$(E - U)^2 = m^2 c^4 + \frac{c^2 L^2}{r^2}.$$

- (b) Explicitly solve the relativistic Binet equation and show that for appropriate choice of the definition of φ , the trajectory is given by:

$$\frac{1}{r(\varphi)} = \frac{\alpha E}{c^2 L^2 - \alpha^2} + \sqrt{\frac{c^2 L^2 E^2}{(c^2 L^2 - \alpha^2)^2} - \frac{m^2 c^4}{c^2 L^2 - \alpha^2}} \cos \left(\varphi \sqrt{1 - \frac{\alpha^2}{c^2 L^2}} \right).$$

It is possible to use this solution to find relativistic generalizations of Kepler's laws.

- (c) Show that unlike the nonrelativistic Kepler problem, the relativistic Kepler problem orbits precess and the orbits don't perfectly close. Define the precession Θ of the orbit as the difference in values of φ at which the maximum value of r is achieved on consecutive orbits minus 2π . Show that the precession of the relativistic Kepler orbit is:

$$\Theta = 2\pi \left(\frac{1}{\sqrt{1 - \frac{\alpha^2}{c^2 L^2}}} - 1 \right).$$

4.4 Lorentz Transformation of the Fields

Now that we know the particle Lagrangian, we again have to find the Lagrangian for the potentials. Hopefully, we will recover equation (3.9.3) as the implications of that Lagrangian set us down this whole path to begin with. Just as before, we consider $\mathfrak{L}_0$, the Lagrangian density for just the potentials as in equation (3.3.3) and Taylor expand it for weak fields. Applying time and space translation symmetry, gauge symmetry, and rotational symmetry in section 3.3 we found that ultimately, before having imposed any notion of boost symmetry, the Lagrangian density becomes equation (3.3.72):

$$\mathfrak{L}_0 = \rho_0 \phi + \frac{\kappa}{2} \vec{A} \cdot \vec{B} + \frac{\epsilon}{2} |\vec{E}|^2 - \frac{1}{2\mu} |\vec{B}|^2 \quad (4.4.1)$$

for some constants ρ_0 , κ , ϵ , and μ . Now we need to impose Lorentz boost symmetry on this Lagrangian density. To do so, we need to understand how the potentials and fields transform. For this, we can simply recycle equations (3.3.9) and (3.3.10):

$$\phi' = \frac{\partial \rho}{\partial \rho'} \phi - \frac{\partial \vec{J}}{\partial \rho'} \cdot \vec{A}, \quad \vec{A}' = -\frac{\partial \rho}{\partial \vec{J}'^T} \phi + \frac{\partial \vec{J}'^T}{\partial \vec{J}'^T} \vec{A}. \quad (4.4.2)$$

Next we need how the charge and current densities transform under a Lorentz boost. We can compute this directly from their definitions. It is easiest to do this by first writing ρ and $\vec{J}$ writing them in a new form. Starting with ρ :

$$\rho(t, \vec{x}) = \sum_n q_n \delta(\vec{x} - \vec{x}_n(t)) = \sum_n q_n \int_{-\infty}^{\infty} \delta(t - t') \delta(\vec{x} - \vec{x}_n(t')) dt' \quad (4.4.3)$$

Let the notation $X = (t, \vec{x})$ indicate an event in spacetime. Using the definition of the proper time, for a given particle we can actually relate the proper time experienced by that particle to its motion in a given frame:

$$d\tau^2 = dt^2 - \frac{|d\vec{x}|^2}{c^2} \implies \frac{d\tau}{dt} = \sqrt{1 - \frac{|\dot{\vec{x}}|^2}{c^2}}. \quad (4.4.4)$$

This gives $\tau(t)$ when integrated which when inverted to find $t(\tau)$ allows us to parameterize the spacetime position of a particle in terms of proper time: $X(\tau) = (t(\tau), \vec{x}(\tau))$. Rewrite ρ in terms of this parameterization:

$$\rho(X) = \sum_n q_n \int_{-\infty}^{\infty} \delta(t - t_n(\tau)) \delta(\vec{x} - \vec{x}_n(\tau)) \frac{dt_n}{d\tau} d\tau \quad (4.4.5)$$

$$\implies \rho(X) = \sum_n q_n \int_{-\infty}^{\infty} \delta(X - X_n(\tau)) \frac{dt_n}{d\tau} d\tau. \quad (4.4.6)$$

Now put $\vec{J}$ into the same form:

$$\vec{J}(t, \vec{x}) = \sum_n q_n \dot{\vec{x}}_n(t) \delta(\vec{x} - \vec{x}_n(t)) = \sum_n q_n \int_{-\infty}^{\infty} \dot{\vec{x}}_n(t') \delta(t - t') \delta(\vec{x} - \vec{x}_n(t')) dt' \quad (4.4.7)$$

$$= \sum_n q_n \int_{-\infty}^{\infty} \delta(t - t_n(\tau)) \delta(\vec{x} - \vec{x}_n(\tau)) \frac{d\vec{x}_n}{dt_n} \frac{dt_n}{d\tau} d\tau \quad (4.4.8)$$

$$\implies \vec{J}(X) = \sum_n q_n \int_{-\infty}^{\infty} \delta(X - X_n(\tau)) \frac{d\vec{x}_n}{d\tau} d\tau. \quad (4.4.9)$$

From (4.4.6) and (4.4.9) we can compute the Lorentz transformations directly. Let $X' = \hat{L}X$ be our boosted point where $\hat{L}$ is our boost transformation. Then:

$$\rho'(X') = \sum_n q_n \int_{-\infty}^{\infty} \delta(\hat{L}(X - X_n(\tau))) \frac{dt'_n}{d\tau} d\tau. \quad (4.4.10)$$

Recall that the Dirac delta satisfies the property:

$$\delta(\hat{M}X) = \frac{\delta(X)}{\det(\hat{M})} \quad (4.4.11)$$

and that $\det(\hat{L}) = 1$ from Theorem 4.1. Then:

$$\rho'(X') = \sum_n q_n \int_{-\infty}^{\infty} \frac{\delta(X - X_n(\tau))}{\det(\hat{L})} \frac{dt'_n}{d\tau} d\tau \quad (4.4.12)$$

$$= \sum_n q_n \int_{-\infty}^{\infty} \delta(X - X_n(\tau)) \left(\gamma \frac{dt}{d\tau} + \frac{\vec{v}}{c^2} \cdot \frac{d\vec{x}}{d\tau} \right) d\tau. \quad (4.4.13)$$

Now using our expressions for ρ and $\vec{J}$:

$$\rho'(X') = \gamma \rho(X) + \gamma \frac{\vec{v} \cdot \vec{J}(X)}{c^2} \quad (4.4.14)$$

Proceeding similarly for $\vec{J}$:

$$\vec{J}'(X') = \sum_n q_n \int_{-\infty}^{\infty} \delta(\hat{L}(X - X_n(\tau))) \frac{d\vec{x}'_n}{d\tau} d\tau = \sum_n q_n \int_{-\infty}^{\infty} \delta(X - X_n(\tau)) \frac{d\vec{x}'_n}{d\tau} d\tau \quad (4.4.15)$$

$$= \sum_n q_n \int_{-\infty}^{\infty} \delta(X - X_n(\tau)) \left((\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \frac{d\vec{x}_n}{d\tau} + \gamma \vec{v} \frac{dt_n}{d\tau} \right) d\tau. \quad (4.4.16)$$

Finally then:

$$\vec{J}'(X') = (\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \vec{J}(X) + \gamma \vec{v} \rho(X). \quad (4.4.17)$$

So we see that up to accounting for the correspondence between the boosted and unboosted point of evaluation, the charge density and current density transform exactly like the differentials $dt, d\vec{x}$. Next we compute the transformations of the potentials. To do so, it is useful to remember that the inverse of the boost by $\vec{v}$ is the boost by $-\vec{v}$ and so:

$$\rho = \gamma \left(\rho' - \frac{\vec{v} \cdot \vec{J}'}{c^2} \right), \quad \vec{J} = (\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \vec{J}' - \gamma \rho' \vec{v}. \quad (4.4.18)$$

Then, the potentials transform as:

$$\phi' = \gamma \left(\phi + \vec{v} \cdot \vec{A} \right), \quad \vec{A}' = (\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \vec{A} + \frac{\vec{v}}{c^2} \phi. \quad (4.4.19)$$

Next we compute the transformation properties of the differential operators using the differentials:

$$\frac{\partial}{\partial t'} = \gamma \frac{\partial}{\partial t} - \gamma \vec{v} \cdot \nabla, \quad \nabla' = (\mathbb{1} + (\gamma - 1)\vec{v}_v \vec{v}_v) \cdot \nabla - \gamma \frac{\vec{v}}{c^2} \frac{\partial}{\partial t}. \quad (4.4.20)$$

Together we now have all of the ingredients necessary to compute the transformation properties of the electric and magnetic fields. With a bit of algebra, we find:

$$\vec{E}' = \gamma \vec{E} - (\gamma - 1)\vec{v}_v \vec{v}_v \cdot \vec{E} - \gamma \vec{v} \times \vec{B}, \quad \vec{B}' = \gamma \vec{B} - (\gamma - 1)\vec{v}_v \vec{v}_v \cdot \vec{B} + \frac{\gamma}{c^2} \vec{v} \times \vec{E}. \quad (4.4.21)$$

We can finally return to the Lagrangian density. Because it is the Lagrangian per unit volume and the Lagrangian is the time derivative of the action, the action is the integral of the Lagrangian density over spacetime:

$$S = \int_0^{t_f} \mathcal{L} dt = \int_{\mathbb{T}} \mathfrak{L} d\mathbb{S} dt = \int_{\mathbb{T}} \mathfrak{L} d\mathbb{T}. \quad (4.4.22)$$

The coordinate invariance of the action and of the spacetime volume element thus imply the invariance of the Lagrangian density. We can directly impose Lorentz boost symmetry on the Lagrangian density in equation (4.4.1). Because it has to have boost symmetry for all values of the boost velocity, we can simply Taylor expand in powers of the velocity and enforce the symmetry at each order in $\vec{v}$. Due to the exponentiation property of the boost, enforcing at linear order actually guarantees that there is symmetry at all orders in the velocity. Applying this:

$$\mathfrak{L}'_0 = \rho_0 \phi' + \frac{\kappa}{2} \vec{A}' \cdot \vec{B}' + \frac{\epsilon}{2} |\vec{E}'|^2 - \frac{|\vec{B}'|^2}{2\mu} \quad (4.4.23)$$

$$= \mathfrak{L}_0 + \rho_0 \vec{v} \cdot \vec{A} + \frac{\kappa}{2c^2} \phi \vec{v} \cdot \vec{B} + \frac{\kappa}{2c^2} \vec{v} \cdot (\vec{E} \times \vec{A}) + \left(\epsilon - \frac{1}{\mu c^2} \right) \vec{v} \cdot (\vec{E} \times \vec{B}) + \mathcal{O}(v^2). \quad (4.4.24)$$

Then, in order for this to be a symmetry, the added terms must be removable by surface terms (at each order in $\vec{v}$):

$$\rho_0 \vec{v} \cdot \vec{A} + \frac{\kappa}{2c^2} \phi \vec{v} \cdot \vec{B} + \frac{\kappa}{2c^2} \vec{v} \cdot (\vec{E} \times \vec{A}) + \left(\epsilon - \frac{1}{\mu c^2} \right) \vec{v} \cdot (\vec{E} \times \vec{B}) = \frac{df_0}{dt} + \nabla \cdot \vec{f}. \quad (4.4.25)$$

However, $\vec{E} \times \vec{B} = -\nabla \phi \times (\nabla \times \vec{A}) - \vec{A} \times (\nabla \times \vec{A})$ and so the left hand side here contains $\partial_a \phi \partial_b A_c$ terms.

From the general surface terms which get added, as shown in (3.3.56), the surface terms cannot produce a $\partial_a \phi \partial_b A_c$ (at least, not without also producing other higher derivatives terms which are not present here). Therefore, the only way the $\vec{E} \times \vec{B}$ term can be a surface term is if its coefficient is 0:

$$\epsilon - \frac{1}{\mu c^2} = 0 \implies \mu = \frac{1}{\epsilon c^2}. \quad (4.4.26)$$

Then, matching the $\dot{\vec{A}}$ term which appears through the $\vec{E} \times \vec{A}$ term on the left hand side against the $\dot{\vec{A}}$ term which appears on the right hand side of equation (3.3.56):

$$\frac{\kappa}{2c^2} \vec{v} \cdot (\vec{A} \times \dot{\vec{A}}) = \frac{\partial F_0}{\partial \vec{A}} \cdot \dot{\vec{A}} \implies \frac{\partial F_0}{\partial \vec{A}} = \frac{\kappa}{2c^2} \vec{v} \times \vec{A} \quad (4.4.27)$$

$$\implies \frac{\partial^2 F_0}{\partial A_a \partial A_b} = -\frac{\kappa}{2c^2} \epsilon^{abc} v_c. \quad (4.4.28)$$

The left hand side is symmetric in interchanging a and b whereas the right hand side is antisymmetric under the same interchange. This is only possible if both are 0. Thus, we must have $\kappa = 0$. Then, (4.4.25) only leaves the $\rho_0 \vec{v} \cdot \vec{A}$ term to be matched. However, to cancel this term the functions F_0 or $\vec{F}$ would have to depend on $\vec{A}$ and in doing so would produce terms which depend on the derivatives of $\vec{A}$ which as we have seen are not present. Thus, this term must be 0 as well in order to be a surface term. Thus, $\rho_0 = 0$. Together then, after applying Lorentz boost symmetry, the Lagrangian density for the potentials when isolated becomes:

$$\mathfrak{L}_0 = \frac{\epsilon}{2} (|\vec{E}|^2 - c^2 |\vec{B}|^2). \quad (4.4.29)$$

Recall from section 3.7 that for electrostatics $\epsilon = \epsilon_0$ is known to be positive because charges of the same sign repel each other and that by choosing our unit of charge, we can impose $\epsilon_0 = 1$. For now we will leave in factors of ϵ_0 for reference sake in comparing to sources in SI units, but later we will set $\epsilon_0 = 1$ permanently. Thus, the free Lagrangian density for the potentials becomes:

$$\boxed{\mathfrak{L}_0 = \frac{\epsilon_0}{2} (|\vec{E}|^2 - c^2 |\vec{B}|^2).} \quad (4.4.30)$$

This is precisely the part of the Lagrangian density which only depends on the potentials coming from equation (3.9.3) and so in fact our original risky leap to consider this new boost symmetry paid off and gave a self consistent theory. Notice as well that unlike in the Galilean case, we did not assume parity symmetry. However, one can see by a quick calculation that in fact this Lagrangian density is parity symmetric anyway. So, in this theory parity symmetry is automatic and we do not add parity symmetry as an independent assumption.

Exercises

Problem 4.15: Parallel and Perpendicular Transformation Laws. Let $\vec{E}_{\parallel}$ and $\vec{B}_{\parallel}$ be the projections of $\vec{E}$ and $\vec{B}$ onto the boost direction $\vec{v}$ in a Lorentz boost and let $\vec{E}_{\perp} = \vec{E} - \vec{E}_{\parallel}$ and $\vec{B}_{\perp} = \vec{B} - \vec{B}_{\parallel}$. Show that under Lorentz boost these pieces transform according to:

$$\vec{E}'_{\parallel} = \vec{E}_{\parallel}, \quad \vec{E}'_{\perp} = \gamma(\vec{E}_{\perp} - \vec{v} \times \vec{B}_{\perp}), \quad \vec{B}'_{\parallel} = \vec{B}_{\parallel}, \quad \vec{B}'_{\perp} = \gamma\left(\vec{B}_{\perp} + \frac{1}{c^2} \vec{v} \times \vec{E}_{\perp}\right).$$

Problem 4.16: Relativistic Particle in a uniform Electric and Magnetic Field. Consider the Lagrangian or Hamiltonian in Theorem 4.2 with the potentials given so that there is a uniform electric field $\vec{E}$ and a uniform magnetic field $\vec{B}$ satisfying $\vec{E} \cdot \vec{B} = 0$.

- Suppose that $|\vec{E}| < c|\vec{B}|$. Show that there exists a Lorentz boost so that in the boosted frame $\vec{E}' = 0$. In that frame solve the equations of motion for the charge. Then, boost back to our original frame to find the solution to the equation of motion. (You will have to write the solution in the original frame implicitly; it cannot be solved in Cartesian coordinates explicitly.)
- Suppose that $|\vec{E}| > c|\vec{B}|$. Show that there exists a Lorentz boost so that in the boosted frame $\vec{B}' = 0$. In that frame solve the equations of motion for the charge. Then, boost back to our original frame to find the solution to the equation of motion. You similarly will have to leave your answer implicit. In order to see how to solve the relativistic particle in a uniform electric and magnetic field for fields of arbitrary strength and without needing to assume $\vec{E} \cdot \vec{B} = 0$ or leave your answer implicit, stick around until the end of the chapter.

4.5 Maxwell's Equations

We have arrived at the Lagrangian proposed in equation (3.9.3) as the unique one at this order of expansion in powers of the fields which is consistent with Lorentz symmetry:

Theorem 4.3: Lagrangian for Maxwell's Equations

The lowest order Lorentz symmetric Lagrangian for the potentials $\phi, \vec{A}$ in background charge and current densities $\rho, \vec{J}$ is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-\rho\phi + \vec{J} \cdot \vec{A} + \frac{\epsilon_0}{2} \left(|\vec{E}|^2 - c^2 |\vec{B}|^2 \right) \right) d\mathbb{S}. \quad (4.5.1)$$

Here c is the Lorentz invariant speed of light.

Let's compute the field equations of motion from our Lagrangian:

$$\frac{\delta \mathcal{L}}{\delta \phi} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\phi}} \stackrel{!}{=} 0 \implies \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \quad (4.5.2)$$

$$\frac{\delta \mathcal{L}}{\delta \vec{A}} - \partial_t \frac{\delta \mathcal{L}}{\delta \dot{\vec{A}}} \stackrel{!}{=} 0 \implies \nabla \times \vec{B} = \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}. \quad (4.5.3)$$

These taken together with the constraints the potentials place on the fields make up what are called Maxwell's equations (the very same equations we found in section 3.9):

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \vec{B} = \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}. \quad (4.5.4)$$

Instead writing these directly in terms of the potentials we find:

$$\nabla \cdot \left(-\nabla \phi - \frac{\partial \vec{A}}{\partial t} \right) = \frac{\rho}{\epsilon_0}, \quad \nabla \times \left(\nabla \times \vec{A} \right) = \mu_0 \vec{J} + \frac{1}{c^2} \frac{\partial}{\partial t} \left(-\nabla \phi - \frac{\partial \vec{A}}{\partial t} \right). \quad (4.5.5)$$

(The middle two of Maxwell's equations, the Solenoid Law and Faraday's Law, are automatic from the potentials.) We know that this theory describes signals which propagate at the speed of light (from equations (3.9.10) and (3.9.15)) and so we may be able to coax these equations into the wave equation. Trying to do so with the first equation we find:

$$-\nabla^2 \phi - \frac{\partial}{\partial t} \nabla \cdot \vec{A} = \frac{\rho}{\epsilon_0} \quad (4.5.6)$$

$$\implies \left[\frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \frac{\rho}{\epsilon_0} + \frac{\partial}{\partial t} \left(\frac{1}{c^2} \frac{\partial \phi}{\partial t} + \nabla \cdot \vec{A} \right) \right]. \quad (4.5.7)$$

Hence we end up with a wave equation with an extra term on the right hand side. Doing the same to the vector equation:

$$\nabla \times (\nabla \times \vec{A}) = \nabla \nabla \cdot \vec{A} - \nabla^2 \vec{A} = \mu_0 \vec{J} - \frac{1}{c^2} \nabla \frac{\partial \phi}{\partial t} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} \quad (4.5.8)$$

$$\implies \left[\frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} = \mu_0 \vec{J} - \nabla \left(\frac{1}{c^2} \frac{\partial \phi}{\partial t} + \nabla \cdot \vec{A} \right) \right]. \quad (4.5.9)$$

And so the vector potential ends up satisfying the wave equation with a similar extra term.

So far, we have been working in an unspecified gauge for the potentials. There is a very convenient gauge, called Lorenz gauge, for solving for the potentials explicitly. Lorenz gauge is defined by setting the extra term in our wave equations to 0:

$$\frac{1}{c^2} \frac{\partial \phi}{\partial t} + \nabla \cdot \vec{A} \stackrel{!}{=} 0. \quad (4.5.10)$$

Let's see that it is possible to pick this gauge in general. Suppose we are in a gauge in which it is not true.

Then, making a gauge transformation:

$$\frac{\partial \phi'}{\partial t} + c^2 \nabla \cdot \vec{A}' = \frac{\partial}{\partial t} \left(\phi - \frac{\partial f}{\partial t} \right) + c^2 \nabla \cdot (\vec{A} + \nabla f) \quad (4.5.11)$$

$$= \frac{\partial \phi}{\partial t} + c^2 \nabla \cdot \vec{A} - \frac{\partial^2 f}{\partial t^2} + c^2 \nabla^2 f \stackrel{!}{=} 0 \quad (4.5.12)$$

$$\Rightarrow \frac{\partial f^2}{\partial t^2} - c^2 \nabla^2 f = \frac{\partial \phi}{\partial t} + c^2 \nabla \cdot \vec{A}. \quad (4.5.13)$$

Hence if we are in a gauge in which equation (4.5.10) is not true and we pick our gauge function f so that it satisfies the wave equation with the left hand side of equation (4.5.10) as the source then in our new gauge, equation (4.5.10) is true. We can always pick such a function by just solving the wave equation for f . And so, the Lorenz gauge exists in general and in that gauge the potentials have the equations of motion:

$$\frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi = \frac{\rho}{\epsilon_0}, \quad \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} = \mu_0 \vec{J}. \quad (4.5.14)$$

These are simply the wave equation, which we have already solved and so:

$$\phi(t, \vec{x}) = \int_{\mathbb{S}'} \frac{\rho \left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}' \right)}{4\pi\epsilon_0 |\vec{x} - \vec{x}'|} d\mathbb{S}', \quad \vec{A}(t, \vec{x}) = \int_{\mathbb{S}'} \frac{\mu_0 \vec{J} \left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}' \right)}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (4.5.15)$$

So the only difference between the solution to the Galilean equations of motion (the Poisson equation) and the Lorentz equations of motion (the wave equation) is that the sources are evaluated with a delay: they are evaluated at time $t - \frac{|\vec{x} - \vec{x}'|}{c}$. This simply accounts for the fact that a signal emitted at time $t' = t - \frac{|\vec{x} - \vec{x}'|}{c}$ at a point $\vec{x}'$ which travels at the speed c would reach the point $\vec{x}$ at time t .

Exercises

Problem 4.17: Jefimenko's Equations. Use equation (4.5.15) together with the definitions of $\vec{E}$ and $\vec{B}$ in terms of the potentials to show that the electric and magnetic fields for arbitrary charge and current distributions are given by:

$$\begin{aligned} \vec{E}(t, \vec{x}) &= \frac{1}{4\pi\epsilon_0} \int_{\mathbb{S}'} \left(\frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} \rho(t_d, \vec{x}') + \frac{1}{c} \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^2} \frac{\partial \rho}{\partial t}(t_d, \vec{x}') - \frac{1}{c^2} \frac{1}{|\vec{x} - \vec{x}'|} \frac{\partial \vec{J}}{\partial t}(t_d, \vec{x}') \right) d^3 \vec{x}' \\ \vec{B}(t, \vec{x}) &= \frac{\mu_0}{4\pi} \int_{\mathbb{S}'} \left(\vec{J}(t_d, \vec{x}') \times \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} + \frac{1}{c} \frac{\partial \vec{J}}{\partial t}(t_d, \vec{x}') \times \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^2} \right) d^3 \vec{x}' \end{aligned}$$

where $t_d = t - \frac{|\vec{x} - \vec{x}'|}{c}$ is called the delayed time. These results are called Jefimenko's equations.

Problem 4.18: Domain of validity of electrostatics and magnetostatics. It is important to understand the conditions under which we expect electrostatics and magnetostatics to hold as they have made many successful predictions.

- Recall that in electrostatics we have Gauss' law and that we can go to electrostatic gauge (meaning we can write $\vec{E} = -\nabla \phi$). Show then from the general Maxwell's equations that the equations of electrostatics are valid whenever the magnetic field does not depend on time.
- Recall that in magnetostatics we have Ampere's law with no additional term. Show from the general Maxwell's equations that the equations of magnetostatics are valid whenever the electric field does not depend on time.

Problem 4.19: Maxwell's Equations in Matter. We would like to model the reaction of the charges in matter to electric and magnetic fields. We have already written equations for a single charge and could generalize directly to N charges. However, in typical matter there are a truly unwieldy number of charges (say 10^{23} or more as we will see in chapter 5) and so this strategy is highly impractical. Instead, we want to find an approximate model for how the charges and currents in a material (called the bound charges and bound currents in that material) depend on the electric and magnetic fields they are experiencing. Typical matter is made of a large number of charge neutral atoms which we will label by an index. Each atom's charge distribution is generally very small compared to the distances between atoms and certainly it is much

smaller than the resolution of typical experiments. As such, it is warranted to describe any specific atom's charge distribution using the exterior multipole expansion. Because the atoms are charge neutral, ρ_b and $\vec{J}_b$ (where b is for bound) begin with dipole moments as the lowest multipole expansion. Because the higher moments are suppressed by powers of the atomic size divided by the atomic separation, we (and most others as well) only treat the response of matter at the level of dipoles and neglect higher moments. As well, there may be other charges in or on the matter which are not bound to the atoms comprising the bulk of the matter. These remaining charges are called “free charges” with densities $\rho_f(t, \vec{x})$ and $\vec{J}_f(t, \vec{x})$ so that by definition the total charge and current densities in the matter are given by:

$$\rho(t, \vec{x}) = \rho_b(t, \vec{x}) + \rho_f(t, \vec{x}), \quad \vec{J}(t, \vec{x}) = \vec{J}_b(t, \vec{x}) + \vec{J}_f(t, \vec{x}).$$

- (a) Consider a charge q at $\vec{y} + \ell \vec{n}(t)$ where $\ell > 0$ and $\vec{n}(t)$ is a unit vector and another charge $-q$ at $\vec{y} - \ell \vec{n}(t)$. Show that $\vec{\varphi}(t) = 2q\ell \vec{n}(t)$ is the electric dipole moment of the charge distribution. Take the limit $\ell \rightarrow 0$ keeping $\vec{\varphi}$ fixed. Show that the charge and current distributions due to the ideal electric dipole are:

$$\rho_{\text{dip}} = -\vec{\varphi} \cdot \nabla \delta(\vec{x} - \vec{y}), \quad \vec{J}_{\text{dip}} = \frac{d\vec{\varphi}}{dt} \delta(\vec{x} - \vec{y}).$$

- (b) Consider a circular current wire of radius R carrying current I with outward pointing normal vector $\vec{n}(t)$ (so that I travels counterclockwise around $\vec{n}$). Show that $\vec{m}(t) = \pi R^2 I \vec{n}(t)$ is the magnetic dipole moment of the charge distribution. Take the limit $R \rightarrow 0$ keeping $\vec{m}$ fixed. Show that the charge and current distributions due to the ideal magnetic dipole are:

$$\rho_{\text{magdip}} = 0, \quad \vec{J}_{\text{magdip}} = -\vec{m} \times \nabla \delta(\vec{x} - \vec{y}).$$

- (c) Now consider our model of matter as composed of electric and magnetic dipoles with the number density of atoms so great that one can reasonably approximate the distribution as continuous. This is reasonable if we are only studying the behavior of electric and magnetic fields on length scales much larger than the atomic separation, which is the typical case. Let $\vec{P}(t, \vec{x})$, called the **polarization** of the matter, be defined as the electric dipole moment per unit volume of the bound charges and let $\vec{M}(t, \vec{x})$, called the **magnetization** of the matter, be defined as the magnetic dipole moment per unit volume of the bound charges. Let $\mathbb{V}$ be the region occupied by the matter. Show using the results of the previous two parts that the bound charge density and bound current density in the matter are given by:

$$\rho_b(t, \vec{x}) = -\nabla \cdot \vec{P}(t, \vec{x}) + \int_{\partial \mathbb{V}} \vec{P}(t, \vec{x}') \delta(\vec{x} - \vec{x}') \cdot d\vec{A}'$$

$$\vec{J}_b(t, \vec{x}) = \frac{\partial \vec{P}}{\partial t}(t, \vec{x}) + \nabla \times \vec{M}(t, \vec{x}) + \int_{\partial \mathbb{V}} \delta(\vec{x} - \vec{x}') \vec{M}(t, \vec{x}') \times d\vec{A}'.$$

Thus, conclude that the bound charge density for points inside the volume of the matter, the bound surface charge density σ_b on the boundary of the volume, the bound current density for points inside the volume of the matter, and the bound surface current $\vec{K}_b$ on the boundary of the volume are given by:

$$\rho_b = -\nabla \cdot \vec{P}, \quad \sigma_b = \vec{P} \cdot \vec{n}, \quad \vec{J}_b = \frac{\partial \vec{P}}{\partial t} + \nabla \times \vec{M}, \quad \vec{K}_b = \vec{M} \times \vec{n}$$

where $\vec{n}$ is the outward pointing normal of the boundary surface.

- (d) Using our found expressions for the bound charge and current densities, show that Maxwell's equations can be rewritten as:

$$\nabla \cdot (\epsilon_0 \vec{E} + \vec{P}) = \rho_f, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \cdot \vec{B} = 0, \quad \nabla \times \left(\frac{\vec{B}}{\mu_0} - \vec{M} \right) = \vec{J}_f + \frac{\partial}{\partial t} (\epsilon_0 \vec{E} + \vec{P}).$$

This form motivates defining the the **Auxiliary Electric Field** $\vec{D}$ and **Auxiliary Magnetic Field**⁵

⁵Some sources, most notably [52], unfortunately refer to $\vec{H}$ as the magnetic field and call $\vec{B}$ the magnetic induction. This is a historical curiosity of language and results in some confusion among what is the “real” magnetic field. Make no mistake: $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields, derived always from the potentials $\phi, \vec{A}$. $\vec{D}$ and $\vec{H}$ are defined purely as a notational convenience and only enter in this specific model for matter. They are by no means “fundamental”. As well, it is $\vec{E}$ and $\vec{B}$ which appear in the equations of motion of any charges and so they are what are directly observed by any device which measures moving charges (such as any circuit).

$\vec{H}$ by:

$$\vec{D} \stackrel{\text{def}}{=} \epsilon_0 \vec{E} + \vec{P}, \quad \vec{H} \stackrel{\text{def}}{=} \frac{\vec{B}}{\mu_0} - \vec{M}.$$

With these definitions we arrive at the famous Maxwell's equations in matter:

$$\nabla \cdot \vec{D} = \rho_f, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{H} = \vec{J}_f + \frac{\partial \vec{D}}{\partial t}.$$

It should be made clear that Maxwell's equations in matter are a special case coming from a particular model of matter. They are strictly less general than the generic Maxwell's equations. As well, even with these equations, we are not yet done with our model. So far, we have no way to figure out $\vec{P}$ or $\vec{M}$. In order to have enough data to solve these differential equations, we need to study how to determine $\vec{P}$ and $\vec{M}$. An equation which determines either of these is called a constitutive relation for the matter.

Problem 4.20: Boundary Conditions in Matter. Consider the boundary of a matter filled region. Let $\vec{n}$ be the outward pointing unit vector of the matter at the point in question. Let $\vec{E}_{\text{in}}$ denote the limit of the electric field as one approaches the boundary of the matter from the inside and $\vec{E}_{\text{out}}$ denote the limit of the electric field as one approaches the boundary of the matter from the outside. As well, let $\vec{E}_{\parallel}$ denote the part of $\vec{E}$ tangential to the boundary (and so orthogonal to $\vec{n}$) and let $E_{\perp}$ denote the component of $\vec{E}$ normal to the boundary (and so in the $\vec{n}$ direction). Similarly define such notation for the other vector fields. Using the arguments from the previous electromagnetic boundary condition questions, show that boundary conditions satisfied across the boundary of the matter are:

$$\begin{aligned} D_{\text{out}\perp} - D_{\text{in}\perp} &= \sigma_f, & \vec{E}_{\text{out}\parallel} &= \vec{E}_{\text{in}\parallel}, \\ \vec{H}_{\text{out}\parallel} - \vec{H}_{\text{in}\parallel} &= \vec{K}_f \times \vec{n}, & B_{\text{out}\perp} &= B_{\text{in}\perp}. \end{aligned}$$

Problem 4.21: Modeling Matter. In this question we will give some basic reasoning on how one may model the polarization and magnetization for matter. We have already assumed matter is well approximated as consisting of densities of electric and magnetic dipoles. The fully general case would be that the polarization and magnetization in the matter depend on the entire history of the electric and magnetic fields experienced by the matter, which in principle one would determine by solving the equations of motion for all of the charges in the matter. But, this is plainly impractical. Instead, we try to apply some of the lessons learned when studying dipoles placed in external fields. This is all modeling; nothing here will be exact.

- Suppose that the magnetic dipoles in the material are close enough and strong enough to very strongly affect each other. Using the results of the dipole-dipole interaction and dipole in an external field questions, explain that one would then expect nearby dipoles to align with each other even when the external magnetic field is removed. Thus, in such a material, a permanent magnetization develops. This phenomenon is called ferromagnetism and only occurs in specific materials (iron, nickel, cobalt).
- Suppose that the electric dipoles in the material are close enough and strong enough to very strongly affect each other. Using the results of the dipole-dipole interaction and dipole in an external field questions, explain that one would then expect nearby dipoles to align with each other even when an external electric field is removed. Thus, in such a material, a permanent polarization develops. This phenomenon is called ferroelectricity. It is a more exotic phenomenon than ferromagnetism in its occurrence in daily life and only occurs in specific materials under the right conditions. Ferromagnetism is much more common than ferroelectricity for reasons we aren't yet fully equipped to describe. The short explanation is that it is possible for the fundamental building blocks of matter to carry a permanent magnetic dipole moment but not possible for them to carry a permanent electric dipole moment without violating parity/time-reversal symmetry.
- Suppose that the dipoles in the material do not have significant interaction with each other and that the dynamics of the dipoles occur on much shorter time scales than the scale over which the applied electric and magnetic fields vary. Explain why you would expect the polarization at $(t, \vec{x})$ to be a function of the electric field at $(t, \vec{x})$: $\vec{P}(\vec{E})$ and similarly the magnetization at $(t, \vec{x})$ to be a function of the magnetic field at $(t, \vec{x})$: $\vec{M}(\vec{B})$. Such matter is said to be "local". As well, argue that you would expect $\vec{P}(0) = \vec{M}(0) = 0$.
- Taking the assumptions of the previous part, show that for weak electric and magnetic fields for some

matrices $\hat{\chi}_e(t, \vec{x})$ and $\hat{\chi}_m(t, \vec{x})$:

$$\vec{P}(t, \vec{x}) = \epsilon_0 \hat{\chi}_e(t, \vec{x}) \vec{E}(t, \vec{x}) + \mathcal{O}(\vec{E}^2), \quad \vec{M}(t, \vec{x}) = \frac{1}{\mu_0} \hat{\chi}_m(t, \vec{x}) \vec{B}(t, \vec{x}) + \mathcal{O}(\vec{B}^2).$$

Whenever the first terms in these Taylor expansions are sufficiently good for describing the matter at hand, the matter is said to be local and “linear”. Here $\hat{\chi}_e$ is called the electric susceptibility tensor and $\hat{\chi}_m$ is called the magnetic susceptibility tensor⁶. Show that the susceptibilities defined here are unitless. One can have linear matter which is not local; as long as the polarization and magnetization are linear functionals of the electric and magnetic fields throughout the material the matter is linear. A particularly useful case of linear but not local matter is whenever instead of the polarization and magnetization being proportional to the electric and magnetic fields, the Fourier transforms of the polarization and magnetization are proportional to the Fourier transforms of the electric and magnetic fields. That is, we will also study:

$$\vec{P}(\omega, \vec{k}) = \hat{\chi}_e(\omega, \vec{k}) \vec{E}(\omega, \vec{k}), \quad \vec{M}(\omega, \vec{k}) = \frac{1}{\mu_0} \hat{\chi}_m(\omega, \vec{k}) \vec{B}(\omega, \vec{k}).$$

Such matter is called “Fourier-local” as it is “local in the Fourier domain”. The matrices appearing here are named the same as in the local case as there is no ambiguity given that the two cases only apply at the same time if the matrices are completely constant in which case they are the same anyway.

- (e) Consider local linear matter in which the susceptibilities do not depend on time or position. Such matter is called “homogeneous”. Show that such matter is also Fourier-local and that the Fourier susceptibilities and susceptibilities match. Thus, one may consider local linear homogeneous matter as a special case of Fourier-local linear matter.
- (f) Consider Fourier-local linear matter in which the internal dipoles are fully allowed to orient themselves in any direction without preference. Such matter is called “isotropic”. Explain based on the results of the dipole in an external field question then that one expects that the direction of $\vec{P}$ should be the same as $\vec{E}$ and that the direction of $\vec{M}$ should be the same as $\vec{B}$. From this, show that the susceptibility tensors can be written as multiples of the identity matrix and thus that for some scalar functions $\chi_e(\omega, \vec{k})$ and $\chi_m(\omega, \vec{k})$:

$$\vec{P}(\omega, \vec{k}) = \epsilon_0 \tilde{\chi}_e(\omega, \vec{k}) \vec{E}(\omega, \vec{k}), \quad \vec{M}(\omega, \vec{k}) = \frac{1}{\mu_0} \tilde{\chi}_m(\omega, \vec{k}) \vec{B}(\omega, \vec{k}).$$

Here we have used the notation that $\vec{E}$ symbolizes that it is both a vector (the arrow) and the Fourier transform (the squiggle) of $\vec{E}$. You may expect that the susceptibilities should be positive (and most often the electric susceptibility is) but there are some microscopic effects which can contribute negative contributions to either so that for some materials under some conditions either of the susceptibilities may be slightly negative. This is more common with the magnetic susceptibility, in which case it is called a diamagnetic material (and when it is positive it is a paramagnetic material). Because we will return to these assumptions, it is useful for brevity to define the notion of “simple” matter as matter which is local, linear, homogeneous, and isotropic. As well, it is useful to define “semisimple” matter as matter which is Fourier-local, linear, and isotropic. As we have shown, simple matter is a special case of semisimple matter.

Problem 4.22: Maxwell's Equations in Local Linear Matter. Consider local linear matter. Show that Maxwell's equations become:

$$\nabla \cdot (\hat{\epsilon} \vec{E}) = \rho_f, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times (\hat{\mu}^{-1} \vec{B}) = \vec{J}_f + \frac{\partial}{\partial t}(\hat{\epsilon} \vec{E})$$

where:

$$\hat{\epsilon} \stackrel{\text{def}}{=} \epsilon_0 (\mathbb{1} + \hat{\chi}_e), \quad \hat{\mu}^{-1} \stackrel{\text{def}}{=} \frac{1}{\mu_0} (\mathbb{1} - \hat{\chi}_m).$$

As well, show that if one takes Maxwell's equations in general written in terms of ϵ_0 and μ_0 and makes the replacements $\epsilon_0 \rightarrow \hat{\epsilon}$, $\mu_0 \rightarrow \hat{\mu}$, $\rho \rightarrow \rho_f$, $\vec{J} \rightarrow \vec{J}_f$ then one arrives precisely at these equations. Thus, here $\hat{\epsilon}$

⁶Very commonly, one will see the magnetic susceptibility instead defined as the linear term in the expansion of $\vec{M}$ as a function of $\vec{H}$ instead of $\vec{B}$. This is again a historical curiosity. One can always switch between the two conventions with very brief algebra.

is called the material permittivity tensor and $\hat{\mu}$ is similarly called the permeability tensor. Note that this is only a valid replacement rule at the level of Maxwell's equations for local linear matter. It is not true for all matter and even for local linear matter if you simply perform this replacement in the action you will get the wrong equations of motion in general. Therefore, you can't simply make these replacements in formulas for the energy of momentum of the electromagnetic fields and get the right answers. Later we will see that if some further restrictions on the matter are placed then in that more specific case we can make a replacement rule that works at the level of the action. In the event that the matter is isotropic, the $\hat{\epsilon}$ and $\hat{\mu}$ tensors are proportional to the identity matrix and so one defines ϵ and μ so that $\hat{\epsilon} = \epsilon \mathbb{1}$ and $\hat{\mu} = \mu \mathbb{1}$.

Problem 4.23: Maxwell's Equations for Fourier-Local Linear Matter. Consider Fourier-local linear matter. Show that the Fourier transforms of Maxwell's equations become:

$$i\vec{k} \cdot (\hat{\epsilon} \vec{E}) = \tilde{\rho}_f, \quad i\vec{k} \cdot \vec{B} = 0, \quad i\vec{k} \times \vec{E} = i\omega \vec{B}, \quad i\vec{k} \times (\hat{\mu}^{-1} \vec{B}) = \vec{J}_f - i\omega \hat{\epsilon} \vec{E}$$

where:

$$\hat{\epsilon}(\omega, \vec{k}) \stackrel{\text{def}}{=} \epsilon_0 \left(\mathbb{1} + \hat{\chi}_e(\omega, \vec{k}) \right), \quad \hat{\mu}^{-1}(\omega, \vec{k}) \stackrel{\text{def}}{=} \frac{1}{\mu_0} \left(\mathbb{1} - \hat{\chi}_m(\omega, \vec{k}) \right).$$

As well, show that if one takes the Fourier transforms of Maxwell's equations in general written in terms of ϵ_0 and μ_0 and makes the replacements $\epsilon_0 \rightarrow \hat{\epsilon}$, $\mu_0 \rightarrow \hat{\mu}$, $\rho \rightarrow \rho_f$, $\vec{J} \rightarrow \vec{J}_f$ then one arrives precisely at these equations. Thus, $\hat{\epsilon}$ and $\hat{\mu}$ retain the same name as in the local linear case. Again there is no confusion as whenever the two definitions simultaneously apply, they match. In the event that the matter is moreover isotropic, these tensors are proportional to the identity matrix and so one defines ϵ and μ so that $\hat{\epsilon} = \epsilon \mathbb{1}$ and $\hat{\mu} = \mu \mathbb{1}$.

Problem 4.24: Dielectric Ball in a Background Electric Field. Consider a ball of simple matter of radius R and $\epsilon > 1$, $\mu = 1$ (matter satisfying these conditions is called a dielectric) to be placed in a background uniform static electric field $\vec{E}_0$.

- (a) Show by using Maxwell's equations for simple matter and boundary conditions that the electric field inside the ball is given by:

$$\vec{E}_{\text{in}} = \frac{\vec{E}_0}{1 + \frac{\chi_e}{3}}.$$

- (b) Show that the electric dipole moment induced in the ball is:

$$\vec{\rho} = \frac{4\pi\epsilon_0 R^3 \chi_e}{3 + \chi_e} \vec{E}_0.$$

Problem 4.25: Electric field of a uniformly polarized ball. Consider a ball of matter of radius R which has fixed uniform polarization $\vec{P}$ throughout the ball. Show using Maxwell's equations and boundary conditions that the electric field inside the ball is given by:

$$\vec{E}_{\text{in}} = -\frac{\vec{P}}{3}$$

and that the electric field outside the ball is exactly the electric field of an electric dipole with dipole moment matching the total dipole moment of the ball.

Problem 4.26: Magnetic Scalar Potential. Consider a simply connected region of matter in which there is no free current. Assume $\rho = 0$ everywhere for all times. Show that $\nabla \times \vec{H} = 0$ in this region and that there exists a function ψ so that in this region $\vec{H} = -\nabla\psi$. Such a ψ is called a magnetic scalar potential. However, it should be understood that it is simply a problem solving tool for the very specific class of scenarios mentioned here and does not exist in general. As well, show that in this region:

$$-\nabla^2 \psi = \rho_{\text{mfic}}$$

where $\rho_{\text{mfic}} \stackrel{\text{def}}{=} -\nabla \cdot \vec{M}$ is called the "fictitious magnetic charge". This allows one to make an analogy to the equations of electrostatics for these special magnetic scenarios which is useful because we already know how to solve the Poisson equation. However, note that this is only valid in a contractible region of matter. If $\nabla \times \vec{H} = 0$ in a noncontractible region, you have no reason at all to believe that a scalar potential for $\vec{H}$ exists.

Problem 4.27: Magnetizable Ball in a Background Magnetic Field. Consider a ball of simple matter of radius R and $\epsilon = 1$, $\mu \neq 1$ to be placed in a background uniform static magnetic field $\vec{B}_0$.

- (a) Show by using Maxwell's equations for simple matter and boundary conditions that the magnetic field inside the ball is given by:

$$\vec{B}_{\text{in}} = \frac{\vec{B}_0}{1 + \frac{\chi_m}{3}}.$$

- (b) Show that the magnetic dipole moment induced in the ball is:

$$\vec{m} = \frac{4\pi R^3 \chi_m}{\mu_0(3 + \chi_m)} \vec{B}_0.$$

Problem 4.28: Magnetic Field of a Uniformly Magnetized Ball. Consider a ball of matter of radius R which has fixed uniform magnetization $\vec{M}$ throughout the ball. Show using Maxwell's equations and boundary conditions that the magnetic field inside the ball is given by:

$$\vec{B}_{\text{in}} = \frac{2}{3} \mu_0 \vec{M}$$

and that the magnetic field outside the ball is exactly the magnetic field of a magnetic dipole with dipole moment matching the total dipole moment of the ball.

Problem 4.29: Conducting Sphere in Background Fields. Consider an empty perfectly conducting sphere of radius R placed in a uniform static electric field $\vec{E}_0$ and a uniform static magnetic field $\vec{B}_0$. Show using Maxwell's equations and boundary conditions that the electric and magnetic fields inside the sphere vanish, that the electric and magnetic fields outside of the sphere are the sums of the externally applied fields and exactly the field of an electric/magnetic dipole with the dipole moments given by:

$$\vec{\phi} = 4\pi R^3 \epsilon_0 \vec{E}_0, \quad \vec{m} = -\frac{2\pi R^3}{\mu_0} \vec{B}_0.$$

To do so, recall that charges in a conductor are allowed to move freely and thus when experiencing background fields the charges will come to a stable equilibrium in which the Lorentz force on them vanishes under all perturbations consistent with remaining in the conductor. Use this to show that the electric field tangential to a conducting surface and the magnetic field normal to a conducting surface both vanish in this equilibrium.

Problem 4.30: Effective Action for Maxwell's equations in Matter. Consider a region of spacetime $\mathbb{M}$ which is occupied by matter. Let the rest of spacetime not occupied by that matter be called $\mathbb{T}/\mathbb{M}$.

- (a) Take the variation of the full action for Maxwell's equations (corresponding to theorem 4.3) and use our expressions for the bound charge and current densities in matter and the definitions of $\vec{D}$ and $\vec{H}$ to show that the variation is given by:

$$\delta S = \int_{\mathbb{T}} \left(\vec{D} \cdot \delta \vec{E} - \vec{H} \cdot \delta \vec{B} + \vec{J}_f \cdot \delta \vec{A} - \rho_f \delta \phi \right) d^3 \vec{x} dt$$

where we have used that outside of matter, there is no bound charge or current density by definition.

- (b) If our model for matter is such that $\vec{D} \cdot \delta \vec{E} - \vec{H} \cdot \delta \vec{B}$ can be written as the variation of some functional $S_M(\vec{E}, \vec{B})$ then one can use the effective action for such matter:

$$S_{\text{eff}} = S_M[\vec{E}, \vec{B}] + \int_{\mathbb{T}} \left(\vec{J}_f \cdot \vec{A} - \rho_f \phi \right) d^3 \vec{x} dt$$

where:

$$\vec{D} = \frac{\delta S_M}{\delta \vec{E}}, \quad \vec{H} = -\frac{\delta S_M}{\delta \vec{B}}.$$

Matter for which S_M exists is called integrable (because the constitutive relations which give $\vec{D}$ and $\vec{H}$ in terms of $\vec{E}$ and $\vec{B}$ are approximate and averaged over different scales in practice, it may be the case that the resulting approximation is not integrable even though the solution-insertion theorem guarantees that the full exact result with all of its initial and final condition dependence is). Show that if in addition to being integrable the matter is also local, then S_M can be written as the integral of a Lagrangian density $\mathcal{L}_{\text{eff}}(t, \vec{x}, \vec{E}, \vec{B})$ so that:

$$S_{\text{eff}} = \int_{\mathbb{T}} \left(\mathcal{L}_{\text{eff}}(t, \vec{x}, \vec{E}, \vec{B}) + \vec{J}_f \cdot \vec{A} - \rho_f \phi \right) d^3 \vec{x} dt$$

where:

$$\vec{D} = \frac{\partial \mathfrak{L}_{\text{eff}}}{\partial \vec{E}}, \quad \vec{H} = -\frac{\partial \mathfrak{L}_{\text{eff}}}{\partial \vec{B}}.$$

- (c) Consider local linear matter for which the susceptibilities are symmetric matrices (we then would say the matter is symmetric). Show that this local linear symmetric matter is integrable and in particular show that the effective action is given by:

$$S_{\text{eff}} = \int_{\mathbb{T}} \left(\frac{1}{2} \vec{E}^T \hat{\epsilon} \vec{E} - \frac{1}{2} \vec{B}^T \hat{\mu}^{-1} \vec{B} + \vec{J}_f \cdot \vec{A} - \rho_f \phi \right) d^3 \vec{x} dt.$$

4.6 Electromagnetic Hamiltonian

Now let us find the Hamiltonian formulation of electromagnetism. We start with the Legendre transformation:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-\rho\phi + \vec{J} \cdot \vec{A} + \frac{\epsilon_0}{2} |\nabla\phi + \dot{\vec{A}}|^2 - \frac{1}{2\mu_0} |\nabla \times \vec{A}|^2 \right) d\mathbb{S} \quad (4.6.1)$$

$$\implies P_\phi = \frac{\delta\mathcal{L}}{\delta\dot{\phi}} = 0, \quad \vec{P}_A = \frac{\delta\mathcal{L}}{\delta\dot{\vec{A}}} = \epsilon_0(\nabla\phi + \dot{\vec{A}}) = -\epsilon_0\vec{E}. \quad (4.6.2)$$

The conjugate momentum of the scalar potential vanishes! At first, this seems like an issue as it means we cannot complete the Legendre transformation and find $\dot{\phi}$ in terms of P_ϕ . However, notice that because $\mathcal{L}$ does not depend on $\dot{\phi}$ the Euler-Lagrange equation for ϕ reads simply:

$$\frac{\delta\mathcal{L}}{\delta\phi} = 0. \quad (4.6.3)$$

Hence, the ϕ equation of motion is essentially the equation of motion of a Lagrange multiplier as it just demands that the Lagrangian's variation with respect to it vanishes. In particular that ϕ equation of motion is:

$$\frac{\delta\mathcal{L}}{\delta\phi} = -\rho + \epsilon_0 \nabla \cdot \vec{E} = -\rho - \nabla \cdot \vec{P}_A \stackrel{!}{=} 0. \quad (4.6.4)$$

This is not a condition on ϕ , it is a condition on $\vec{P}_A$. Therefore, the ϕ equation of motion produces a phase space constraint on the phase space $(\vec{A}, \vec{P}_A)$ of the vector potential. In terms of the Hamiltonian, this equivalently becomes:

$$\frac{\delta\mathcal{H}}{\delta\phi} = -\frac{\partial P_\phi}{\partial t} = -\partial_t \frac{\delta\mathcal{L}}{\delta\dot{\phi}} = -\frac{\delta\mathcal{L}}{\delta\phi} = 0. \quad (4.6.5)$$

Thus, in the Hamiltonian as well ϕ enters as a Lagrange multiplier rather than a canonical coordinate. That is, the Hamiltonian for electromagnetism is actually a function on the phase space $(\vec{A}, \vec{P}_A)$ and the scalar potential ϕ is a Lagrange multiplier which imposes a phase space constraint on this system.

Continuing with the calculation of the Hamiltonian:

$$\mathcal{H} = \int_{\mathbb{S}} \left(P_\phi \dot{\phi} + \vec{P}_A \cdot \dot{\vec{A}} \right) d\mathbb{S} - \mathcal{L} \quad (4.6.6)$$

$$= \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{|\nabla \times \vec{A}|^2}{2\mu_0} - \vec{J} \cdot \vec{A} + \rho\phi - \vec{P}_A \cdot \nabla\phi \right) d\mathbb{S} \quad (4.6.7)$$

$$= \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{|\nabla \times \vec{A}|^2}{2\mu_0} - \vec{J} \cdot \vec{A} + \phi \left(\rho + \nabla \cdot \vec{P}_A \right) \right) d\mathbb{S}. \quad (4.6.8)$$

This is the Hamiltonian for electromagnetism. Its equations of motion are given as always by Hamilton's equations:

$$\frac{\partial \vec{A}}{\partial t} = \frac{\delta\mathcal{H}}{\delta \vec{P}_A}, \quad \frac{\partial \vec{P}_A}{\partial t} = -\frac{\delta\mathcal{H}}{\delta \vec{A}}, \quad \frac{\delta\mathcal{H}}{\delta\phi} = 0. \quad (4.6.9)$$

Let us verify explicitly the equations of motion:

$$\frac{\partial \vec{A}}{\partial t} = \frac{\delta\mathcal{H}}{\delta \vec{P}_A} = \frac{\vec{P}_A}{\epsilon_0} - \nabla\phi \implies \vec{P}_A = -\epsilon_0\vec{E}. \quad (4.6.10)$$

$$\frac{\partial \vec{P}_A}{\partial t} = -\frac{\delta\mathcal{H}}{\delta \vec{A}} = -\frac{1}{\mu_0} \nabla \times (\nabla \times \vec{A}) + \vec{J} = -\frac{1}{\mu_0} \nabla \times \vec{B} + \vec{J} \quad (4.6.11)$$

$$\implies \nabla \times \vec{B} = \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} + \mu_0 \vec{J}. \quad (4.6.12)$$

$$0 = \frac{\delta\mathcal{H}}{\delta\phi} = \rho + \nabla \cdot \vec{P}_A \implies \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}. \quad (4.6.13)$$

Hence the canonical equations of motion give back the Maxwell-Ampere law and the Lagrange multiplier gives Gauss' Law!

Let us now be slightly more careful about our treatment of constraints. We have the Hamiltonian:

$$\mathcal{H}[\phi, \vec{A}, \vec{P}_A] = \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{|\nabla \times \vec{A}|^2}{2\mu_0} - \vec{J} \cdot \vec{A} + \phi \left(\rho + \nabla \cdot \vec{P}_A \right) \right) d\mathbb{S} \quad (4.6.14)$$

where the ϕ equation of motion imposes a constraint. By the logic of section 2.8.3 we should check the consistency condition for this constraint (in equation (2.8.55)):

$$\frac{d}{dt} \left(\rho + \nabla \cdot \vec{P}_A \right) = \frac{\partial \rho}{\partial t} + \{ \rho + \nabla \cdot \vec{P}_A, \mathcal{H} \} \stackrel{!}{=} 0 \quad (4.6.15)$$

$$\implies \frac{\partial \rho}{\partial t} - \nabla \cdot \frac{\delta \mathcal{H}}{\delta \vec{A}} \stackrel{!}{=} 0 \quad (4.6.16)$$

$$\implies \frac{\partial \rho}{\partial t} + \nabla \cdot \left(\vec{J} - \frac{1}{\mu_0} \nabla \times \vec{B} \right) \stackrel{!}{=} 0 \quad (4.6.17)$$

$$\implies \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} \stackrel{!}{=} 0. \quad (4.6.18)$$

Hence the consistency condition just imposes the continuity equation on the sources. So, Maxwell's equations only make sense for theories with local charge conservation. However, the continuity equation says nothing about the phase space $(\vec{A}, \vec{P}_A)$. Because this is not a new constraint on the phase space, no new constraints are generated. Therefore, the only constraint is $\rho + \nabla \cdot \vec{P}_A \stackrel{!}{=} 0$. Being more careful, this provides a constraint at each $\vec{x}$. This constraint at each $\vec{x}$ Poisson commutes with the constraint at each other $\vec{x}'$ and so at each $\vec{x}$ this is a first class constraint. Because these are first class constraints, $\phi(t, \vec{x})$ as a Lagrange multiplier is a completely arbitrary function and is wholly undetermined by the equations of motion and consistency conditions. We know from section 2.8.3 that a linear combination of the constraint functions with time dependent coefficients generates the gauge transformations of the theory. And so, any linear combination of $\rho + \nabla \cdot \vec{P}_A$ generates some gauge transformation. Because of this, the most general gauge transformation in this theory is given by a generator G dependent on some arbitrary function $f(t, \vec{x})$ as:

$$G = - \int f(t, \vec{x}) (\rho + \nabla \cdot \vec{P}_A) d^3 \vec{x}. \quad (4.6.19)$$

Let the parameter associated to this transformation be called ε . Then, under this transformation by equation (2.8.132):

$$\mathcal{D}\phi = -\dot{f}, \quad \mathcal{D}\vec{A} = \{\vec{A}, G\} = \nabla f, \quad \mathcal{D}\vec{P}_A = \{\vec{P}_A, G\} = 0. \quad (4.6.20)$$

This is precisely the usual gauge transformation property of the potentials! Thus, the theory of phase space constraints is exactly consistent with and reproduces our understanding of gauge transformations.

The fact that Gauss' law is a first class constraint really means that it is a constraint on the legally allowed initial conditions for the theory. To see this, let us take the divergence of the Maxwell-Ampere law and recall the continuity equation for the charge density:

$$\nabla \cdot \nabla \times \vec{B} = \epsilon_0 \mu_0 \nabla \cdot \frac{\partial \vec{E}}{\partial t} + \mu_0 \nabla \cdot \vec{J} \quad (4.6.21)$$

$$\implies 0 = \frac{\partial}{\partial t} \left(\nabla \cdot \vec{E} - \frac{\rho}{\epsilon_0} \right) \quad (4.6.22)$$

$$\implies \nabla \cdot \vec{E}(t, \vec{x}) - \frac{\rho(t, \vec{x})}{\epsilon_0} = \nabla \cdot \vec{E}(0, \vec{x}) - \frac{\rho(0, \vec{x})}{\epsilon_0}. \quad (4.6.23)$$

So, without applying Gauss' law, the Maxwell-Ampere equation already implies that $\nabla \cdot \vec{E} - \frac{\rho}{\epsilon_0}$ is constant. All Gauss' law does is impose a restriction on the initial condition $\vec{E}(0, \vec{x})$ that its divergence must be so that this combination vanishes initially. Gauss' law gives no new dynamical information, it simply very slightly constrains the initial conditions.

You might consider the presence of the Lagrange multiplier annoying as it requires us to carry around ϕ as an additional variable to our canonical coordinates $(\vec{A}, \vec{P}_A)$. We know from our study of phase space constraints that the Lagrange multipliers associated to first class constraints can be selected arbitrarily. So, we can always select a gauge in which $\phi = 0$ identically for all times and positions. To prove that this exists in general, suppose we initially are in a gauge in which it is not true $\phi(t, \vec{x}) \neq 0$. Define $\phi'(t, \vec{x})$ by gauge

transformation with the gauge fixing function:

$$f(t, \vec{x}) = \int_{t_0}^t \phi(t', \vec{x}) dt' + g(\vec{x}) \quad (4.6.24)$$

where t_0 is an arbitrary real number and $g(\vec{x})$ is an arbitrary function. Then:

$$\phi'(t, \vec{x}) = \phi(t, \vec{x}) - \frac{\partial f}{\partial t} = \phi - \phi = 0. \quad (4.6.25)$$

Hence, after such a gauge transformation $\phi = 0$ everywhere and always. Because this simplifies the Hamiltonian so much, it is called Hamiltonian gauge. In this gauge we have:

$$\mathcal{H} = \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{|\nabla \times \vec{A}|^2}{2\mu_0} - \vec{J} \cdot \vec{A} \right) d\mathbb{S}. \quad (4.6.26)$$

As well, the equation of motion for $\vec{A}$ becomes:

$$\frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} + \nabla \nabla \cdot \vec{A} - \nabla^2 \vec{A} = \mu_0 \vec{J}. \quad (4.6.27)$$

This last equation of motion is called the transverse wave equation. While the Hamiltonian gauge is nice for eliminating the scalar potential, we ought to be careful and remember that Gauss' law is still true and thus it still implies a constraint on the allowed initial conditions for $\vec{P}_A$. That is, $\vec{P}_A(0, \vec{x})$ must satisfy:

$$\nabla \cdot \vec{P}_A(0, \vec{x}) + \rho(0, \vec{x}) = 0. \quad (4.6.28)$$

All dynamical evolution is then given from Hamiltonian with $\phi = 0$. This gives:

Theorem 4.4: Hamiltonian for Maxwell's Equations

The Hamiltonian for Maxwell's Equations in any gauge is given by:

$$\mathcal{H} = \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{|\nabla \times \vec{A}|^2}{2\mu_0} - \vec{J} \cdot \vec{A} + \phi \left(\rho + \nabla \cdot \vec{P}_A \right) \right) d\mathbb{S} \quad (4.6.29)$$

with equations of motion:

$$\frac{\partial \vec{A}}{\partial t} = \frac{\delta \mathcal{H}}{\delta \vec{P}_A}, \quad \frac{\partial \vec{P}_A}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \vec{A}}, \quad \frac{\delta \mathcal{H}}{\delta \phi} = 0 \quad (4.6.30)$$

on the phase space $(\vec{A}, \vec{P}_A)$ and $\phi(t, \vec{x})$ acting as a Lagrange multiplier enforcing Gauss' Law as a first class constraint. If one uses the Hamiltonian gauge $\phi = 0$, one can equivalently use the simpler Hamiltonian:

$$\mathcal{H} = \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2}{2\epsilon_0} + \frac{c^2 |\nabla \times \vec{A}|^2}{2} - \vec{J} \cdot \vec{A} \right) d\mathbb{S} \quad (4.6.31)$$

where the supplied initial conditions for $\vec{P}_A$ must satisfy:

$$\nabla \cdot \vec{P}_A(0, \vec{x}) + \rho(0, \vec{x}) = 0. \quad (4.6.32)$$

Using Hamiltonian thinking, and the resultant Poisson bracket, we can give a precise mathematical meaning to causality. Locality requires that the equations of motion of our theory are local, meaning that the equation of motion for a field $\Phi(X)$ in our theory at an event X can be expressed in a way which depends only on the values of quantities at that event and a finite number of spatial derivatives of quantities at that event. Causality requires that the results of an experiment depend only on data in the past light cone of that experiment, and so the solution to the equation of motion depends only on initial data in the past lightcone. Suppose $\Phi^a(X)$ are all of the fields in our theory (point particles can be snuck in as fields by having a density field $\rho(t, \vec{x}) = \delta(\vec{x} - \vec{z}(t))$ where $\vec{z}(t)$ is the position of the particle). Suppose further that we solve the equations of motion so that we can fully express $\Phi^a(t, \vec{x})$ in terms of initial conditions $\Phi^a(0, \vec{x})$:

$$\Phi^a(t, \vec{x}) = U^a(t, \Phi_0). \quad (4.6.33)$$

We know how to take the Poisson bracket of two quantities evaluated at the same time (just use the standard Poisson bracket). Using the solution of the equations of motion, we can then define the Poisson bracket

between quantities at different times. Precisely:

$$\{\Phi^a(t_1, \vec{x}_1), \Phi^b(t_2, \vec{x}_2)\} = \{U^a(t_1, \Phi_0), U^b(t_2, \Phi_0)\}. \quad (4.6.34)$$

In this last expression, all fields are evaluated at $t = 0$, so we can use the standard Poisson bracket.

Let $F(X), G(X)$ be gauge invariant functions of the fields $\Phi^a(X)$ and a finite number of spatial derivatives all evaluated at the event X . The Poisson bracket $\{\cdot, F(X)\}$ of a quantity represents how that quantity changes under the canonical transformation generated by $F(X)$. Therefore, if two quantities are to be unable to affect each other experimentally, they must have vanishing Poisson bracket. Because of this, locality requires that if the events X_1 and X_2 are spacelike separated (so that neither is in the past light cone of the other), then for all such $F(X)$ and $G(X)$:

$$\{F(X_1), G(X_2)\} = 0. \quad (4.6.35)$$

Sometimes we have physical interest in quantities that depend on many events, such as a time-average of a rapidly oscillating quantity. Let F and G now be gauge invariant functionals which each depend only on data on a subset of spacetime, $\mathbb{T}_1$ and $\mathbb{T}_2$ respectively. Further, suppose that the no point of $\mathbb{T}_1$ is in the past lightcone of any point in $\mathbb{T}_2$ and no point in $\mathbb{T}_2$ is in the past lightcone of any point in $\mathbb{T}_1$. Then, causality requires:

$$\{F, G\} = 0. \quad (4.6.36)$$

It is important to require that these quantities are gauge invariant because it is possible to choose gauges which are acausal, in the sense of depending on conditions that use data outside of the relevant past lightcone but such acausal choices drop out of any physical effects. For example, the Coulomb gauge $\nabla \cdot \vec{A} = 0$ causes Gauss' law to become the Poisson equation for ϕ and the solution to the Poisson equation is acausal, because it gives an expression for $\phi(t, \vec{x})$ that depends on $\rho(t, \vec{x}')$ for all $\vec{x}'$ which are all outside the past lightcone of $(t, \vec{x})$. This acausal gauge artifact can be eliminated in the resulting expressions for $\vec{E}$ or $\vec{B}$.

Exercises

Problem 4.31: ★ Electromagnetic Energy Conservation. Consider the Lagrangian of N charges interacting with electromagnetism:

$$\mathcal{L} = \sum_{n=1}^N \left(-m_n c^2 \sqrt{1 - \frac{|\dot{\vec{x}}_n|^2}{c^2}} + q_n \dot{\vec{x}}_n \cdot \vec{A}(t, \vec{x}_n) - q_n \phi(t, \vec{x}_n) \right) + \int_{\mathbb{S}} \left(\frac{\epsilon_0}{2} |\vec{E}|^2 - \frac{|\vec{B}|^2}{2\mu_0} \right) d\mathbb{S}.$$

(a) From Noether's theorem, show that the total energy of the system is given by:

$$E = \sum_{n=1}^N \frac{m_n c^2}{\sqrt{1 - \frac{|\dot{\vec{x}}_n|^2}{c^2}}} + \int_{\mathbb{S}} \left(\frac{\epsilon_0}{2} |\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu_0} \right) d\mathbb{S}$$

and that it is conserved. And so, the energy very cleanly decomposes into the sum of free energies for each particle and the free energy for the electromagnetic fields. One may find this surprising as certainly for an interacting theory the sum of free Hamiltonians is not the total Hamiltonian. This is true but recall that in the Legendre transformation the expression for the particle's momenta depends on $\vec{A}$ and so the conjugate momentum of the free and interacting theories are different. This allows it to be possible that the free Hamiltonians, expressed in terms of coordinates and momenta, do not add up to the total Hamiltonian while the free energies, expressed in terms of the coordinates and velocities, do add up to the total energy.

(b) From the above, one can⁷ identify the electromagnetic energy density $\mathcal{E}$ to be:

$$\mathcal{E} = \frac{\epsilon_0}{2} |\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu_0}.$$

Show using Maxwell's equations that the electromagnetic energy density then satisfies:

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \vec{S} = -\vec{J} \cdot \vec{E}$$

⁷This choice is not unique from our analysis so far. One could modify the quantity by adding a total divergence and such a choice would disappear after integration. However, we will understand later that the choice made here is the unique one satisfying the correct Poisson brackets with other quantities of interest.

where $\vec{S} \stackrel{\text{def}}{=} \frac{1}{\mu_0} \vec{E} \times \vec{B}$ is called the Poynting vector. As well, show using the Lorentz force that $\vec{J} \cdot \vec{E}$ is the work done per unit time per unit volume by electromagnetism on the charges. Thus, one can see that the electromagnetic energy density satisfies a continuity equation with a source term in which the electromagnetic energy current density is given by the Poynting vector and the source term corresponds to the rate at which energy leaves the electromagnetic fields and enters the charges at that location.

Problem 4.32: ★ Electromagnetic Linear Momentum Conservation. Consider the same Lagrangian of N charges interacting with electromagnetism.

- (a) From Noether's theorem, show that the total linear momentum of the system is given by:

$$\vec{P} = \sum_{n=1}^N \frac{m_n \dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}_n|^2}{c^2}}} + \int_{\mathbb{S}} \epsilon_0 \vec{E} \times \vec{B} d\mathbb{S}$$

and that it is conserved. And so, the momentum very cleanly decomposes into the sum of free linear momentum for each particle and the free linear momentum for the electromagnetic fields. In order to do this, you will have to use that after translating a function $f(t, \vec{x})$ in space by the amount $\vec{a}$, we mean that the translated function f' should take the same value as the untranslated function but at the translated position: $f'(t, \vec{x}') \stackrel{!}{=} f(t, \vec{x})$ thus $f'(t, \vec{x} + \vec{a}) = f(t, \vec{x})$ and so $f'(t, \vec{x}) = f(t, \vec{x} - \vec{a})$.

- (b) From the above, one can identify the electromagnetic linear momentum density $\vec{\varphi}$ to be:

$$\vec{\varphi} = \epsilon_0 \vec{E} \times \vec{B} = \frac{1}{c^2} \vec{S}.$$

Thus, the Poynting vector (up to factors of c^2) is also the electromagnetic linear momentum density. Show using Maxwell's equations that the electromagnetic linear momentum density then satisfies:

$$\frac{\partial \vec{\varphi}}{\partial t} - \nabla \cdot \hat{\sigma} = -\rho \vec{E} - \vec{J} \times \vec{B}$$

where:

$$\hat{\sigma} = \epsilon_0 \vec{E} \vec{E}^T + \frac{1}{\mu_0} \vec{B} \vec{B}^T - \left(\frac{\epsilon_0}{2} |\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu_0} \right) \mathbb{1}$$

is called the electromagnetic stress tensor. As well, show that the $\rho \vec{E} + \vec{J} \times \vec{B}$ term on the right hand side is the force per unit volume by electromagnetism on the charges. Thus, one can see that the electromagnetic momentum density satisfies a continuity equation with a source term in which the electromagnetic momentum current density is given by the negative of the stress tensor and the source term corresponds to the rate at which linear momentum is transferred from the electromagnetic fields to the charges.

Problem 4.33: ★ Electromagnetic Angular Momentum Conservation. Consider the same Lagrangian of N charges interacting with electromagnetism.

- (a) From Noether's theorem, show that the total angular momentum of the system is given by:

$$\vec{J} = \sum_{n=1}^N \vec{x}_n \times \frac{m_n \dot{\vec{x}}}{\sqrt{1 - \frac{|\dot{\vec{x}}_n|^2}{c^2}}} + \int_{\mathbb{S}} \vec{x} \times (\epsilon_0 \vec{E} \times \vec{B}) d\mathbb{S}$$

and that it is conserved. And so, the angular momentum very cleanly decomposes into the sum of free angular momentum for each particle and the free angular momentum for the electromagnetic fields. In order to do this, you will have to use that after rotating a vector field $\vec{A}(t, \vec{x})$ in by $\hat{R}$, we mean that the rotated function $\vec{A}'$ should take the rotated value of the unrotated field but at the rotated position: $\vec{A}'(t, \vec{x}') \stackrel{!}{=} \hat{R} \vec{A}(t, \vec{x})$ thus $\vec{A}'(t, \hat{R} \vec{x}) = \hat{R} \vec{A}(t, \vec{x})$ and so $\vec{A}'(t, \vec{x}) = \hat{R} \vec{A}(t, \hat{R}^{-1} \vec{x})$.

- (b) In deriving the above, you may have noticed that the electromagnetic angular momentum can be decomposed into a piece which depends on the origin and a piece which does not reference the origin. In particular, show that equivalently the electromagnetic angular momentum can be written as:

$$\int_{\mathbb{S}} \vec{x} \times (\epsilon_0 \vec{E} \times \vec{B}) d\mathbb{S} = \epsilon_0 \int_{\mathbb{S}} \vec{E} \times \vec{A} d\mathbb{S} + \epsilon_0 \int_{\mathbb{S}} \vec{x} \times \left(\vec{A} \nabla \cdot \vec{E} + E_a \nabla A^a \right) d\mathbb{S}.$$

Here the first integral on the right is sometimes called the “spin angular momentum” as it does not depend on the origin while the second integral is sometimes called the “orbital angular momentum”. Show that neither are gauge invariant, but that the total is; pieces shuffle back and forth between

these two terms under gauge transformation. This sometimes leads to sources claiming there is no gauge invariant way to define spin angular momentum and orbital angular momentum separately. It is certainly true that there is no local gauge invariant expression for spin angular momentum density or orbital angular momentum density while there is for total angular momentum density. However, later we will find gauge invariant expressions for the total spin angular momentum of electromagnetism and total orbital angular momentum.

- (c) From the above, one can identify the electromagnetic angular momentum density $\vec{\mathcal{J}}$ to be:

$$\vec{\mathcal{J}} = \vec{x} \times (\epsilon_0 \vec{E} \times \vec{B}) = \vec{x} \times \vec{\varphi}$$

using the linear momentum density found before. Show using Maxwell's equations that the electromagnetic angular momentum density then satisfies:

$$\frac{\partial \vec{\mathcal{J}}}{\partial t} - \nabla \cdot (\hat{\sigma} \times \vec{x}) = -\vec{x} \times (\rho \vec{E} + \vec{J} \times \vec{B}).$$

As well, show that the $\vec{x} \times (\rho \vec{E} + \vec{J} \times \vec{B})$ term on the right hand side is the torque per unit volume by electromagnetism on the charges. Thus, one can see that the electromagnetic angular momentum density satisfies a continuity equation with a source term in which the electromagnetic angular momentum current density is given by the negative of the stress tensor crossed with position (where the cross product of a matrix and a vector is defined through applying matrix multiplication with the matrix definition of $\vec{x} \times$) and the source term corresponds to the rate at which angular momentum is transferred from the electromagnetic fields to the charges.

Problem 4.34: ★ Electromagnetic Dynamic Energy Moment Conservation. Consider the same Lagrangian of N charges interacting with electromagnetism.

- (a) From Noether's theorem, show that the generator of Lorentz boosts of the whole system (called the dynamic energy moment) is given by:

$$\vec{K} = ct\vec{P} - \frac{1}{c} \left(\sum_{n=1}^N E_n \vec{x}_n + \int_{\mathbb{S}} \mathcal{E} \vec{x} d\mathbb{S} \right)$$

(where E_n is the free energy of particle n) and that it is conserved. And so, the dynamic energy moment very cleanly decomposes into the sum of free moments for each particle and the free moment for the electromagnetic fields. In order to do this, you will have to generalize Noether's theorem as proven in chapter 1 to apply for fields. Following the steps of section 1.10 with this additional stipulation will lead to the correct generalization. As well, you must apply the same transformation argument as applied for rotations in the previous question.

- (b) Define the center of momentum (also called the center of energy) position of the system by:

$$\vec{x}_{\text{COM}} \stackrel{\text{def}}{=} \frac{\sum_{n=1}^N E_n \vec{x}_n + \int_{\mathbb{S}} \mathcal{E} \vec{x} d\mathbb{S}}{E}.$$

Show that the conservation law for $\vec{K}$ implies that the center of momentum position moves at constant velocity given by:

$$\dot{\vec{x}}_{\text{COM}} = \frac{c^2 \vec{P}}{E}.$$

Thus, the Lorentz boost symmetry guarantees that the center of momentum of the system moves at constant velocity.

- (c) From the above, one can identify the electromagnetic dynamic energy moment density $\vec{\mathcal{K}}$ to be:

$$\vec{\mathcal{K}} = ct\epsilon_0 \vec{E} \times \vec{B} - \frac{\epsilon_0}{2c} \left(|\vec{E}|^2 + c^2 |\vec{B}|^2 \right) \vec{x} = ct\vec{\varphi} - \frac{\mathcal{E}}{c} \vec{x}.$$

Show using Maxwell's equations that the electromagnetic dynamic energy moment density then satisfies:

$$\frac{\partial \vec{\mathcal{K}}}{\partial t} + \nabla \cdot (ct\hat{\sigma} - \vec{\varphi} \vec{x}) = \frac{1}{c} \vec{J} \cdot \vec{E} \vec{x} - ct(\rho \vec{E} + \vec{J} \times \vec{B}).$$

Thus, one can see that the electromagnetic dynamic energy moment density satisfies a continuity equation with a source term as written. (As well, one can see that the source term depends on the rate at which energy and momentum are transferred from electromagnetism to matter.)

Problem 4.35: Alternative way of deriving the Electromagnetic Stress Tensor. Starting from the total electromagnetic force on a distribution of charge in a region of space $\mathbb{M}$:

$$\vec{F} = \int_{\mathbb{M}} (\rho \vec{E} + \vec{J} \times \vec{B}) d\mathbb{S}$$

show using Maxwell's equations that this expression can be rewritten in terms of the electromagnetic stress tensor as:

$$\vec{F} = \int_{\partial\mathbb{M}} \hat{\sigma} \cdot d\vec{\mathbb{A}}.$$

Problem 4.36: ★ Dispersion Relations and Fourier Amplitudes. Consider a system of inhomogeneous time and space translationally symmetric linear partial differential equations for some functions $\phi^a(t, \vec{x})$ and inhomogeneities $\eta^a(t, \vec{x})$. Such a system, for some matrix function of components $\mathcal{L}^a_b$, can be written as:

$$\mathcal{L}^a_b \left(\frac{\partial}{\partial t}, \nabla \right) \phi^b(t, \vec{x}) = \eta^a(t, \vec{x}).$$

(You may want to take some examples we have covered, such as Maxwell's equations, and put them in this form to see how it works.)

- (a) We will consider this differential equation on all of space with initial conditions which decay sufficiently quickly away from the origin for the Fourier transform to converge. Show that if we define the spatial Fourier transforms of $\phi^a(t, \vec{x})$ and $\eta^a(t, \vec{x})$ as:

$$\phi_F^a(t, \vec{k}) = \int_{\mathbb{S}} \frac{e^{-i\vec{k} \cdot \vec{x}}}{(2\pi)^{\frac{3}{2}}} \phi^a(t, \vec{x}) d^3\vec{x}, \quad \eta_F^a(t, \vec{k}) = \int_{\mathbb{S}} \frac{e^{-i\vec{k} \cdot \vec{x}}}{(2\pi)^{\frac{3}{2}}} \eta^a(t, \vec{x}) d^3\vec{x}$$

then the differential equation becomes:

$$\mathcal{L}^a_b \left(\frac{\partial}{\partial t}, i\vec{k} \right) \phi_F^b(t, \vec{k}) = \eta_F^a(t, \vec{k}).$$

- (b) The result of the previous part is now a system of inhomogeneous linear ordinary differential equations for the time dependence of $\phi_F^a(t, \vec{k})$ and thus we can apply the standard theory of ODE's. As such, we know the solution can be written as the sum of a homogeneous part $\phi_H^a(t, \vec{k})$ and an inhomogeneous part $\phi_I^a(t, \vec{k})$ satisfying:

$$\begin{aligned} \phi_F^a(t, \vec{k}) &= \phi_H^a(t, \vec{k}) + \phi_I^a(t, \vec{k}), \\ \mathcal{L}^a_b \left(\frac{\partial}{\partial t}, i\vec{k} \right) \phi_H^b(t, \vec{k}) &= 0, \quad \mathcal{L}^a_b \left(\frac{\partial}{\partial t}, i\vec{k} \right) \phi_I^b(t, \vec{k}) = \eta_F^a(t, \vec{k}). \end{aligned}$$

Using the theory of ODE's, show that $\phi_H^a(t, \vec{k})$ can be written in the form:

$$\phi_H^a(t, \vec{k}) = \sum_{b=1}^B \xi_b^a(\vec{k}) e^{-i\Omega_b(\vec{k})t}$$

where $\xi_b^a(\vec{k})$ and $\Omega_b(\vec{k})$ satisfy:

$$\mathcal{L}^a_c \left(-i\Omega_b(\vec{k}), i\vec{k} \right) \xi_b^c(\vec{k}) = 0.$$

and B is the number of linearly independent solutions to this equation⁸. This equation is of the form of a matrix multiplied onto a vector returning the 0 vector. Thus, the determinant of the matrix must be 0 and the vector must be in the null space of the matrix. As such, each $\Omega_b(\vec{k})$ must satisfy:

$$\det(\mathcal{L}(-i\Omega_b(\vec{k}), i\vec{k})) = 0.$$

This equation is called the **dispersion relation** for this system of differential equations; as you can see, it provides the relationship between the frequencies and wavenumbers in the homogeneous part of the system. The solutions, $\Omega_b(\vec{k})$ are called the “branches” of the dispersion relation. The vectors ξ_b with components ξ_b^a are then called the “polarizations” corresponding to each branch.

⁸We will assume B does not depend on $\vec{k}$. We generally deal with differential equations which are polynomials in the time derivative, thus giving a polynomial dispersion relation with constant degree, and so by the fundamental theorem of algebra for such differential equations B is automatically independent of $\vec{k}$.

- (c) Take the time Fourier transform of $\phi_I^a(t, \vec{k})$ and $\eta_F^a(t, \vec{k})$ defined by:

$$\tilde{\phi}_I^a(\omega, \vec{k}) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{2\pi}} \phi_I^a(t, \vec{k}) dt, \quad \tilde{\eta}_F^a(\omega, \vec{k}) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{2\pi}} \eta_F^a(t, \vec{k}) dt$$

to show that the inhomogeneous solution can be taken to be:

$$\phi_I^a(t, \vec{k}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')}}{\sqrt{2\pi}} (\mathcal{L}^{-1}(-i\omega, i\vec{k}))^a_b \eta_F^b(t', \vec{k}) d\omega dt'$$

where here $\mathcal{L}^{-1}(-i\omega, i\vec{k})$ is a pseudo-inverse of the matrix $\mathcal{L}(-i\omega, i\vec{k})$ (meaning an inverse on the subspace on which it is invertible; the choice of behavior of $\mathcal{L}^{-1}$ on the subspace on which $\mathcal{L}$ is not invertible is not unique).

- (d) Show then altogether that the full solution to the differential equation is given in the form:

$$\phi^a(t, \vec{x}) = \int_{\mathbb{K}} \sum_{\underline{b}=1}^B \xi_{\underline{b}}^a(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{b}}(\vec{k})t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} + \int_{-\infty}^{\infty} \int_{\mathbb{S}} G^a_b(t-t', \vec{x}-\vec{x}') \eta^b(t', \vec{x}') d^3 \vec{x}' dt'$$

where

$$G^a_b(t, \vec{x}) = \int_{-\infty}^{\infty} \int_{\mathbb{K}} e^{i(\vec{k} \cdot \vec{x} - \omega t)} (\mathcal{L}^{-1}(-i\omega, i\vec{k}))^a_b \frac{d^3 \vec{k} d\omega}{(2\pi)^2}$$

is called the Green's function for the system. Thus, such a system of differential equations is solved by a linear combination of plane-waves satisfying the dispersion relation and an inhomogeneous term produced by this Green's function. The nonuniqueness of $\mathcal{L}^{-1}$ leads to nonuniqueness in the Green's function, and the uniqueness issues can be resolved by specifying boundary conditions on your solution.

- (e) Suppose that the fields $\phi^a(t, \vec{x})$ and sources $\eta^a(t, \vec{x})$ are real-valued functions. Consequently, show that $\mathcal{L}^a_b$ is also real-valued (for real arguments) and that the Green's function $G^a_b(t, \vec{x})$ is real-valued. From this, conclude that the linear combination of plane waves which satisfy the dispersion relation found in the previous part is real-valued and so show that $\phi^a(t, \vec{x})$ can be written:

$$\phi^a(t, \vec{x}) = \text{Re} \int_{\mathbb{K}} \sum_{\underline{b}=1}^B \xi_{\underline{b}}^a(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{b}}(\vec{k})t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} + \int_{-\infty}^{\infty} \int_{\mathbb{S}} G^a_b(t-t', \vec{x}-\vec{x}') \eta^b(t', \vec{x}') d^3 \vec{x}' dt'$$

where $\text{Re}(z)$ gives the real part of the complex number z .

- (f) Assuming the conditions of the previous part, using the dispersion relation, show that if $\Omega_b(\vec{k})$ solves the dispersion relation then $-\Omega_b^*(-\vec{k})$ does as well. Thus, the solutions come in two types: solutions for which the two elements of this pair are distinct and solutions for which they are the same. Let B_s be the number of solutions which satisfy $\Omega_b(\vec{k}) = -\Omega_b^*(-\vec{k})$ and let B_d be the number of pairs of distinct solutions. Thus, $B = B_s + 2B_d$. Let b_s as an index run through all of the B_s solutions. Show that in a pair of distinct solutions to the dispersion relation, one element of the pair has positive (or zero) real part and the other has negative (or zero) real part. Let b_d as an index run through all of the solutions in pairs of distinct solutions for which $\Omega_{b_d}(\vec{k})$ has positive (or zero) real part and let b'_d be the other solution in the associated pair. Show that:

$$\xi_{b'_d}^a(\vec{k}) = \xi_{b_d}^{*a}(-\vec{k})$$

and that the homogeneous part of $\phi^a(t, \vec{x})$ can be written as:

$$\text{Re} \int_{\mathbb{K}} \sum_{\underline{b}=1}^B \xi_{\underline{b}}^a e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{b}} t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} = \text{Re} \int_{\mathbb{K}} \sum_{\underline{b}_s} \xi_{\underline{b}_s}^a e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{b}_s} t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} + \text{Re} \int_{\mathbb{K}} \sum_{\underline{b}_d} 2\xi_{\underline{b}_d}^a e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{b}_d} t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}$$

Then, let $P = B_s + B_d$ indicate the number of pairs of solutions (whether their entries are distinct or not) and let:

$$\tilde{\phi}_b^a(\vec{k}) = \begin{cases} \xi_b^a(\vec{k}), & \Omega_b(\vec{k}) = -\Omega_b^*(-\vec{k}) \\ 2\xi_b^a(\vec{k}), & \Omega_b(\vec{k}) \neq -\Omega_b^*(-\vec{k}) \end{cases}.$$

These $\tilde{\phi}_b(\vec{k})$ are called the “Fourier-Amplitudes” for the wave $\phi(t, \vec{x})$. Unfortunately, it is just common notation that makes them look so similar to the Fourier transform even though they are quite distinct. Watch for context to tell which one is actually being referred to. Show then finally that for these Fourier amplitudes (determined by initial conditions), the final solution to our differential equation can be

written:

$$\phi^a(t, \vec{x}) = \operatorname{Re} \int_{\mathbb{K}} \sum_{\underline{p}=1}^P \tilde{\phi}_{\underline{p}}^a(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega_{\underline{p}}(\vec{k})t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} + \int_{-\infty}^{\infty} \int_{\mathbb{S}} G^a_b(t - t', \vec{x} - \vec{x}') \eta^b(t', \vec{x}') d^3 \vec{x}' dt'.$$

Problem 4.37: Electromagnetic Waves in Empty Space. Consider Maxwell's equations with no sources. Using the result of the previous question, show that the general solutions for the electric and magnetic fields can be written as:

$$\vec{E}(t, \vec{x}) = \operatorname{Re} \int_{\mathbb{K}} \tilde{\vec{E}}(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}, \quad \vec{B}(t, \vec{x}) = \operatorname{Re} \int_{\mathbb{K}} \tilde{\vec{B}}(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}$$

where the Fourier-amplitudes satisfy:

$$\vec{k} \cdot \tilde{\vec{E}} = 0, \quad \vec{k} \times \tilde{\vec{E}} = \Omega \tilde{\vec{B}}, \quad \vec{k} \cdot \tilde{\vec{B}} = 0, \quad \vec{k} \times \tilde{\vec{B}} = -\frac{\Omega}{c^2} \tilde{\vec{E}}$$

and the dispersion relation is given by:

$$\Omega(\vec{k}) = c|\vec{k}|.$$

Show that these Maxwell's equations for Fourier amplitudes together imply that $\tilde{\vec{E}}$ and $\tilde{\vec{B}}$ are orthogonal to $\vec{k}$ (and thus the waves are said to be “transverse”) and that $\vec{k}, \tilde{\vec{E}}, \tilde{\vec{B}}$ form an orthogonal basis.

Problem 4.38: Time Averaged Power, Intensity, and Pressure. Consider pure electromagnetic plane-waves normalized as:

$$\vec{E}(t, \vec{x}) = \operatorname{Re} \left(\tilde{\vec{E}} e^{i(\vec{k} \cdot \vec{x} - \omega t)} \right), \quad \vec{B}(t, \vec{x}) = \operatorname{Re} \left(\tilde{\vec{B}} e^{i(\vec{k} \cdot \vec{x} - \omega t)} \right)$$

where these $\tilde{\vec{E}}, \tilde{\vec{B}}$, and ω satisfy the Fourier transformed Maxwell's equations in empty space. We will have much interest in pure plane-wave solutions in the coming questions because as we have just found, a generic solution to Maxwell's equations in empty space can be written as a linear combination of them and as we will see they individually have many nice properties.

(a) Show that the time averaged value of the Poynting vector is given by:

$$\mathbb{T}(\vec{S}) = \frac{1}{2\mu_0} \operatorname{Re}(\tilde{\vec{E}} \times \tilde{\vec{B}}^*) = \frac{c\epsilon_0}{2} |\tilde{\vec{E}}|^2 \hat{k}$$

where $\hat{k}$ is the unit vector in the direction of $\vec{k}$. It is very common to consider time-averaged electromagnetic quantities because the solutions are often periodic and in practical setups the frequencies involved are very high. Often experimental equipment only has the time-resolution to respond to the averaged behavior; the short term fluctuations occur on such brief scales that they are essentially inaccessible in many cases.

(b) Consider a surface whose normal vector is parallel to $\vec{k}$. Show that the intensity of light through the surface (defined as the time averaged power transferred through the surface per unit area) is given by:

$$\mathcal{I} = |\mathbb{T}(\vec{S})| = \frac{c\epsilon_0}{2} |\tilde{\vec{E}}|^2.$$

(c) Consider a surface whose unit normal vector $\vec{n}$ has an angle θ between it and $\vec{k}$. That is, $\vec{n} \cdot \hat{k} = \cos \theta$. Show that the time averaged pressure on the surface (defined as the force on the surface in the direction into the surface per unit area) is given by:

$$p = -\mathbb{T}(\vec{n} \cdot \hat{\sigma} \cdot \vec{n}) = \frac{\epsilon_0 |\tilde{\vec{E}}|^2}{2} \cos^2 \theta = \frac{|\mathbb{T}(\vec{S})|}{c} \cos^2 \theta.$$

(d) Show that the time averaged energy density $\mathcal{E}$ of the plane wave is:

$$\mathbb{T}(\mathcal{E}) = \frac{\epsilon_0}{2} |\tilde{\vec{E}}|^2 \implies \mathbb{T}(\vec{S}) = c\mathbb{T}(\mathcal{E})\hat{k}.$$

(e) Now consider the electric and magnetic fields to be a sum of two plane waves of different angular frequencies ω_1, ω_2 ($|\omega_1| \neq |\omega_2|$). Show that the time averaged energy densities and Poynting vectors

add. That is:

$$\mathbb{T}(\mathcal{E}) = \mathbb{T}(\mathcal{E}_1) + \mathbb{T}(\mathcal{E}_2), \quad \mathbb{T}(\vec{S}) = \mathbb{T}(\vec{S}_1) + \mathbb{T}(\vec{S}_2).$$

Problem 4.39: Electromagnetic Waves in Simple Media. Consider the effective action we found for simple matter:

$$S_{\text{eff}} = \int_{\mathbb{T}} \left(\frac{\epsilon}{2} |\vec{E}|^2 - \frac{|\vec{B}|^2}{2\mu} + \vec{J}_f \cdot \vec{A} - \rho_f \phi \right) d^3\vec{x} dt.$$

- (a) Show that in the absence of free charges and currents the Maxwell's equations for Fourier Amplitudes become:

$$\vec{k} \cdot \vec{E} = 0, \quad \vec{k} \times \vec{E} = \Omega \vec{B}, \quad \vec{k} \cdot \vec{B} = 0, \quad \vec{k} \times \vec{B} = -\mu\epsilon\Omega \vec{E}$$

and that consequently the general solutions can be written as:

$$\vec{E}(t, \vec{x}) = \text{Re} \int_{\mathbb{K}} \vec{E}(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega t)} \frac{d^3\vec{k}}{(2\pi)^{\frac{3}{2}}}, \quad \vec{B}(t, \vec{x}) = \text{Re} \int_{\mathbb{K}} \vec{B}(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega t)} \frac{d^3\vec{k}}{(2\pi)^{\frac{3}{2}}}$$

where the dispersion relation is given as:

$$\Omega(\vec{k}) = \frac{|\vec{k}|}{\sqrt{\mu\epsilon}}.$$

Thus, Maxwell's equations in simple matter evolve in time just as in empty space except with the speed of light replaced with an effective speed $v = \frac{1}{\sqrt{\mu\epsilon}}$.

- (b) It is typical to define the index of refraction n in matter as the ratio between the speed of light and this effective speed:

$$n \stackrel{\text{def}}{=} \frac{c}{v} = c\sqrt{\mu\epsilon}.$$

As well, it is typical to define the material impedance⁹ Z by:

$$Z = \sqrt{\frac{\mu}{\epsilon}}.$$

The importance of n and Z will reveal themselves over the coming questions and we will see that they are directly experimentally accessible (which is why they are quantities of interest to define). Show that μ and ϵ can be recovered from n and Z by:

$$\epsilon = \frac{n}{cZ}, \quad \mu = \frac{nZ}{c}.$$

- (c) Show that from the effective action, the effective energy conservation law is given by:

$$\frac{\partial \mathcal{E}_{\text{eff}}}{\partial t} + \nabla \cdot \vec{S}_{\text{eff}} = -\vec{E} \cdot \vec{J}_f$$

where the effective energy density $\mathcal{E}_{\text{eff}}$ and effective Poynting vector $\vec{S}_{\text{eff}}$ are given by:

$$\mathcal{E}_{\text{eff}} = \frac{\epsilon}{2} |\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu}, \quad \vec{S}_{\text{eff}} = \frac{1}{\mu} \vec{E} \times \vec{B} = \vec{E} \times \vec{H}.$$

As well, show that the effective momentum conservation law is given by:

$$\frac{\partial \vec{\varphi}_{\text{eff}}}{\partial t} - \nabla \cdot \hat{\sigma}_{\text{eff}} = -\rho_f \vec{E} - \vec{J}_f \times \vec{B}$$

where the effective momentum density $\vec{\varphi}_{\text{eff}}$ and effective stress tensor $\hat{\sigma}_{\text{eff}}$ are given by:

$$\vec{\varphi}_{\text{eff}} = \epsilon \vec{E} \times \vec{B} = \frac{\vec{S}}{v^2}, \quad \hat{\sigma}_{\text{eff}} = \epsilon \vec{E} \vec{E}^T + \frac{1}{\mu} \vec{B} \vec{B}^T - \left(\frac{\epsilon}{2} |\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu} \right) \mathbb{1}.$$

- (d) Show that the time averaged effective Poynting vector of a pure plane-wave solution normalized as in

⁹The name impedance is given because in SI units this combination has the same units as electrical impedance. However, this Z has no relation to electrical impedance in the sense of circuits.

problem 4.38 becomes:

$$\mathbb{T}(\vec{S}_{\text{eff}}) = \frac{|\vec{E}|^2}{2Z} \hat{k}.$$

Please note that while all of these effective results are very nice, their existence requires a tower of additional conditions to apply on top of the usual Maxwell's equations and so these effective quantities provide far less general notions of energy, momentum, stress, and etc. than the completely general formulation given by simply using the full Maxwell's equations with the full charge and current densities. As well, the simple replacement rule of replacing $\epsilon_0, \mu_0, \rho, \vec{J}$ by $\epsilon, \mu, \rho_f, \vec{J}_f$ we see only holds in general as a meaningful thing to do when the matter satisfies every possible simplifying assumption. And importantly, the effective energy density, momentum density, etc. under this rule are not equal to the electromagnetic energy density, momentum density, etc. Instead they are those electromagnetic quantities plus contributions from the energy density, momentum density, etc. due to the interaction of the electromagnetic fields with the matter.

Problem 4.40: The Polarization Ellipse. Consider Maxwell's equations for Fourier amplitudes in simple matter.

- (a) For simplicity, let the z -direction be the direction of $\vec{k}$ and choose the origin of t smartly. Show that for some real numbers $\tilde{E} > 0$, $\varphi \in (-\frac{\pi}{2}, \frac{\pi}{2}]$, and $\theta \in [0, \frac{\pi}{2}]$ a single pure plane-wave solution (called a monochromatic solution) for the electric field to Maxwell's equations can be written as:

$$\vec{E} = \text{Re} \left(\tilde{E} \vec{\xi} e^{i(kz - \omega t)} \right)$$

where the polarization vector $\vec{\xi}$ is given by:

$$\vec{\xi} = e^{-i\varphi} \cos \theta \vec{t}_x + e^{i\varphi} \sin \theta \vec{t}_y.$$

- (b) Show that the x and y components of the electric field are given by:

$$E_x = \tilde{E} \cos \theta \cos(kz - \omega t - \varphi), \quad E_y = \tilde{E} \sin \theta \cos(kz - \omega t + \varphi).$$

- (c) Consider a rotated set of coordinates (x', y', z') rotated by an angle β about the z axis with respect to (x, y, z) . Show that for some constants $\tilde{E}'_x > 0$ and $\tilde{E}'_y$, a smart choice of the origin of the z axis, and a particular choice of β , E'_x and E'_y can be put into the form:

$$E'_x = \tilde{E}'_x \cos(kz - \omega t), \quad E'_y = \tilde{E}'_y \sin(kz - \omega t).$$

- (d) Thus, show that the electric field vector of a plane wave in general traces out an ellipse in the plane orthogonal to its propagation. So, the general polarization of an electromagnetic field is called elliptical polarization. Note that the ellipse is traced out in a right-handed corkscrew about the z -axis for $\tilde{E}'_y < 0$ and in a left-handed corkscrew about the z -axis for $\tilde{E}'_y > 0$.
- (e) Consider the special case $\tilde{E}'_y = 0$. Show that the ellipse actually reduces to a line segment. This special case is called linear (or rectangular) polarization. Show that if ξ is given by any linear combination of $\vec{t}_x$ and $\vec{t}_y$ with real coefficients then the result is linearly polarized.
- (f) Consider the special case of $|\tilde{E}'_y| = \tilde{E}'_x$. Show that the ellipse reduces to a circle. This special case is called circular polarization. Show that the two linearly independent polarization vectors:

$$\vec{\xi}_+ = \frac{\vec{t}_x + i\vec{t}_y}{\sqrt{2}}, \quad \vec{\xi}_- = \frac{\vec{t}_x - i\vec{t}_y}{\sqrt{2}}$$

both give circular polarizations (with $\vec{\xi}_+$ right-handed and $\vec{\xi}_-$ left-handed) and form a basis for a general polarization.

- (g) Show that the circular polarizations satisfy:

$$i\vec{k} \times \vec{\xi}_{\pm} = \pm |\vec{k}| \vec{\xi}_{\pm}.$$

Thus, the circular polarizations are eigenvectors of the cross product. This equation is convenient as it no longer references any specific orientation for $\vec{k}$ and thus serves to define $\vec{\xi}_{\pm}$ when $\vec{k}$ does not point in the z direction. Note: because the cross product $\vec{k} \times$ can be written as a 3x3 anti-symmetric matrix, it does in fact have a third eigenvector ($\vec{k}$ is the eigenvector and it has eigenvalue 0).

Problem 4.41: Polarizers and Jones Calculus. Consider a monochromatic solution to Maxwell's

equation in simple matter so that the electric field takes the form:

$$\vec{E} = \text{Re}(\tilde{\vec{E}} e^{i(\vec{k} \cdot \vec{x} - \omega t)}).$$

Take the z -direction to be the direction of $\vec{k}$ and so for the rest of this question write $\tilde{\vec{E}}$ as:

$$\tilde{\vec{E}} = \begin{pmatrix} \tilde{E} e^{i\varphi_x} \cos \theta \\ \tilde{E} e^{i\varphi_y} \sin \theta \end{pmatrix}$$

for some real parameters $\tilde{E}, \varphi_x, \varphi_y, \theta$ and where it is understood that these two components are in the x, y directions. This form is called the “Jones vector” for the plane wave. Many pieces of experimental equipment act (approximately) linearly on the electromagnetic waves they are intended to manipulate (sometimes naturally and sometimes designed to be so with significant effort). Due to linearity, the action of such a linear component on the Jones vector can be represented by some matrix 2x2 complex matrix $\hat{J}$. Thus, after passing through the component the resulting Jones vector is:

$$\tilde{\vec{E}}' = \hat{J} \tilde{\vec{E}}.$$

- (a) Suppose a plane wave crosses through a sequence of three linear components in the order of $\hat{J}_1$ then $\hat{J}_2$ then $\hat{J}_3$. Show that the resulting Jones vector is:

$$\tilde{\vec{E}}' = \hat{J}_3 \hat{J}_2 \hat{J}_1 \tilde{\vec{E}}.$$

Thus, the effective Jones matrix of a sequence of components is the matrix product of those components in the order in which they are passed through (with the earliest to the right and the latest to the left).

- (b) One of the most common components is a linear polarizer. A linear polarizer is a component which allows a linear polarization in a particular direction to pass through without any effect and which completely blocks the orthogonal linear polarization to the one which is allowed. They can come in many forms including thin sheets of film, certain crystals, or wire grids. Show that the Jones matrix for an x direction linear polarizer is given by:

$$\hat{J}_x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

that the Jones matrix for a y direction linear polarizer is given by:

$$\hat{J}_y = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

and that the Jones matrix for a linear polarizer with allowed direction $\cos \alpha \vec{t}_x + \sin \alpha \vec{t}_y$ is given by:

$$\hat{J} = \begin{pmatrix} \cos^2 \alpha & \sin \alpha \cos \alpha \\ \sin \alpha \cos \alpha & \sin^2 \alpha \end{pmatrix}.$$

- (c) Consider a monochromatic plane wave which is linearly polarized (the x and y components are in-phase with each other). Suppose this wave passes through a linear polarizer which makes an angle θ with respect to the direction of the incoming Jones vector. Show that the intensity $\mathcal{I}'$ of the resulting wave is related to the intensity $\mathcal{I}$ of the incoming wave by:

$$\mathcal{I}' = \mathcal{I} \cos^2 \theta.$$

This result is known as Malus' law.

- (d) The following experiment illustrates a funny consequence of Malus' law which many find surprising before they have become comfortable with the mechanics of polarization. Consider a linearly polarized plane wave in the x direction which then reaches a y linear polarizer. Show that the intensity of the wave which comes out of the other end of the polarizer is 0 (and thus there is no wave which comes out). Now consider placing another linear polarizer before the y polarizer at an angle θ with respect to the x axis. Show that the resulting intensity of the final wave is now:

$$\mathcal{I}' = \frac{\mathcal{I}}{4} \sin^2(2\theta)$$

and so now with a second polarizer placed in front of the first, in fact more light gets through in the end than when no such polarizer was placed. Show that the maximum intensity occurs for $\theta = \frac{\pi}{4}$.

- (e) Consider now a linearly polarized plane wave in the x direction which then reaches a sequence of N

polarizers each rotated by an angle θ/N in the same direction with respect to the polarizer before it. Show that the final intensity of the light after passing through all of the polarizers is given by:

$$\mathcal{I}' = \mathcal{I} \cos^{2N} \left(\frac{\theta}{N} \right).$$

As well, show that in the limit $N \rightarrow \infty$, $\mathcal{I}' = \mathcal{I}$. Thus, in the limit of continuously deforming polarization one can make a device which fully rotates the polarization of the incoming beam by an arbitrary amount without losing any intensity.

- (f) Consider a linear component which performs a perfect polarization rotation by an angle θ without changing the intensity or having any phase effects. Show that its Jones matrix is given by:

$$\hat{J} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

- (g) Another common component is a circular polarizer. Let $\hat{J}_+$ be the Jones matrix for a circular polarizer which projects out only the right-handed circular polarization, not allowing through any left-handed component and $\hat{J}_-$ be likewise with the opposite handedness. Show that they are given by:

$$\hat{J}_{\pm} = \frac{1}{2} \begin{pmatrix} 1 & \mp i \\ \pm i & 1 \end{pmatrix}.$$

- (h) One final component which is very common is a phase modulator, which causes a relative phase shift between different polarizations. Consider a phase modulator $\hat{J}$ which through which an x polarized wave develops a phase of α_x and through which a y polarized wave develops a phase of α_y . Show then that $\hat{J}$ is given by:

$$\hat{J} = \begin{pmatrix} e^{i\alpha_x} & 0 \\ 0 & e^{i\alpha_y} \end{pmatrix}.$$

Problem 4.42: Partially Polarized Light and Density Matrices. Generally, the quantities of interest in electromagnetism depend quadratically on the fields. For example, the energy density, linear momentum density, angular momentum density, dynamic energy moment density, and stress tensor are all quadratic in the fields. As well, we are typically only interested in time-averages of these quantities due to the limited ability to measure instantaneous values of them in experiment.

- (a) Show that a quantity of interest as described above can be written as a quadratic form in the $\vec{E}$ and $\vec{B}$ fields as:

$$G = (\vec{E}^T \quad \vec{B}^T) \hat{g} \begin{pmatrix} \vec{E} \\ \vec{B} \end{pmatrix}$$

where $\hat{g}$ is a real 6x6 symmetric matrix ($\hat{g}^T = \hat{g}$).

- (b) Consider $\vec{E}$ and $\vec{B}$ to be monochromatic solutions to Maxwell's equations in simple matter. Show that for electric field amplitude $\vec{E}$ and some matrix 2x2 complex $\hat{G}$ the time-averaged value of G can be written:

$$\mathbb{T}(G) = \vec{E}^\dagger \hat{G} \vec{E}.$$

where $\vec{E}^\dagger$ is the complex conjugate of the transpose of $\vec{E}$ (called the Hermitian adjoint or just adjoint¹⁰) of $\vec{E}$. Show that because $\mathbb{T}(G)$ is real-valued for all $\vec{E}$, it must be the case that $\hat{G}^\dagger = \hat{G}$. Such a matrix is called Hermitian. By the spectral theorem of linear algebra, Hermitian matrices are diagonalizable by an orthonormal basis of eigenvectors and have real eigenvalues.

- (c) Find the $\hat{G}$ matrix for each of the examples given in the problem preamble. For simplicity, define the z direction to be the direction of the wavenumber vector $\vec{k}$.
- (d) Show that alternatively one can write the time-averaged G as:

$$\mathbb{T}(G) = \text{Tr}(\hat{G}\hat{\rho})$$

where $\hat{\rho} = \vec{E} \vec{E}^\dagger$ is called the density matrix and Tr is the matrix trace. Show in particular that the

¹⁰In general, adjoint has a more general and technical meaning in mathematics but for our purposes it will coincide with the Hermitian adjoint, which is the complex conjugate transpose

density matrix is Hermitian, its eigenvalues are nonnegative, and that its trace is given by:

$$\text{Tr}(\hat{\rho}) = 2Z\mathcal{I}$$

where $\mathcal{I}$ is the intensity of the wave and Z is the material impedance of the medium.

- (e) Consider a source of electromagnetic waves in which the produced wave does not have an exactly predictable $\vec{E}$ due to there being more variables at work in the source than we have accounted for. Consequently, one must model the source as producing the different possible values of $\vec{E}$, which we call $\vec{E}_1, \vec{E}_2, \dots$ each with probability $p_1, p_2, \dots$. Each wave emitted from the source will have some independently selected $\vec{E}$ from this distribution. Explain then that as is typical in experiment by sampling many waves from the source one can measure the expected value of any of the previously mentioned quantities of interest defined by:

$$\mathbb{E}(G) = \sum_n p_n \mathbb{T}(\vec{E}_n^\dagger \hat{G} \vec{E}_n).$$

As well, show that one can **NOT** in general identify a vector $\vec{E}_0$ so that:

$$\mathbb{E}(G) \stackrel{!}{=} \mathbb{T}(\vec{E}_0^\dagger \hat{G} \vec{E}_0)$$

and thus that there is no way to define an effective Fourier amplitude for a probabilistic source. However, show that one can in general define the density matrix $\hat{\rho}$ so that:

$$\hat{\rho} = \sum_n p_n \vec{E}_n \vec{E}_n^\dagger, \quad \mathbb{E}(G) = \text{Tr}(\hat{G} \hat{\rho}).$$

As well, show that in addition to reducing to the original expression given for the density matrix in the case that only one value of $\vec{E}$ is possible, this general density matrix is also Hermitian, has nonnegative eigenvalues, and has trace given by:

$$\text{Tr}(\hat{\rho}) = 2Z\mathbb{E}(\mathcal{I}).$$

Thus, while the Fourier-amplitude description cannot be generalized to the case of a probabilistic source, the density matrix description can. Many sources are effectively probabilistic, such as light bulbs or the Sun (which essentially produce all polarizations uniformly often), due to them having very complicated internal dynamics and little if any bias toward any particular directions of polarizations. Thus, for modeling real equipment the density matrix formalism is often a necessity.

- (f) Show that if light from such a source passes through a linear component with Jones matrix $\hat{J}$ the density matrix afterward is given by:

$$\hat{\rho}' = \hat{J} \hat{\rho} \hat{J}^\dagger.$$

As well, show that if a sequence of multiple (say 3) components of Jones matrices $\hat{J}_1, \hat{J}_2, \hat{J}_3$ are passed through in that order the resulting density matrix is:

$$\hat{\rho}' = \hat{J}_3 \hat{J}_2 \hat{J}_1 \hat{\rho} \hat{J}_1^\dagger \hat{J}_2^\dagger \hat{J}_3^\dagger.$$

- (g) Show that there exists an effective Fourier amplitude $\vec{E}_0$ for a given density matrix (meaning $\hat{\rho} = \vec{E}_0 \vec{E}_0^\dagger$) if and only if $\text{Tr}(\hat{\rho}^2) = (\text{Tr}(\hat{\rho}))^2$ or (because $\hat{\rho}$ is a 2x2 matrix) equivalently if and only if $\det(\hat{\rho}) = 0$. Such a source is called completely polarized.
- (h) Consider a light source which produces all polarizations uniformly. That is, the parameters φ_x, φ_y , and θ defined for a Jones vector sampled from it are uniformly distributed. Show that the corresponding density matrix is proportional to the identity matrix. Such a light source is called “unpolarized”. Show that unpolarized light produces the same expected values $\text{Tr}(\hat{G} \hat{\rho})$ as a light source which takes x and y linear polarizations each with probability 1/2 or as well a light source which takes each of the two circular polarizations each with probability 1/2.
- (i) Using that $\hat{\rho}$ is a 2x2 Hermitian matrix, show that for real parameters S_0, S_1, S_2, S_3 (called Stokes’

parameters) the density matrix can be written:

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} S_0 + S_3 & S_1 - iS_2 \\ S_1 + iS_2 & S_0 - S_3 \end{pmatrix}.$$

Show that $S_0 = Z\mathbb{E}(\mathcal{I})$. Let d , the “degree of polarization” be defined by:

$$d = \frac{\sqrt{S_1^2 + S_2^2 + S_3^2}}{S_0}.$$

Show that $0 \leq d \leq 1$ with $d = 0$ if and only if the source is unpolarized and $d = 1$ if and only if the source is completely polarized.

- (j) Show that the density matrix can be written as the sum of a completely unpolarized part of intensity $\mathcal{I}_u$ and a completely polarized part of intensity $\mathcal{I}_p$ and polarization $\vec{\xi}$ as:

$$\hat{\rho} = Z\mathcal{I}_u \mathbb{1} + 2Z\mathcal{I}_p \vec{\xi} \vec{\xi}^\dagger$$

and find the relationship between $\mathcal{I}_u, \mathcal{I}_p$, the Jones parameters which define $\vec{\xi}$, and the four Stokes parameters. As well, show that the total expected intensity is given by $\mathbb{E}\mathcal{I} = \mathcal{I}_u + \mathcal{I}_p$ and that the degree of polarization can be reexpressed as:

$$d = \frac{\mathcal{I}_p}{\mathcal{I}_p + \mathcal{I}_u}$$

and thus can be understood as the fraction of the total intensity which is due to polarized light.

Problem 4.43: Stokes Vectors and Mueller Calculus. Consider a beam of light with polarization state represented by the density matrix $\hat{\rho}$ as in the previous problem. Define the following matrices:

$$\sigma^0 = \mathbb{1}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- (a) Show that any 2x2 Hermitian matrix $\hat{G}$ can be written for some real coefficients G_0, G_1, G_2, G_3 as:

$$\hat{G} = G_0\sigma^0 + G_1\sigma^1 + G_2\sigma^2 + G_3\sigma^3 = G_\mu\sigma^\mu$$

where the index μ is used for implicit summation and ranges from 0 to 3.

- (b) Show that:

$$\text{Tr}(\sigma^\mu \sigma^\nu) = 2\delta^{\mu\nu}.$$

- (c) Define for a Hermitian matrix $\hat{G}$ the 4 dimensional vector $\vec{G} = (G_0, G_1, G_2, G_3)$ and define the Stokes vector $\vec{S} = (S_0, S_1, S_2, S_3)$ so that $S_\mu = \mathbb{E}(\sigma_\mu)$. Show then that:

$$\mathbb{E}(G) = \text{Tr}(\hat{\rho}\hat{G}) = S_\mu G_\mu = \vec{G} \cdot \vec{S}, \quad S_\mu = \text{Tr}(\sigma^\mu \hat{\rho}), \quad G_\mu = \frac{1}{2} \text{Tr}(\sigma^\mu \hat{G}).$$

- (d) Show that if light from a source of Stokes vector $\vec{S}$ passes through a linear component with Jones matrix $\hat{J}$ the resultant Stokes vector satisfies:

$$\vec{S}' = \hat{M}\vec{S}$$

where the real 4x4 matrix $\hat{M}$, called the Mueller matrix, has components given by:

$$M_{\mu\nu} = \frac{1}{2} \text{Tr}(\sigma_\mu \hat{J} \sigma_\nu \hat{J}^\dagger).$$

- (e) Find the Mueller matrix for each of the following: a linear polarizer at angle θ with respect to the x direction, a polarization rotator which rotates by an angle θ , a left circular polarizer, a right circular polarizer, and a phase modulator.
- (f) Sometimes, even the components of a system will be probabilistic in their macroscopic behavior due to their complicated internal dynamics. As such, it is sometimes appropriate to model a linear component as having Jones matrix $\hat{J}_1$ with probability p_1 , $\hat{J}_2$ with probability p_2 , and so on. Let $\hat{\rho}'_n$ be the density matrix of a source with incoming density matrix $\hat{\rho}$ after passing through such a component when it had Jones matrix $\hat{J}_n$. Because the component has probabilistic behavior, it is necessary to now sample many times results and use statistical averages to make experimental measurements. So, for a quantity of interest G (with associated $\hat{G}$) for the light after passing through the component define the expected

value $\mathbb{E}(G)$ by averaging over the possible results of the component:

$$\mathbb{E}(G) = \sum_n p_n \text{Tr}(\hat{G}\hat{\rho}'_n).$$

Show that equivalently one may write:

$$\mathbb{E}(G) = \text{Tr}(\hat{G}\hat{\rho}')$$

where the effective density matrix $\hat{\rho}'$ is given by:

$$\hat{\rho}' = \sum_n p_n \hat{\rho}'_n.$$

As well, show that $\hat{\rho}'$ is Hermitian, has nonnegative eigenvalues, and has trace:

$$\text{Tr}(\hat{\rho}') = 2Z\mathbb{E}(\mathcal{I}).$$

Thus, even in the case of probabilistic Jones matrix, one can identify an effective density matrix.

(g) Show that the $\hat{\rho}'$ of the previous part is related to $\hat{\rho}$ by:

$$\hat{\rho}' = \sum_n p_n \hat{J}_n \hat{\rho} \hat{J}_n^\dagger$$

and thus explain that it is **NOT** in general possible to define an effective Jones matrix $\hat{J}_0$ for a probabilistic component so that:

$$\hat{\rho}' \stackrel{!}{=} \hat{J}_0 \hat{\rho} \hat{J}_0^\dagger.$$

However, show that the Stokes vector $\vec{S}'$ corresponding to $\hat{\rho}'$ is related to the Stokes vector $\vec{S}$ corresponding to $\hat{\rho}$ by:

$$\vec{S}' = \hat{M} \vec{S}$$

where $\hat{M}$ has components given by:

$$M_{\mu\nu} = \sum_n \frac{1}{2} p_n \text{Tr}(\sigma_\mu \hat{J}_n \sigma_\nu \hat{J}_n^\dagger).$$

Thus, in the case of probabilistic components, while it is typically not possible to define an effective Jones matrix it is possible to define an effective Mueller matrix. So, probabilistic sources demand the density matrix formalism and probabilistic components demand the Stokes vector and Mueller matrix formalism.

Problem 4.44: ★ Normal Mode Decomposition of the Electromagnetic Hamiltonian. We have found that the Fourier transform leads to very helpful simplifications at the level of the equations of motion. Here we will see that it is equally helpful at the level of the Hamiltonian.

(a) Define for a function $f(t, \vec{x})$ the spatial Fourier transform $\tilde{f}(t, \vec{k})$:

$$\tilde{f}(t, \vec{k}) = \int_{\mathbb{S}} e^{-i\vec{k} \cdot \vec{x}} f(t, \vec{x}) \frac{d^3 \vec{x}}{(2\pi)^{\frac{3}{2}}} \implies f(t, \vec{x}) = \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \tilde{f}(t, \vec{k}) \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}.$$

Show that for real-valued functions $f(t, \vec{x})$ and $g(t, \vec{x})$:

$$\begin{aligned} f^*(t, -\vec{k}) &= f(t, \vec{k}) \\ \int_{\mathbb{S}} f(t, \vec{x}) g(t, \vec{x}) d^3 \vec{x} &= \int_{\mathbb{K}} \tilde{f}^*(t, \vec{k}) \tilde{g}(t, \vec{k}) d^3 \vec{k}. \end{aligned}$$

(b) Show that the electromagnetic Hamiltonian in terms of Fourier components becomes:

$$\mathcal{H} = \int_{\mathbb{K}} \left(\frac{|\tilde{P}_A(t, \vec{k})|^2}{2\epsilon_0} + \frac{|i\vec{k} \times \tilde{A}(t, \vec{k})|^2}{2\mu_0} - \tilde{J}^*(t, \vec{k}) \cdot \tilde{A}(t, \vec{k}) + \tilde{\phi}^*(t, \vec{k}) \left(\tilde{\rho}(t, \vec{k}) + i\vec{k} \cdot \tilde{P}_A(t, \vec{k}) \right) \right) d^3 \vec{k}.$$

(c) Let $\vec{\xi}_0(\vec{k}) = i\frac{\vec{k}}{|\vec{k}|}$, $\vec{\xi}_1(\vec{k}) = \vec{\xi}_+(\vec{k})$, $\vec{\xi}_{-1}(\vec{k}) = \vec{\xi}_-(\vec{k})$ where $\vec{\xi}_\pm(\vec{k})$ are the circular polarization vectors found at the end of problem 4.40. Show that:

$$i\vec{k} \times \vec{\xi}_m = m|\vec{k}|\vec{\xi}_m, \quad \vec{\xi}_m^*(-\vec{k}) = \vec{\xi}_m(\vec{k}), \quad \vec{\xi}_m^\dagger \vec{\xi}_{m'} = \delta_{mm'}, \quad \sum_{m=-1}^1 \vec{\xi}_m \vec{\xi}_m^\dagger = \mathbb{1}.$$

Here m is called the “helicity” of $\vec{\xi}_m$.

(d) For a vector field $\vec{f}(t, \vec{k})$, define:

$$\vec{f}_m(t, \vec{k}) = \vec{\xi}_m^\dagger(\vec{k}) \vec{f}(t, \vec{k}) \implies \vec{f}(t, \vec{k}) = \sum_m \vec{f}_m(t, \vec{k}) \vec{\xi}_m(\vec{k}).$$

This is called the helicity basis representation of $\vec{f}$. Show that in the helicity basis the electromagnetic Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{K}} \left(\sum_{h \in \{-1, 1\}} \left(\frac{|\tilde{P}_{Ah}|^2}{2\epsilon_0} + \frac{\epsilon_0 c^2 |\vec{k}|^2 |\tilde{A}_h|^2}{2} - \tilde{J}_h^* \tilde{A}_h \right) + \frac{|\tilde{P}_{A0}|^2}{2\epsilon_0} - \tilde{J}_0^* \tilde{A}_0 + \tilde{\phi}^* (\tilde{\rho} - |\vec{k}| \tilde{P}_{A0}) \right) d^3 \vec{k}$$

with the Poisson brackets:

$$\{\tilde{A}_m(t, \vec{k}), \tilde{A}_{m'}(t, \vec{k}')\} = 0, \quad \{\tilde{A}_m(t, \vec{k}), \tilde{P}_{Am'}(t, \vec{k}')\} = \delta_{mm'} \delta(\vec{k} + \vec{k}'), \quad \{\tilde{P}_{Am}(t, \vec{k}), \tilde{P}_{Am'}(t, \vec{k}')\} = 0.$$

As well, show that under a gauge transformation so that:

$$\phi'(t, \vec{x}) = \phi(t, \vec{x}) - \frac{\partial f}{\partial t}(t, \vec{x}), \quad \vec{A}'(t, \vec{x}) = \vec{A}(t, \vec{x}) + \nabla f(t, \vec{x})$$

it follows that:

$$\tilde{\phi}' = \tilde{\phi} - \frac{\partial \tilde{f}}{\partial t}, \quad \tilde{A}'_{-1} = \tilde{A}_{-1}, \quad \tilde{A}'_0 = \tilde{A}_0 + |\vec{k}| \tilde{f}, \quad \tilde{A}'_1 = \tilde{A}_1.$$

Thus only the component parallel to the wavevector (called the “longitudinal mode”) of the vector potential is not gauge invariant.

(e) Define now the mode vector $\vec{a}(t, \vec{k})$ for $h \in \{-1, 1\}$ by:

$$\vec{a}(t, \vec{k}) = a_{-1}(t, \vec{k}) \vec{\xi}_{-1}(\vec{k}) + a_1(t, \vec{k}) \vec{\xi}_1(\vec{k})$$

$$a_h(t, \vec{k}) = \sqrt{\frac{\epsilon_0 c |\vec{k}|}{2}} \tilde{A}_h(t, \vec{k}) + \frac{i}{\sqrt{2\epsilon_0 c |\vec{k}|}} \tilde{P}_{Ah}(t, \vec{k}).$$

Show that:

$$\tilde{A}_h(t, \vec{k}) = \frac{a_h(t, \vec{k}) + a_h^*(t, -\vec{k})}{\sqrt{2\epsilon_0 c |\vec{k}|}}, \quad \tilde{P}_{Ah}(t, \vec{k}) = \frac{1}{i} \sqrt{\frac{\epsilon_0 c |\vec{k}|}{2}} (a_h(t, \vec{k}) - a_h^*(t, -\vec{k}))$$

$$\mathcal{H} = \int_{\mathbb{K}} \left(\sum_h \left(c |\vec{k}| a_h^* a_h - \sqrt{\frac{2}{\epsilon_0 c |\vec{k}|}} \text{Re}(\tilde{J}_h^* a_h) \right) + \frac{|\tilde{P}_{A0}|^2}{2} - \tilde{J}_0^* \tilde{A}_0 + \tilde{\phi}^* (\tilde{\rho} - |\vec{k}| \tilde{P}_{A0}) \right) d^3 \vec{k}$$

with the Poisson brackets:

$$\{a_h(t, \vec{k}), a_{h'}(t, \vec{k}')\} = 0, \quad \{a_h(t, \vec{k}), a_{h'}^*(t, \vec{k}')\} = -i \delta_{hh'} \delta(\vec{k} - \vec{k}'), \quad \{a_h, \tilde{A}_0\} = \{a_h, \tilde{P}_{A0}\} = 0.$$

(f) Show that the equations of motion of the above Hamiltonian are:

$$\frac{\partial \tilde{A}_0}{\partial t} + |\vec{k}| \tilde{\phi} = \tilde{P}_{A0} = \frac{\tilde{\rho}}{|\vec{k}|}, \quad i \frac{\partial a_h}{\partial t} = c |\vec{k}| a_h - \frac{\tilde{J}_h}{\sqrt{2\epsilon_0 c |\vec{k}|}}.$$

Thus, in these coordinates the different helicities and wavenumbers decouple from each other. As well, take the time derivative of the a_h equation of motion to show that it satisfies:

$$\frac{\partial^2 a_h}{\partial t^2} + c^2 |\vec{k}|^2 a_h = \sqrt{\frac{c |\vec{k}|}{2\epsilon_0}} \tilde{J}_h + \frac{i}{\sqrt{2\epsilon_0 c |\vec{k}|}} \dot{\tilde{J}}_h.$$

Thus, a_h in fact evolves as a driven harmonic oscillator and the original equation of motion is just the way to write a driven harmonic oscillator in complex coordinates. And so, Maxwell’s equations truly consist of a constraint equation to conserve charge and infinitely many independent harmonically oscillating Fourier modes.

(g) Consider the case of free electromagnetism ($\rho = 0, \vec{J} = 0$). Show that one can take by gauge

transformation $\tilde{A}_0 = \tilde{\phi} = 0$ and that in this gauge:

$$\begin{aligned}\vec{A}(t, \vec{x}) &= \text{Re} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \vec{a}(t, \vec{k}) \sqrt{\frac{2}{\epsilon_0 c |\vec{k}|}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} = \text{Re} \int_{\mathbb{K}} e^{i(\vec{k} \cdot \vec{x} - c|\vec{k}|t)} \vec{a}(0, \vec{k}) \sqrt{\frac{2}{\epsilon_0 c |\vec{k}|}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} \\ \vec{E}(t, \vec{x}) &= -\frac{\vec{P}_A(t, \vec{x})}{\epsilon_0} = -\text{Im} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \vec{a}(t, \vec{k}) \sqrt{\frac{2c|\vec{k}|}{\epsilon_0}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} = -\text{Im} \int_{\mathbb{K}} e^{i(\vec{k} \cdot \vec{x} - c|\vec{k}|t)} \vec{a}(0, \vec{k}) \sqrt{\frac{2c|\vec{k}|}{\epsilon_0}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} \\ \vec{B}(t, \vec{x}) &= -\text{Im} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \hat{k} \times \vec{a}(t, \vec{k}) \sqrt{\frac{2|\vec{k}|}{\epsilon_0 c}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} = -\text{Im} \int_{\mathbb{K}} e^{i(\vec{k} \cdot \vec{x} - c|\vec{k}|t)} \hat{k} \times \vec{a}(0, \vec{k}) \sqrt{\frac{2|\vec{k}|}{\epsilon_0 c}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}\end{aligned}$$

where $\hat{k} = \frac{\vec{k}}{|\vec{k}|}$. Thus, show that $\vec{a}(0, \vec{k})$ is in fact related to the electric field Fourier amplitude by:

$$\tilde{E}(\vec{k}) = i\vec{a}(0, \vec{k}) \sqrt{\frac{2c|\vec{k}|}{\epsilon_0}}.$$

- (h) Show that the energy, linear momentum, angular momentum, and dynamic energy moment for free electromagnetism can be expressed in terms of the mode vector as:

$$\begin{aligned}E &= \int_{\mathbb{K}} c|\vec{k}| \vec{a}^\dagger \vec{a} d^3 \vec{k} \\ \vec{P} &= \int_{\mathbb{K}} \vec{k} \vec{a}^\dagger \vec{a} d^3 \vec{k} \\ \vec{J} &= \int_{\mathbb{K}} \sum_h \left(h\hat{k} a_h^* a_h - a_h^* \left(i\vec{k} \times \frac{\partial}{\partial \vec{k}} \right) a_h \right) d^3 \vec{k} \\ \vec{K} &= ct\vec{P} - \text{Re} \int_{\mathbb{K}} \sum_h a_h^* i|\vec{k}| \frac{\partial a_h}{\partial \vec{k}} d^3 \vec{k}.\end{aligned}$$

Thus, all of the conserved quantities written as wavenumber integrals are proportional to $\vec{a}^\dagger, \vec{a}$.

- (i) Show that the angular momentum formula found in the previous question implies gauge invariant expressions for the total spin angular momentum and total orbital angular momentum of free electromagnetism:

$$\vec{S} = \int_{\mathbb{K}} \sum_h h\hat{k} a_h^* a_h d^3 \vec{k}, \quad \vec{L} = \int_{\mathbb{K}} \sum_h a_h^* \left(-i\vec{k} \times \frac{\partial}{\partial \vec{k}} \right) a_h d^3 \vec{k}$$

where both of these have the required corresponding dependence on the coordinate origin.

Problem 4.45: ★ Phase Velocity, Wave-Packet Velocity, Group Velocity. As waves travel across space, one may wish to identify the “velocity” of the wave. However, as waves are not point objects, to do so is not as straightforward as simply differentiating the position of that single point with respect to time.

- (a) We found in Problem 4.36 that in general a wave freely propagating with no sources in a linear theory has solution of the form:

$$\phi^a(t, \vec{x}) = \text{Re} \int_{\mathbb{K}} \sum_{b=1}^B \xi_b^a(\vec{k}) e^{i(\vec{k} \cdot \vec{x} - \Omega_b(\vec{k})t)} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}.$$

Thus, because the solution can be expanded in terms of plane-waves, we may seek a notion of the velocity of a plane-wave. Consider a function $f(t, \vec{x})$ of the form:

$$f(t, \vec{x}) = F(\vec{x} - \vec{v}t)$$

for some function F and constant $\vec{v}$. Explain that graphically $f(t, \vec{x})$ represents the shape of $F(\vec{x})$ moving at fixed shape at velocity $\vec{v}$. Thus, conclude that a plane-wave moves at velocity:

$$\vec{v}_\varphi(\vec{k}) = \frac{\Omega(\vec{k})}{|\vec{k}|} \hat{k}$$

where $\hat{k} = \frac{\vec{k}}{|\vec{k}|}$. This velocity is called the “phase velocity” as it could equivalently be understood as the velocity at which one would have to move in order for the phase of the plane-wave one is traveling in the presence of to be constant along one’s motion. The phase velocity we will find has useful mathematical

applications however it is not actually a good representative for the actual velocity of a general wave. In the first place, it is defined specifically for a plane wave and it is not clear what would be the correct generalization for a linear combination of plane waves. As well, the phase velocity turns out not to be the velocity at which the energy or linear momentum or any other experimentally useful quantities are propagated at by waves. This is because plane-waves are infinite in their extent; they do not decay at all in any direction whereas actual wave solutions produced experimentally are compactly supported – they do not extend arbitrarily far out. This essential difference in form between plane-waves and real waves¹¹ makes the velocity of plane-waves essentially irrelevant for characterizing the velocity of real wave packets. The index of refraction n in general for light is defined as the ratio of the speed of light c to the magnitude of the phase velocity:

$$n = \frac{c}{|\vec{v}_\varphi|}.$$

It will turn out that the main use of the phase velocity is through the index of refraction, which is essential for understanding the propagation of light through material interfaces.

- (b) We found in Problem 4.44 that the quantities of interest in electromagnetism can be written as integrals over wavenumber of quantities of the form $\vec{a}^\dagger G\left(\vec{k}, \frac{\partial}{\partial \vec{k}}\right) \vec{a}$ where G is determined by the particular quantity. In fact, this structure generalizes and as we will prove in section 8.2; the Hamiltonian of any linear order stable wave theory with translational symmetry can be (by canonical transformation) be put into the form of:

$$\mathcal{H} = \int_{\mathbb{K}} \sum_n \Omega_n a_n^*(t, \vec{k}) a_n(t, \vec{k}) d^3 \vec{k}$$

and in general the generators of transformations of this theory are of the form:

$$\mathcal{G} = \int_{\mathbb{K}} \sum_n a_n^*(t, \vec{k}) G_n\left(\vec{k}, \frac{\partial}{\partial \vec{k}}\right) a_n(t, \vec{k}) d^3 \vec{k}.$$

As such, we can see that any generator can essentially be computed by a weighted integral of some functions G_n weighted by these factors of a_n^* and a_n . By construction, these a_n satisfy the Poisson brackets:

$$\{a_n(t, \vec{k}), a_{n'}(t, \vec{k}')\} = 0, \quad \{a_n(t, \vec{k}), a_{n'}^*(t, \vec{k}')\} = -i\delta_{nn'}\delta(\vec{k} - \vec{k}').$$

Show that the equation of motion for these $a_n(t, \vec{k})$ are:

$$i \frac{\partial a_n}{\partial t} = \Omega_n(\vec{k}) a_n(t, \vec{k})$$

and thus these $a_n(t, \vec{k})$ evolve as complex harmonic oscillators and are decoupled from each other at different values of n and $\vec{k}$.

- (c) Because the a_n decouple for each different n , we can consider each n separately (which is equivalent to considering a theory with only one value of n). So, take:

$$\mathcal{H} = \int_{\mathbb{K}} \Omega(\vec{k}) a^*(t, \vec{k}) a(t, \vec{k}) d^3 \vec{k}.$$

This $a(t, \vec{k})$ is defined on wavenumber space; in experiment though we work with waves in actual position space. So, define the wavefunction $\psi(t, \vec{x})$ by the inverse Fourier transform of $a(t, \vec{k})$:

$$\psi(t, \vec{x}) = \int_{\mathbb{K}} \frac{e^{i\vec{k} \cdot \vec{x}}}{(2\pi)^{\frac{3}{2}}} a(t, \vec{k}) d^3 \vec{k}.$$

Then, using our previous integral facts about the Fourier transform, show that all generators $\mathcal{G}$ can be rewritten for some functions $G'(\vec{x}, \frac{\partial}{\partial \vec{x}})$ as:

$$\mathcal{G} = \int_{\mathbb{K}} \psi^*(t, \vec{x}) G'\left(\vec{x}, \frac{\partial}{\partial \vec{x}}\right) \psi(t, \vec{x}) d^3 \vec{x}.$$

As such, in position space we can see all generators are given by weighted integrals by ψ^* and ψ . Show

¹¹Here by real waves we mean waves which take finite energy to produce. Plane waves by virtue of not decaying at all with distance lead to non-converging energy integrals; they generically take infinite energy to produce. To see this, attempt to compute the total energy of a plane-wave solution to Maxwell's equations.

that the total wave intensity, given by directly integrating these weighing functions:

$$\mathcal{I} = \int_{\mathbb{K}} \psi^*(t, \vec{x}) \psi(t, \vec{x}) d^3 \vec{x} = \int_{\mathbb{K}} a^*(t, \vec{k}) a(t, \vec{k}) d^3 \vec{k}$$

is constant. Let $\vec{y}(t)$ called the “Wave-Packet position” be given by the intensity-weighted averaged position of the wave:

$$\vec{y}(t) = \frac{\int_{\mathbb{K}} \vec{x} \psi^* \psi d^3 \vec{x}}{\int_{\mathbb{K}} \psi^* \psi d^3 \vec{x}}.$$

This $\vec{y}(t)$ is analogous to center of mass or center of energy position of a continuous distribution of matter where instead of weighing by the mass density of the material, we have weighed by $\psi^* \psi$ (in fact, we will see that often this quantity literally corresponds to mass density). We have chosen this weight specifically because it is of the form identified above to be of relevance in these coordinates. One can see that if the wave ψ is essentially localized near a position $\vec{x}_0$ so that $\psi^* \psi$ is small for $\vec{x}$ away from $\vec{x}_0$, then $\vec{y} \approx \vec{x}_0$. Show then that the “Wave-Packet velocity” defined as the time derivative of $\vec{y}$ is given by:

$$\dot{\vec{y}} = \frac{\int_{\mathbb{K}} \frac{\partial \Omega(\vec{k})}{\partial \vec{k}} a^* a d^3 \vec{k}}{\int_{\mathbb{K}} a^* a d^3 \vec{k}}.$$

and explain that this is the same form of average described before. By definition, this velocity is the velocity at which the “center” or representative position of the wave-packet actually moves. Because of this, this velocity is generally a much better representation of the velocity of an actual wave than any particular application of the phase velocity. Whenever a wave consists mostly of only a narrow band of wavenumbers so that $a^*(\vec{k}) a(\vec{k})$ is small for $\vec{k}$ away from $\vec{k}_0$, show that we can approximate the wave-packet velocity by:

$$\dot{\vec{y}} \approx \frac{\partial \Omega(\vec{k}_0)}{\partial \vec{k}_0}.$$

This right hand side then defines the “group velocity”:

$$\vec{v}_g(\vec{k}) = \frac{\partial \Omega(\vec{k})}{\partial \vec{k}}.$$

So, the phase velocity is a mathematically useful tool giving the velocity of a plane-wave but is irrelevant for real waves. The Wave-Packet velocity is the exact velocity at which the intensity-weighted position of a wave-packet moves and in the event that that wave-packet is essentially localized in wave-number space, that wave-packet velocity can be approximated by the group velocity.

- (d) Show that for Maxwell’s equations in simple matter the phase velocity and group velocity coincide. This will not always be the case! In fact, show that the only dispersion relation for which the phase velocity and group velocity coincide is one of the form $\Omega(\vec{k}) = v|\vec{k}|$ for some constant v .

Problem 4.46: Waves in Ohmic Matter. Consider Maxwell’s equations in an Ohmic medium (meaning one which satisfies Ohm’s law) with conductivity σ in the rest frame of that medium. Otherwise, the medium is simple with relative permittivity $\epsilon = 1$ and permeability $\mu = 1$.

- (a) Show that Maxwell’s equations in this medium become:

$$\nabla \cdot \vec{E} = \frac{\rho_f}{\epsilon_0}, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \vec{B} = \mu_0 \sigma \vec{E} + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t}.$$

- (b) Show that the free charge density in the medium satisfies:

$$\frac{\partial \rho_f}{\partial t} + \frac{\sigma}{\epsilon_0} \rho_f = 0$$

and thus show that any initial charge distribution in the medium exponentially leaves the volume by accumulating on the surface. Thus, we typically take the free charge density in Ohmic matter to be 0 as any initial non-zero amount quickly dissipates. (We assume that before any wave source is applied this dissipation has already happened.)

- (c) Show that Maxwell’s equations for Fourier Amplitudes in this medium become:

$$\vec{k} \cdot \vec{E} = 0, \quad \vec{k} \cdot \vec{B} = 0, \quad \vec{k} \times \vec{E} = \Omega \vec{B}, \quad \vec{k} \times \vec{B} = -\frac{1}{c^2} \left(\Omega + i \frac{\sigma}{\epsilon_0} \right) \vec{E}$$

and that the dispersion relation is given by:

$$\Omega^2 + i\frac{\sigma}{\epsilon_0}\Omega - c^2|\vec{k}|^2 = 0$$

and that these are equivalent to the case of simple matter if one replaces the permittivity in simple matter by the complex effective permittivity:

$$\epsilon_{\text{eff}}(\vec{k}) = \epsilon_0 - i\frac{\sigma}{\Omega(\vec{k})}$$

and thus Ohmic matter can be understood as a particular form of semisimple matter.

- (d) If there is an initial electric and magnetic field in the medium, those fields can be Fourier decomposed and then their time evolution predicted by solving the equations of motion as done in Problem 4.36. Then, the wavevector will be real (due to being from a Fourier transform). In this case, show that the angular frequency $\Omega(\vec{k})$ (with real part $\Omega_R(\vec{k})$ and imaginary part $\Omega_I(\vec{k})$) is given by:

$$\Omega = \pm \sqrt{c^2|\vec{k}|^2 - \frac{\sigma^2}{4\epsilon_0^2}} - i\frac{\sigma}{2\epsilon_0}.$$

- (e) There is a critical wavelength λ_c so that for wavelengths longer than λ_c , $\Omega_R(\vec{k}) = 0$ while for $\lambda < \lambda_c$, $\Omega_R \neq 0$. Show that:

$$\lambda_c = \frac{4\pi\epsilon_0 c}{\sigma}$$

and that for $\lambda > \lambda_c$:

$$\Omega_I = -\frac{\sigma}{2\epsilon_0} \pm \sqrt{\frac{\sigma^2}{4\epsilon_0^2} - c^2|\vec{k}|^2}.$$

Further, show that in general $\Omega_I < 0$ and that consequently the resulting solution exponentially decays in time.

- (f) Suppose now that $\lambda < \lambda_c$. Show that:

$$\Omega_R = \pm \sqrt{c^2|\vec{k}|^2 - \frac{\sigma^2}{4\epsilon_0^2}}, \quad \Omega_I = -\frac{\sigma}{2\epsilon_0}$$

and thus for short wavelengths the solutions decay exponentially with characteristic lifetime $\tau = \frac{2\epsilon_0}{\sigma}$ while oscillating.

- (g) If instead there is an electric or magnetic field source at one end of the medium, that source may drive the system with input waves at fixed real frequency ω . In this case, the wavenumber which will develop will in general be complex¹². Let $k = \sqrt{\vec{k} \cdot \vec{k}} = k_R + ik_I$ where k_R and k_I are real. Show that:

$$k = \sqrt{\frac{\omega^2}{c^2} + i\frac{\sigma}{c^2}\omega}$$

$$k_R = \frac{\omega}{c} \sqrt{\frac{\sqrt{1 + \frac{\sigma^2}{\epsilon_0^2 \omega^2}} + 1}{2}}, \quad k_I = \frac{\omega}{c} \sqrt{\frac{\sqrt{1 + \frac{\sigma^2}{\epsilon_0^2 \omega^2}} - 1}{2}}$$

and that the wave decays with distance as one goes deeper into the medium at characteristic length scale $d(\omega) = \frac{1}{k_I}$. This $d(\omega)$ is called the skin-depth of the medium.

Problem 4.47: Waves in a Neutral Non-Relativistic Collisionless Plasma. Consider a medium in which there are two kinds of charges. The first is a uniform background of very heavy positive charges with number density n and charge q per particle so that the charge density due to them is qn . Because they are very heavy, we take them to be stationary. The other is a uniform background of much lighter negative charges with the same number density n and charge $-q$ per particle but with mass m per particle. These charges are able to be moved and so let the local average velocity of charges at location $\vec{x}$ be $\vec{v}(t, \vec{x})$. An interacting collection of many flowing charges and the electromagnetic fields is called a plasma.

¹²To derive this from the original equation of motion, one would take that equation of motion and Fourier transform with respect to time instead of position and solve the position differential equation for an oscillating source.

- (a) Show that at the lowest order in the velocity $\vec{v}$:

$$m \frac{\partial \vec{v}}{\partial t}(t, \vec{x}) = -q \vec{E}(t, \vec{x}).$$

Thus, show that the total charge and current densities in the medium for small charge velocities (this is why it is called a “non-relativistic” plasma) satisfy:

$$\rho = 0, \quad \frac{\partial \vec{J}}{\partial t} = \frac{q^2 n}{m} \vec{E}.$$

Because $\rho = 0$ this is a “neutral” plasma and because we will not account for any interactions between the charges we are considering the plasma to be “collisionless”.

- (b) Show that Maxwell’s equations in this plasma become (after taking an additional time derivative of the Maxwell-Ampere equation):

$$\nabla \cdot \vec{E} = 0, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \frac{\partial \vec{B}}{\partial t} = \frac{q^2 n}{m \epsilon_0 c^2} \vec{E} + \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2}.$$

- (c) Show that Maxwell’s equations for Fourier Amplitudes in this medium become:

$$\vec{k} \cdot \vec{E} = 0, \quad \vec{k} \cdot \vec{B} = 0, \quad \vec{k} \times \vec{E} = \Omega \vec{B}, \quad \vec{k} \times \vec{B} = \left(\frac{q^2 n}{m \epsilon_0 c^2 \Omega} - \frac{\Omega}{c^2} \right) \vec{E}$$

and that the dispersion relation is given by:

$$\Omega^2 = c^2 |\vec{k}|^2 + \omega_p^2$$

where the plasma frequency ω_p is defined by:

$$\omega_p = \sqrt{\frac{q^2 n}{m \epsilon_0}}.$$

- (d) Show that the above is equivalent to the case of semisimple matter with effective permittivity:

$$\epsilon_{\text{eff}} = \epsilon_0 \left(1 - \frac{\omega_p^2}{\Omega^2} \right).$$

- (e) Show that the group and phase velocities in this medium are given by:

$$\vec{v}_g = \frac{c^2 \vec{k}}{\sqrt{c^2 |\vec{k}|^2 + \omega_p^2}}, \quad \vec{v}_\varphi = \sqrt{c^2 + \frac{\omega_p^2}{|\vec{k}|^2}} \hat{k}.$$

As well, show that the group speed $|\vec{v}_g| < c$ and that the phase speed $|\vec{v}_\varphi| > c$. It may be surprising that the phase speed may exceed the speed of light but remember that a wave packet moves at the group velocity; the phase velocity is not the velocity of a wave. Show that the index of refraction for this plasma is:

$$n = \sqrt{1 - \frac{\omega_p^2}{\Omega^2}}.$$

- (f) If there is an initial electric and magnetic field in the medium, those fields can be Fourier decomposed and then their time evolution predicted by solving the equations of motion as done in Problem 4.36. Then, the wavevector will be real (due to being from a Fourier transform). In this case, show that the angular frequency $\Omega(\vec{k})$ is real and thus the system oscillates with no decay.
- (g) If instead there is an electric or magnetic field source at one end of the medium, that source may drive the system with input waves at fixed real frequency ω . In this case, the wavenumber which will develop will in general be complex. Let $k = \sqrt{\vec{k} \cdot \vec{k}} = k_R + i k_I$ where k_R and k_I are real. Show that:

$$k = \frac{1}{c} \sqrt{\omega^2 - \omega_p^2}.$$

Further, suppose $|\omega| < \omega_p$. Show that:

$$k_R = 0, \quad k_I = \frac{1}{c} \sqrt{\omega_p^2 - \omega^2}$$

and thus explain that the wave decays with distance as one goes deeper into the medium with skin-depth

$d = \frac{1}{k_I}$. Instead, suppose $|\omega| > \omega_p$. Show that:

$$k_R = \frac{1}{c} \sqrt{\omega^2 - \omega_p^2}, \quad k_I = 0$$

and thus explain that the wave oscillates with no decay in the medium. Thus, this plasma can only transmit waves deep into the medium if those waves have angular frequency above the cut-off frequency ω_p .

Problem 4.48: Electromagnetic Transmission and Reflection at an interface. Consider space to be split in half by a plane (called the interface) such that on one side of the plane, the space is filled with simple matter with $\vec{D} = \epsilon_1 \vec{E}$ and $\vec{H} = \vec{B}/\mu_1$ and on the other side of the plane, the space is filled with simple matter with $\vec{D} = \epsilon_2 \vec{E}$ and $\vec{H} = \vec{B}/\mu_2$. Let n_1, n_2, Z_1, Z_2 be the indices of refraction and material impedances of each side. Let $\vec{\ell}$ be the vector normal to the interface pointing from region 1 to region 2.

(a) Show that in both regions away from the interface, the electric and magnetic fields satisfy:

$$\frac{1}{v^2} \frac{\partial^2 \vec{E}}{\partial t^2} = \nabla^2 \vec{E}, \quad \frac{1}{v^2} \frac{\partial^2 \vec{B}}{\partial t^2} = \nabla^2 \vec{B}$$

where v is the phase velocity in that region. Thus, in each region provided one is away from the interface, the local evolution of the electric and magnetic fields is identical to just simple matter. So, in each region we can apply our plane wave solutions and we must somehow relate our plane wave solutions in each of the two regions to develop the full solution.

- (b) Consider a wave-packet solution which initially is in region 1 and getting closer to the interface (meaning it is a linear combination of plane-waves with wavenumbers $\vec{k}$ satisfying $\vec{k} \cdot \vec{\ell} > 0$). Initially the electric and magnetic fields are 0 in the second region. Using the concept of group or phase velocity, show that the portion of the wave-packet which reaches region 2 will also be a linear combination of plane-waves with wavenumbers $\vec{k}$ satisfying $\vec{k} \cdot \vec{\ell} > 0$.
- (c) Explain, based on the results of the previous parts then that an outgoing (meaning wavenumber away from the interface) plane-wave solution in region 2 (called the transmitted wave) then requires that in region 1 there is an incoming (meaning wavenumber toward the interface, called the incident wave) and outgoing plane-wave (called the reflected wave) so that the full electric and magnetic fields are of the form:

$$\vec{E}(t, \vec{x}) = \begin{cases} \text{Re} \left(\vec{E}_0 e^{i(\vec{k}_0 \cdot \vec{x} - \omega_0 t)} + \vec{E}_r e^{i(\vec{k}_r \cdot \vec{x} - \omega_r t)} \right), & \vec{x} \in \text{Region 1} \\ \text{Re} \left(\vec{E}_t e^{i(\vec{k}_t \cdot \vec{x} - \omega_t t)} \right), & \vec{x} \in \text{Region 2} \end{cases}$$

$$\vec{B}(t, \vec{x}) = \begin{cases} \text{Re} \left(\vec{B}_0 e^{i(\vec{k}_0 \cdot \vec{x} - \omega_0 t)} + \vec{B}_r e^{i(\vec{k}_r \cdot \vec{x} - \omega_r t)} \right), & \vec{x} \in \text{Region 1} \\ \text{Re} \left(\vec{B}_t e^{i(\vec{k}_t \cdot \vec{x} - \omega_t t)} \right), & \vec{x} \in \text{Region 2} \end{cases}$$

where $\vec{k}_0 \cdot \vec{\ell} > 0$, $\vec{k}_r \cdot \vec{\ell} < 0$, $\vec{k}_t \cdot \vec{\ell} > 0$.

- (d) Let the x -direction be the direction of $\vec{\ell}$ and let the xy plane be the plane spanned by $\vec{k}_0$ and $\vec{\ell}$. Further, let θ_0 be the angle between $\vec{k}_0$ and $\vec{\ell}$. Show then that $\vec{k}_0 = |\vec{k}_0|(\cos \theta_0, \sin \theta_0, 0)$ and that the boundary conditions on the interface at $x = 0$ for all y, z, t are:

$$\epsilon_1 E_{1x} = \epsilon_2 E_{2x}, \quad B_{1x} = B_{2x}, \quad E_{1y} = E_{2y}, \quad E_{1z} = E_{2z}, \quad \frac{B_{1y}}{\mu_1} = \frac{B_{2y}}{\mu_2}, \quad \frac{B_{1z}}{\mu_1} = \frac{B_{2z}}{\mu_2}.$$

- (e) Use that these boundary conditions are true for all y, z, t to conclude that all of the frequencies coincide $\omega \stackrel{\text{def}}{=} \omega_0 = \omega_r = \omega_t$ and that the y and z components of the wavevectors each individually coincide: $k_{0y} = k_{ry} = k_{ty}$, $k_{0z} = k_{rz} = k_{tz}$. From this and the dispersion relations satisfied by each wave, conclude that the reflected wavevector $\vec{k}_r$ can be written:

$$\vec{k}_r = |\vec{k}_0|(-\cos \theta_0, \sin \theta_0, 0)$$

and thus the angle of reflection (clockwise above the axis orthogonal to the interface) equals the angle of incidence. As well, show that the transmitted wavevector can be written:

$$\vec{k}_t = |\vec{k}_t|(\cos \theta_t, \sin \theta_t, 0)$$

where the transmitted angle θ_t satisfies “Snell’s Law”:

$$n_1 \sin \theta_0 = n_2 \sin \theta_t.$$

Thus, $\vec{k}_0, \vec{k}_r$, and $\vec{k}_t$ are all coplanar.

- (f) Deduce from the boundary conditions and Maxwell’s equations for Fourier amplitudes that the field amplitudes may be written as:

$$\begin{aligned}\vec{E}_0 &= (-E_{p0} \sin \theta_0, E_{p0} \cos \theta_0, E_{s0}), & \vec{B}_0 &= \frac{1}{v_1} (E_{s0} \sin \theta_0, -E_{s0} \cos \theta_0, E_{p0}) \\ \vec{E}_r &= (-E_{pr} \sin \theta_0, -E_{pr} \cos \theta_0, E_{sr}), & \vec{B}_r &= \frac{1}{v_1} (E_{sr} \sin \theta_0, E_{sr} \cos \theta_0, E_{pr}) \\ \vec{E}_t &= (-E_{pt} \sin \theta_t, E_{pt} \cos \theta_t, E_{st}), & \vec{B}_t &= \frac{1}{v_2} (E_{st} \sin \theta_t, -E_{st} \cos \theta_t, E_{pt})\end{aligned}$$

where the “s-polarization” coefficients E_{s0}, E_{sr}, E_{st} and the “p-polarization” coefficients E_{p0}, E_{pr}, E_{pt} satisfy:

$$\begin{aligned}E_{st} &= E_{s0} + E_{sr}, & \frac{E_{st}}{Z_2} \cos \theta_t &= \frac{E_{s0} - E_{sr}}{Z_1} \cos \theta_0 \\ \frac{E_{pt}}{Z_2} &= \frac{E_{p0} + E_{pr}}{Z_1}, & E_{pt} \cos \theta_t &= (E_{p0} - E_{pr}) \cos \theta_0.\end{aligned}$$

Thus, there are two linearly independent incident polarizations: the s-polarization, also called “Transverse Electric” as it involves an electric field which is orthogonal to the plane spanned by $\vec{i}$ and $\vec{k}_0$, and the p-polarization, also called “Transverse Magnetic” as it involves a magnetic field which is orthogonal to that same plane¹³.

- (g) Show that the reflected and transmitted field components are proportional to the incident fields of the same polarization (thus there is a sort of “conservation of polarization” at the interface) with reflection and transmission (amplitude) coefficients r and s given by:

$$\begin{aligned}r_s &\stackrel{\text{def}}{=} \frac{E_{sr}}{E_{s0}} = \frac{Z_2 \cos \theta_0 - Z_1 \cos \theta_t}{Z_2 \cos \theta_0 + Z_1 \cos \theta_t}, & t_s &\stackrel{\text{def}}{=} \frac{E_{st}}{E_{s0}} = \frac{2Z_2 \cos \theta_0}{Z_2 \cos \theta_0 + Z_1 \cos \theta_t} \\ r_p &\stackrel{\text{def}}{=} \frac{E_{pr}}{E_{p0}} = \frac{Z_1 \cos \theta_0 - Z_2 \cos \theta_t}{Z_1 \cos \theta_0 + Z_2 \cos \theta_t}, & t_p &\stackrel{\text{def}}{=} \frac{E_{pt}}{E_{p0}} = \frac{2Z_2 \cos \theta_0}{Z_1 \cos \theta_0 + Z_2 \cos \theta_t}.\end{aligned}$$

These results are known as the “Fresnel relations”.

- (h) Consider the time-averaged power delivered to or emitted from the interface from each of the component waves (incident, reflected, and transmitted, and of each polarization). Define the the power reflection coefficients R_s and R_p as the time averaged reflected power per time averaged incident power for each polarization and similarly define the power transmission coefficients T_s and T_p as the time averaged transmitted power per time averaged incident power for each polarization. Show that they are related to the amplitude coefficients by:

$$R_s = |r_s|^2, \quad R_p = |r_p|^2, \quad T_s = \frac{Z_1 \cos \theta_t}{Z_2 \cos \theta_0} |t_s|^2, \quad T_p = \frac{Z_1 \cos \theta_t}{Z_2 \cos \theta_0} |t_p|^2.$$

As well, show that $R_s + T_s = R_p + T_p = 1$. Explain why this result was necessarily true in consideration of energy conservation.

- (i) Consider the two media to be non-magnetic ($\mu = \mu_0$). Show that there is a critical angle at which r_p is 0 and thus the reflected light is perfectly s-polarized and find that angle in terms of n_1, n_2 . This angle is known as Brewster’s angle and allows us to use a dielectric crystal as a linear polarizer.

Problem 4.49: Birefringence. Consider a crystal medium in which $\mu = \mu_0$ and $\vec{D} = \hat{\epsilon} \vec{E}$ where $\hat{\epsilon}$ is a real symmetric matrix. Let the eigenvalues of the $\hat{\epsilon}$ matrix be $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3$.

- (a) Show that one can choose coordinates so that $\hat{\epsilon}$ is diagonal. Consider plane waves in this medium with phase speed v_φ and let $\vec{l} = \frac{\vec{k}}{|\vec{k}|}$ and $v_a = c\sqrt{\frac{\epsilon_0}{\epsilon_a}}$. Show that for $v_\varphi \notin \{v_1, v_2, v_3\}$ the dispersion relation

¹³The name s-polarization is from the German word for orthogonal, senkrecht, and p-polarization is from the German word for parallel, parallel.

for the system is equivalent to:

$$\frac{\iota_1^2}{v_\varphi^2 - v_1^2} + \frac{\iota_2^2}{v_\varphi^2 - v_2^2} + \frac{\iota_3^2}{v_\varphi^2 - v_3^2} = 0.$$

As well, show that there are two linearly independent polarizations of solutions in this system, that the $\vec{D}$ for these two solutions are orthogonal, and that for each phase velocity in the range $[v_3, v_1]$ there exists a direction $\vec{t}$ so that there are solutions to this system with that phase velocity.

- (b) Consider an incident wave to this crystal which has its wavevector pointing in the direction of the ϵ_3 eigenvector. Show that a phase difference develops between the components of the electric field amplitude parallel to the ϵ_1 and ϵ_2 eigenvectors so that upon exiting the crystal on the other side a total phase difference of:

$$\Delta\varphi = \omega\ell \left(\frac{1}{v_2} - \frac{1}{v_1} \right).$$

As well, suppose that the crystal in that direction has a thickness of ℓ . Explain that if an incident electric field is as above and incident 45° between the ϵ_1 and ϵ_2 axes and ℓ is such that a phase difference of 90° develops, then the outgoing wave will be circularly polarized.

Problem 4.50: ★ Wave-packet solutions. As in problem 4.45 consider a linear wave system with wavefunction $\psi(t, \vec{x})$ and generators of the form:

$$\mathcal{G} = \int_{\mathbb{S}} \psi^*(t, \vec{x}) G' \left(\vec{x}, \frac{\partial}{\partial \vec{x}} \right) \psi(t, \vec{x}) d^3 \vec{x}.$$

In particular, consider a Hamiltonian which may not have translational symmetry:

$$\mathcal{H} = \int_{\mathbb{S}} \psi^*(t, \vec{x}) \Omega \left(\vec{x}, -i \frac{\partial}{\partial \vec{x}} \right) \psi(t, \vec{x}) d^3 \vec{x}.$$

- (a) Show using the conventions of problem 4.45 that the equation of motion for $\psi(t, \vec{x})$ is given by:

$$i \frac{\partial \psi}{\partial t} = \Omega \left(\vec{x}, -i \frac{\partial}{\partial \vec{x}} \right) \psi(t, \vec{x}).$$

for some Ω . This is known as the Schrödinger equation; it is generically the equation of motion for any stable linear wave theory in the correct coordinates. Identify that this Ω is a generalization of the dispersion relation function defined previously (and that it coincides with that function whenever it does not depend on position).

- (b) Let the wave-packet position $\vec{y}(t)$ be defined exactly as problem 4.45. Show that the previous result holds. Namely, that if the wavefunction is such that $|a(t, \vec{k})|^2$ is small except for $\vec{k}$ very near a particular wavenumber $\vec{K}(t)$ and $|\psi(t, \vec{x})|^2$ is small except for $\vec{x}$ very near $\vec{y}$ then:

$$\frac{d\vec{y}}{dt} \approx \frac{\partial \Omega(\vec{y}, \vec{K})}{\partial \vec{K}}.$$

- (c) Show further that the particular wavenumber $\vec{K}$ can be defined as:

$$\vec{K}(t) = \frac{\int_{\mathbb{K}} \vec{k} a^* a d^3 \vec{k}}{\int_{\mathbb{K}} a^* a d^3 \vec{k}}$$

and that from this expression its time derivative is given by:

$$\frac{d\vec{K}}{dt} \approx - \frac{\partial \Omega(\vec{y}, \vec{K})}{\partial \vec{y}}.$$

- (d) Thus, show that for wave-packet solutions (solutions for which the wave is approximately localized around a particular position and a particular wavenumber) to first approximation that position and wavenumber satisfy Hamilton's equations with $\vec{K}$ acting as the conjugate momentum and the dispersion relation $\Omega(\vec{y}, \vec{K})$ acting as the Hamiltonian. This analogy being wave propagation and mechanics, known as the opticommechanical analogy, allows us to study waves through decomposing them as linear combinations of wave-packets.
- (e) Show that the effective Hamiltonian/dispersion relation for Maxwell's equations in a vacuum is $\Omega = c|\vec{K}|$ and that this is exactly analogous to a relativistic particle of mass $m = 0$. As well, show using the

results of problem 4.44 that in this wave-packet approximation the energy E and linear momentum $\vec{P}$ of the wave-packet are:

$$E = \hbar\Omega, \quad \vec{P} = \hbar\vec{K}$$

where here $\hbar$ is defined by:

$$\hbar = \int_{\mathbb{K}} \vec{a}^\dagger \vec{a} d^3\vec{k}.$$

as well show that $\hbar$ is conserved and that using $\vec{y}$ and $\vec{P}$ as conjugate variables with E as the Hamiltonian produces the correct equations of motion for the wave-packet. Thus, literally an electromagnetic wave-packet genuinely has the energy and momentum of a relativistic particle of mass $m = 0$ (meaning $\mathcal{H} = c|\vec{p}|$). Although we will not fully explain it until Part II, this construction here of a particle-like propagating electromagnetic wave-packet is essentially the “photon”.

Problem 4.51: Fermat’s Principle.

- (a) Consider a plane wave in simple matter in an initial region called region 1 which is reflected off of and transmitted through an interface into a second region called region 2 of simple matter in the same way as in problem 4.48. Show that in crossing the interface:

$$\Delta \left(\frac{|\vec{k}|}{n} \right) = 0, \quad \Delta (n \sin \theta) = 0, \quad \Delta \vec{k}_\parallel = 0$$

where Δf is the difference in the function f evaluated in region 2 minus f evaluated in region 1, n is the index of refraction, θ is the angle of incidence in region 1 and the angle of transmission in region 2, and $\vec{k}_\parallel$ is the part of $\vec{k}$ which lays in the plane of interface separating regions 1 and 2. As well, show that together these imply:

$$\Delta \vec{k} = \Delta (|\vec{k}| \cos \theta) \vec{\tau}$$

where $\vec{\tau}$ is the unit vector pointing from region 1 into region 2.

- (b) Consider a wave-packet solution analogous to the previous question for a system which has a spatially varying index of refraction and so dispersion relation give by: $\Omega(\vec{y}, \vec{k}) = \frac{c}{n(\vec{y})} |\vec{k}|$. Using Hamilton’s first equation for this system show that $\frac{\vec{k}}{|\vec{k}|} = \frac{d\vec{y}}{ds}$ where $ds = |d\vec{y}|$ and we have parameterized the path of the solution $\vec{y}$ by the arclength s it has traveled from some starting position. Treating regions 1 and 2 in the previous part as being arbitrarily close together, show that the result of the previous part is:

$$\frac{d\vec{k}}{ds} = \frac{|\vec{k}|}{n} \frac{dn}{ds} \frac{\vec{\tau}}{\cos \theta}.$$

where $\vec{\tau} = \frac{\nabla n}{|\nabla n|}$.

- (c) Show that the result of the previous part is also implied by the combination of Hamilton’s equations of motion using the given dispersion relation. Thus, Snell’s law is correctly captured by this effective wave-packet Hamiltonian.
- (d) Show by combining Hamilton’s equations that:

$$\frac{d}{ds} \left(n \frac{d\vec{y}}{ds} \right) = \nabla n.$$

- (e) Show that the final equation for the path $\vec{y}(s)$ from the previous part is equivalent to the equation of motion gotten from requiring the stationary variation of the action:

$$T[y] = \frac{1}{c} \int_s n(\vec{y}) |d\vec{y}(s)|,$$

As well, show that when the variation of this action is stationary this action is in fact at a minimum and that the numerical value of this action is the total time taken for the wave-packet to travel from its initial location to its final location. Thus, we have Fermat’s principle: a ray of light traveling through a material will take the path of least time between its initial and final locations.

Problem 4.52: Paraxial Optics and Ray Transfer Matrices. Consider a wave-packet of light moving across space. Let the x axis be called the “optical axis” and let us assume that the displacement of the wave-packet from the optical axis is very small and that the velocity of the wave-packet is very nearly aligned

with the optical axis. (This is known as the paraxial approximation.) Suppose that when the wave packet is at a particular value of x , it is a displacement y away from the optical axis and moving with an angle θ relative to the optical axis. The paraxial approximation then is that we will only keep expressions to linear order in y and θ . Because the path traced by the wave-packet is specified by its position and velocity, we can represent the state of the wave-packet at a particular x by the “ray state” $\vec{R}(x)$:

$$\vec{R}(x) = \begin{pmatrix} y(x) \\ \theta(x) \end{pmatrix}.$$

- (a) Suppose the wave-packet moves through free space so that its new position along the x axis is $x + d$. Show that (to linear order in θ) its new ray state is:

$$\vec{R}(x + d) = \begin{pmatrix} y(x) + d\theta(x) \\ \theta(x) \end{pmatrix}.$$

Thus, show that the act of propagating across space by a distance d is given by multiplying the ray state by the matrix:

$$\hat{M} = \begin{pmatrix} 1 & d \\ 0 & 1 \end{pmatrix}.$$

We will see that many processes can be represented by multiplying the ray state by a matrix. Those such matrices are called ray transfer matrices.

- (b) Suppose the wave-packet is moving through a region with index of refraction n_1 . The wave-packet comes across a plane interface which has the optical axis as its normal vector and on the other side of the interface is a region with index of refraction n_2 . Show that crossing this interface multiplies the ray state by the ray transfer matrix:

$$\hat{M} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{n_1}{n_2} \end{pmatrix}.$$

- (c) Suppose a wave-packet in its propagation goes through multiple processes with ray transfer matrices $\hat{M}_1, \hat{M}_2, \hat{M}_3$ in the order 1, then 2, then 3. Show that the ray transfer matrix for the entire process is:

$$\hat{M} = \hat{M}_3 \hat{M}_2 \hat{M}_1.$$

- (d) Suppose the wave-packet is moving through a region with index of refraction n_1 . It comes across a surface with radius of curvature R (defined so that if $R > 0$ the surface curves away from the incoming wave-packet) and on the other side of this interface is a region with index of refraction n_2 . Define the x axis so that it runs through the center of curvature of this surface. Show that crossing this interface multiplies the ray state by the ray transfer matrix:

$$\hat{M} = \begin{pmatrix} 1 & 0 \\ -\frac{n_2 - n_1}{n_2 R} & \frac{n_1}{n_2} \end{pmatrix}.$$

- (e) Suppose the wave-packet in free space comes across a surface with radius of curvature R_1 defined with the same sign convention as in the previous part and that on the other side of this interface is a region with index of refraction n . Then, it quickly leaves this region through a surface of radius of curvature R_2 , again with the same convention of sign, to return to free space. This device made of two curved surfaces filled with a material of index of refraction not equal to 1 is called a lens. Because we assume that the wave-packet hits the second surface immediately after the first, this is a “thin lens” (to make a thick lens of thickness d , one needs to include propagation by a distance d between the two surfaces). Show that the ray transfer matrix of the thin lens is:

$$\hat{M} = \begin{pmatrix} 1 & 0 \\ -\frac{1}{f} & 1 \end{pmatrix}$$

where the lens’ focal length f is given by:

$$\frac{1}{f} = (n - 1) \left(\frac{1}{R_1} - \frac{1}{R_2} \right).$$

This is known as the lens maker’s equation.

- (f) Consider a light emitting object which extends from the optical axis up to a distance y_{obj} above the optical axis and is a distance d_{obj} along the optical axis away from a lens of focal length f (which is centered on the optical axis by definition). The object will emit light in many different directions which will then reach the lens. Show that all of the rays which came from the top of the object and went

through the lens will converge at a point a distance d_{img} away from the lens along the optical axis and at a displacement y_{img} from the optical axis where d_{img} is given by:

$$\frac{1}{d_{\text{obj}}} + \frac{1}{d_{\text{img}}} = \frac{1}{f}$$

(this is known as the thin lens equation) and y_{img} is given by:

$$y_{\text{img}} = -\frac{d_{\text{img}}}{d_{\text{obj}}} y_{\text{obj}}.$$

- (g) Explain that the above implies an “image” of the light emitting object is formed by the lens at the x value d_{img} and that the size of the image is $|y_{\text{img}}|$. Thus explain that the magnification factor of the image (the size of the image compared to the object, with a sign flip if the image is upside down) is:

$$m = \frac{y_{\text{img}}}{y_{\text{obj}}} = -\frac{d_{\text{img}}}{d_{\text{obj}}}.$$

- (h) Show that if an object is placed extremely far away from a lens with focal length f then the image formed by that object will be that distance f away from the lens. (This provides the geometric interpretation of the focal length.)

Problem 4.53: Maxwell’s equations with Magnetic Charge. We found before that magnetic monopoles are inconsistent with the potentials being formulated on full Euclidean space. For now in this question we will “abandon” the potentials and simply consider the electric and magnetic fields without assuming that they are derived from any potentials. (This is brazen given what we have learned, but let us see what happens.)

- (a) Suppose there were such a thing as magnetic charge and that it was described by magnetic charge density ρ_m and magnetic current density $\vec{J}_m$ so that for the same reasons as electric charge it satisfies the continuity equation:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \vec{J}_m = 0.$$

By magnetic charge we mean that the Solenoid law of Maxwell’s equations becomes instead the Gauss’ law for magnetism:

$$\nabla \cdot \vec{B} = \mu_0 \rho_m.$$

Show that in order for Maxwell’s equations to be consistent with this modification Faraday’s law must also be modified so that the full set of equations becomes:

$$\begin{aligned} \nabla \cdot \vec{E} &= \frac{\rho}{\epsilon_0}, & \nabla \cdot \vec{B} &= \mu_0 \rho_m, \\ \nabla \times \vec{E} &= -\mu_0 \vec{J}_m - \frac{\partial \vec{B}}{\partial t}, & \nabla \times \vec{B} &= \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}. \end{aligned}$$

These are known as Maxwell’s equations with magnetic charge.

- (b) Show that Maxwell’s equations with magnetic charge have symmetry under the “duality rotation” by a general angle θ :

$$\begin{aligned} \vec{E}' &= \vec{E} \cos \theta - c \vec{B} \sin \theta & \vec{B}' &= \vec{B} \cos \theta + \frac{\vec{E}}{c} \sin \theta \\ \rho' &= \rho \cos \theta - \frac{\rho_m}{c} \sin \theta & \rho'_m &= \rho_m \cos \theta + c \rho \sin \theta \\ \vec{J}' &= \vec{J} \cos \theta - \frac{\vec{J}_m}{c} \sin \theta & \vec{J}'_m &= \vec{J}_m \cos \theta + c \vec{J} \sin \theta. \end{aligned}$$

- (c) We have Maxwell’s equations for magnetic charge, but what about the Lorentz force law? Suppose we wish to add some terms to the Lorentz force law proportional to the magnetic charge of an object (so that those terms do not affect anything magnetically unchanged). As well, let us assume that the total force is to also have symmetry under the duality rotation. Show that the Lorentz force law on a point with electric charge q and magnetic charge q_m must be:

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) + q_m \left(\vec{B} - \frac{1}{c^2} \vec{v} \times \vec{E} \right).$$

- (d) Suppose we now have a continuous distribution of electric and magnetic charge in a region $\mathbb{M}$ of space.

Show (using the Lorentz force law for magnetic charge) that the force on the region can be written as:

$$\vec{F} = \int_{\partial\mathbb{M}} \hat{\sigma} \cdot d\vec{A}$$

where $\hat{\sigma}$ is the same stress tensor found in problem 4.32. Use this stress tensor and the Lorentz force for magnetic charge to show that the electromagnetic linear momentum density which satisfies a continuity equation for this theory is the same one as without magnetic charge. As well, show using the work done by the Lorentz force for magnetic charge that the electromagnetic energy density which satisfies a continuity equation for this theory is the same one as without the magnetic charge. With these results, show that the various continuity equations found in problems 4.31(b), 4.32(b), 4.33(c), and 4.34(c) need to simply have their source term updated to include the full Lorentz force for magnetic charge and then they all remain true with or without magnetic charge.

- (e) All of these facts we have seen working together has given many hope that magnetic charge is real. However, we have discarded the potentials so far and we only know how to derive Maxwell's equations from an action through the potentials. It is time to try to put the potentials back. Suppose we introduce "magnetopotentials" in addition to the familiar potentials so that in terms of the standard scalar and vector potentials and the new magneto scalar potential ϕ_m and magneto vector potential $\vec{A}_m$ the electric and magnetic fields are defined as:

$$\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t} - c^2\nabla \times \vec{A}_m, \quad \vec{B} = -\nabla\phi_m - \frac{\partial\vec{A}_m}{\partial t} + \nabla \times \vec{A}.$$

Show that the action:

$$S = \int \left(\frac{\epsilon_0}{2} |\vec{E}|^2 - \frac{|\vec{B}|^2}{2\mu_0} + \vec{J} \cdot \vec{A} - \rho\phi - \vec{J}_m \cdot \vec{A}_m + \rho_m\phi_m \right) d\mathbb{T}$$

with the electric and magnetic fields defined in terms of the potentials $\phi, \vec{A}, \phi_m, \vec{A}_m$ gives all of Maxwell's equations with magnetic charge correctly. However, show that the Lorentz force law for magnetic charge predicted by this action does **NOT** agree with that found in part (c), does not have the duality rotation symmetry, and cannot even be written in terms of just $\vec{E}$ and $\vec{B}$. As well, show that this action does not produce the energy density, linear momentum density, or stress tensor we would expect from our analysis in part (c). In fact, it is a theorem [97] that there is no action that can produce both Maxwell's equations with magnetic charge and the Lorentz force law with magnetic charge given in part (c) unless there simply is no magnetic charge¹⁴. This is another reason to be skeptical of the existence of fundamental magnetic charge besides its lack of experimental evidence (fundamental magnetic charge means magnetic charge not from holes in space or as the effective magnetic charge of a sort of effective magnetic field).

Problem 4.54: Darwin Theory. For many practical applications, only the first correction from the Lorentz theory over the Galilean theory is necessary. Let us develop a Lagrangian corresponding to such a theory.

- (a) Consider Maxwell's equations for the potentials in the Coulomb gauge ($\nabla \cdot \vec{A} = 0$). Show that in this gauge the equations of motion for the potentials become:

$$-\nabla^2\phi = \rho, \quad \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} = \frac{1}{c^2} \left(\vec{J} - \frac{\partial\phi}{\partial t} \right).$$

- (b) Consider solutions to the above equations expanded as a series in inverse powers of c and assume the homogeneous solution to the equations is 0 (there are no incoming electromagnetic waves in the system). Show that the resulting equations are to lowest order:

$$-\nabla^2\phi = \rho, \quad -\nabla^2 \vec{A} = \frac{1}{c^2} \left(\vec{J} - \frac{\partial\nabla\phi}{\partial t} \right) + \mathcal{O}\left(\frac{1}{c^4}\right).$$

¹⁴It may be surprising that no such action could exist when we have proven before that by doubling your number of variables one can produce any equations of motion you like from an action. It is in fact true that you can always do that but in doing so the extra variables will in general appear in the interaction terms of the action and thus affect the force law predicted. As well, such an action in the free limit ($q \rightarrow 0, q_m \rightarrow 0$) does not reduce to the free action for a relativistic particle. So, one can throw it together but it does not reduce to our established theories in appropriate limits nor reproduce what is already experimentally well established.

- (c) Show that for a point charge q at position $\vec{y}(t)$ in this approximation the resulting potentials are:

$$\phi(t, \vec{x}) = \frac{q}{4\pi\epsilon_0|\vec{x} - \vec{y}(t)|}, \quad \vec{A}(t, \vec{x}) = \frac{q}{4\pi\epsilon_0 c^2 |\vec{x} - \vec{y}(t)|} \left(\mathbb{1} + \frac{\vec{x} - \vec{y}}{|\vec{x} - \vec{y}|} \frac{\vec{x} - \vec{y}}{|\vec{x} - \vec{y}|} \right) \cdot \dot{\vec{y}} + \mathcal{O}\left(\frac{1}{c^4}\right).$$

- (d) Consider two point charges q_1 and q_2 , with positions $\vec{y}_1(t)$ and $\vec{y}_2(t)$. Write down the equations of motion corresponding to these charges interacting due to the fields they produce, ignoring the effect of a charge's field on itself, up through order $\frac{1}{c^2}$. Show that the resulting equations of motion are exactly those produced from the Lagrangian:

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}m_1|\dot{\vec{y}}_1|^2 + \frac{1}{8c^2}m_1|\dot{\vec{y}}_1|^4 + \frac{1}{2}m_2|\dot{\vec{y}}_2|^2 + \frac{1}{8c^2}m_2|\dot{\vec{y}}_2|^4 \\ & - \frac{q_1 q_2}{4\pi\epsilon_0|\vec{y}_1 - \vec{y}_2|} + \frac{q_1 q_2}{8\pi\epsilon_0 c^2 |\vec{y}_1 - \vec{y}_2|} \dot{\vec{y}}_1 \cdot \left(\mathbb{1} + \frac{\vec{y}_1 - \vec{y}_2}{|\vec{y}_1 - \vec{y}_2|} \frac{\vec{y}_1 - \vec{y}_2}{|\vec{y}_1 - \vec{y}_2|} \right) \cdot \dot{\vec{y}}_2 \end{aligned}$$

and that this Lagrangian is exactly the Lagrangian for two particles expanded to order $\frac{1}{c^2}$ using the potentials we found before. This Lagrangian is known as the Darwin Lagrangian and as we see it produces the lowest order Lorentz correction to the Galilean theory.

- (e) Show that the associated Hamiltonian to this Lagrangian is given by:

$$\mathcal{H} = \left(1 - \frac{|\vec{p}_1|^2}{4m_1^2 c^2}\right) \frac{|\vec{p}_1|^2}{2m_1} + \left(1 - \frac{|\vec{p}_2|^2}{4m_2^2 c^2}\right) \frac{|\vec{p}_2|^2}{2m_2} + \frac{q_1 q_2}{4\pi\epsilon_0 r} - \frac{q_1 q_2}{8\pi\epsilon_0 m_1 m_2 c^2 r} \vec{p}_1 \cdot (\mathbb{1} + \hat{r}\hat{r}) \cdot \vec{p}_2$$

where $r = |\vec{y}_1 - \vec{y}_2|$ and $\hat{r} = \frac{\vec{y}_1 - \vec{y}_2}{|\vec{y}_1 - \vec{y}_2|}$.

Problem 4.55: Near and Far Field Solutions to Maxwell's Equations.

- (a) Recall Jefimenko's equations from problem 4.17 as the exact solutions for the electric and magnetic fields from arbitrary sources:

$$\begin{aligned} \vec{E}(t, \vec{x}) = & \int_{\mathbb{S}} \left(\frac{\rho\left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}'\right)}{4\pi\epsilon_0 |\vec{x} - \vec{x}'|^3} (\vec{x} - \vec{x}') + \frac{\frac{\partial \rho}{\partial t}\left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}'\right)}{4\pi\epsilon_0 c |\vec{x} - \vec{x}'|^2} (\vec{x} - \vec{x}') - \frac{\frac{\partial \vec{J}}{\partial t}\left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}'\right)}{4\pi\epsilon_0 c^2 |\vec{x} - \vec{x}'|} \right) d\mathbb{S}' \\ \vec{B}(t, \vec{x}) = & \int_{\mathbb{S}} \left(\frac{\vec{J}\left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}'\right) \times (\vec{x} - \vec{x}')}{4\pi\epsilon_0 c^2 |\vec{x} - \vec{x}'|^3} + \frac{\frac{\partial \vec{J}}{\partial t}\left(t - \frac{|\vec{x} - \vec{x}'|}{c}, \vec{x}'\right) \times (\vec{x} - \vec{x}')}{4\pi\epsilon_0 c^3 |\vec{x} - \vec{x}'|^2} \right) d\mathbb{S}'. \end{aligned}$$

Show that the first term in each of the electric and magnetic fields dominates the others for small $|\vec{x} - \vec{x}'|$. Thus, nearby the source charges and current densities these terms produce the leading effects and are called the “near-fields”.

- (b) Now let us consider the far-field behavior of these solutions. That is, consider the charge and current distributions to be in a region near the origin and the point of evaluation $\vec{x}$ to be very far away from the origin. Define $r = |\vec{x}|$ and $\hat{r} = \frac{\vec{x}}{|\vec{x}|}$. Show that:

$$\phi(t, \vec{x}) = \frac{\int_{\mathbb{S}} \rho\left(t - \frac{r}{c} + \frac{\hat{r} \cdot \vec{x}'}{c}, \vec{x}'\right) d^3 \vec{x}'}{4\pi\epsilon_0 r} + \mathcal{O}\left(\frac{1}{r^2}\right), \quad \vec{A}(t, \vec{x}) = \frac{\int_{\mathbb{S}} \vec{J}\left(t - \frac{r}{c} + \frac{\hat{r} \cdot \vec{x}'}{c}, \vec{x}'\right) d^3 \vec{x}'}{4\pi\epsilon_0 c^2 r} + \mathcal{O}\left(\frac{1}{r^2}\right)$$

and that the resulting electric and magnetic fields are:

$$\vec{E}(t, \vec{x}) = \frac{\mu_0}{4\pi r} \hat{r} \times (\hat{r} \times \vec{\alpha}(t, \vec{x})) + \mathcal{O}\left(\frac{1}{r^2}\right), \quad \vec{B}(t, \vec{x}) = -\frac{\mu_0}{4\pi c r} \hat{r} \times \vec{\alpha}(t, \vec{x}) + \mathcal{O}\left(\frac{1}{r^2}\right)$$

where the radiation vector $\vec{\alpha}(t, \vec{x})$ is defined as:

$$\vec{\alpha}(t, \vec{x}) = \int_{\mathbb{S}} \frac{\partial \vec{J}}{\partial t} \left(t + \frac{\hat{r} \cdot \vec{x}'}{c} - \frac{r}{c}, \vec{x}' \right) d^3 \vec{x}'.$$

Thus, in the far-field region, the electric and magnetic fields are completely determined by $\vec{\alpha}$ and decay with distance as $\frac{1}{r}$.

Problem 4.56: Radiated Electromagnetic Power. Consider a charge and current distribution which are localized in some finite region of space.

- (a) Consider a sphere of radius R which completely encloses the charge and current. Let $\frac{dP}{d\Omega}(t, \theta, \varphi)$ be the electromagnetic power through this sphere per unit solid-angle of the sphere. Let $\hat{r}(\theta, \varphi) = \frac{\vec{x}}{|\vec{x}|}$. Show

this power is given by:

$$\frac{d\mathcal{P}}{d\Omega} = R^2 \hat{r} \cdot \vec{S}$$

where $\vec{S}$ is the Poynting vector.

- (b) Show using the far-field results from the previous problem then that in the limit $R \rightarrow \infty$:

$$\frac{d\mathcal{P}}{d\Omega} = \frac{\mu_0 |\hat{r} \times \vec{\alpha}_*|^2}{16\pi^2 c}$$

where:

$$\vec{\alpha}_*(t, \theta, \varphi) = \lim_{R \rightarrow \infty} \vec{\alpha}(t, R\hat{r}(\theta, \varphi))$$

and $\vec{\alpha}$ is the radiation vector. Thus, this expression gives the power radiated out to distances arbitrarily far away from the source per solid angle by an electromagnetic system.

Problem 4.57: Larmor Formula. Consider a point charge q moving with trajectory $\vec{y}(t)$.

- (a) Show that the $\vec{\alpha}(t, \vec{x})$ defined above is given by:

$$\vec{\alpha}(t, \vec{x}) = q \frac{\ddot{\vec{y}}(t_d) + \hat{r} \cdot \ddot{\vec{y}}(t_d) \dot{\vec{y}}(t_d) - \hat{r} \cdot \dot{\vec{y}}(t_d) \ddot{\vec{y}}(t_d)}{\left(1 - \frac{\hat{r} \cdot \dot{\vec{y}}(t_d)}{c}\right)^3}$$

where t_d , called the delayed time, is defined implicitly by:

$$t_d = t + \frac{\hat{r} \cdot \vec{y}(t_d)}{c} - \frac{r}{c}.$$

- (b) Show that the power radiated per unit solid angle is:

$$\frac{d\mathcal{P}}{d\Omega} = \frac{\mu_0 q^2}{16\pi^2 c} \left(\frac{|\ddot{\vec{y}}|^2}{\left(1 - \frac{\hat{r} \cdot \dot{\vec{y}}}{c}\right)^4} + \frac{\frac{2}{c} \dot{\vec{y}} \cdot \ddot{\vec{y}} \ddot{\vec{y}} \cdot \hat{r}}{\left(1 - \frac{\hat{r} \cdot \dot{\vec{y}}}{c}\right)^5} - \frac{(\hat{r} \cdot \ddot{\vec{y}})^2}{\left(1 - \frac{\hat{r} \cdot \dot{\vec{y}}}{c}\right)^6} \left(1 - \frac{|\dot{\vec{y}}|^2}{c^2}\right) \right).$$

- (c) The above gives the electromagnetic energy per unit time per unit solid angle incident on an arbitrarily large sphere surrounding the region in which the charge is moving at the time the energy reaches that sphere. By energy conservation, that energy reaching far away is compensated for by energy lost by the charge. Explain then that (assuming there are no other ways in which the charge gains or loses energy) the rate of energy loss of the charge at time t_0 is related to the radiated power per solid angle by:

$$-\frac{dE_{\text{charge}}}{dt_0} = \int_{\Omega} \frac{d\mathcal{P}}{d\Omega} \frac{dt}{dt_0} d\Omega = \int_{\Omega} \frac{d\mathcal{P}}{d\Omega} \left(1 - \frac{\hat{r} \cdot \dot{\vec{y}}}{c}\right) d\Omega$$

where $\dot{\vec{y}}$ and $\ddot{\vec{y}}$ are evaluated at the time t_0 in the distant past when the radiation was emitted. It isn't exactly right to assume that no other energy is emitted or absorbed by the charge as the radiated power only accounts for energy which escapes arbitrarily far away and thus neglects energy the charge may give off to an electromagnetic field but which then may in turn return to that charge through its interaction with the electromagnetic field. As such, this expression is really only to be taken seriously on time scales much longer than the time scale of emission and reabsorption of electromagnetic waves by the charge.

- (d) Using our above formula for the radiated power, integrate this result to show that:

$$\frac{dE}{dt}(t) = -\frac{\mu_0 q^2 \gamma^4}{6\pi c} \left(|\ddot{\vec{y}}(t)|^2 + \frac{\gamma^2}{c^2} (\dot{\vec{y}}(t) \cdot \ddot{\vec{y}}(t))^2 \right).$$

This result is known as the (relativistic) Larmor formula and as we see it is the predicted rate of energy loss by a charge due to accelerating while interacting with the electromagnetic field. Because we now see that energy is radiated by the charge, such an effect should be present in its equation of motion to produce this (as all dynamical results come ultimately from the equations of motion). This is the first sign that in the Lorentz theory, unlike the Galilean one, the effect of a point charge on itself is nonzero. We will analyze this in detail later in section 4.8.

Problem 4.58: Cerenkov Radiation. Consider a charge q moving in a straight line with speed v through a medium in which there is an effective speed of light less than c due to having an index of refraction n . Due

to the interaction of this charge with the electromagnetic field, electromagnetic waves moving at speed $\frac{c}{n}$ are constantly being emitted by this charge from its location. Show that if v is greater than the speed of light in this medium, then the envelope of all of the waves emitted by the charge as it moves forms a cone with the point charge at the nose (called the Cerenkov Radiation cone) and that the opening angle of that cone is given by:

$$\sin \theta = \frac{c}{nv}.$$

Problem 4.59: Electromagnetic Scattering. Just like the scattering of particles, we can scatter electromagnetic waves. For particles, we had an incoming distribution of particles in a beam and an outgoing distribution of particles scattered onto the sphere surrounding the scattering center. For electromagnetic waves, we have an incoming distribution of electromagnetic energy in a beam and an outgoing distribution of electromagnetic energy scattered onto the sphere surrounding the scattering center. So, for wave scattering, define the differential scattering cross section by the ratio of the time averaged power per unit solid angle coming out of the event to the time averaged power per unit area of the beam coming into the event:

$$\frac{d\sigma}{d\Omega} = \frac{\mathbb{T}\left(\frac{d\mathcal{P}_{\text{out}}}{d\Omega}\right)}{\mathbb{T}\left(\frac{d\mathcal{P}_{\text{in}}}{d\mathbb{A}}\right)}.$$

- (a) Show that for an incoming electromagnetic plane wave with electric Fourier amplitude $\vec{E}$, the incoming power distribution is given by:

$$\mathbb{T}\left(\frac{d\mathcal{P}_{\text{in}}}{d\mathbb{A}}\right) = \frac{\epsilon_0 c}{2} |\vec{E}|^2.$$

- (b) Show that for an incoming electromagnetic plane wave with polarization $\vec{\xi}$, the outgoing power distribution is given by:

$$\mathbb{T}\left(\frac{d\mathcal{P}_{\text{out}}}{d\Omega}\right) = \vec{\xi}^\dagger \hat{G} \vec{\xi}$$

for some $\hat{G}$. As well, show that if the system's response to the incoming wave is linear then $\hat{G}$ does not depend on the polarization and the resulting cross section does not depend on $|\vec{E}|$.

- (c) Show that if one considers an unpolarized cross section (meaning averaged uniformly over all possible polarizations) under the hypotheses of the previous part then the result is equivalent to half of the sum of the cross sections for any two orthonormal polarizations of the incoming wave.

Problem 4.60: Thomson Scattering. Consider a point charge q which is otherwise free and moving slowly (so consider only the first order deviation from stationary) to experience an unpolarized beam of incoming electromagnetic plane waves. Show that at leading order in powers of $1/c$ the scattering cross section for this interaction is given by:

$$\frac{d\sigma}{d\Omega} = \left(\frac{\mu_0 q^2}{4\pi m}\right)^2 \frac{1 + \cos^2 \theta}{2}$$

where in spherical coordinates θ is the zenith angle and the $\theta = 0$ axis is the direction in which the beam points.

Problem 4.61: Rayleigh Scattering. Consider a point charge q which is affected by a linear restoring force so that it would have natural angular frequency ω_0 and moving slowly (so consider only the first order deviation from stationary) to experience an unpolarized beam of incoming electromagnetic plane waves.

- (a) Show that at leading order in powers of $1/c$ the scattering cross section for this interaction is given by:

$$\frac{d\sigma}{d\Omega} = \left(\frac{\mu_0 q^2}{4\pi m}\right)^2 \left(\frac{\omega^2}{\omega_0^2 - \omega^2}\right)^2 \frac{1 + \cos^2 \theta}{2}.$$

- (b) Show that in the high-frequency limit this reduces to Thomson scattering result. So, if the incident beam oscillates much more quickly than the charge's natural frequency the charge is essentially free.
- (c) Show that in the low-frequency limit this result is proportional to ω^4 and thus low frequencies scatter more weakly than higher frequencies. It turns out that the electric charges in the atmosphere, due to the pressure they exert on each other, experience such linear restoring forces and have a natural frequency much higher than those which correspond to light we can see. Thus, the light from the

sun is scattered with the higher frequencies scattered more strongly. The higher frequency light thus bounces around the entire sky whereas the lower frequencies scatter less and come more straight at us. The higher frequency light corresponds to blue light in our vision and this is the reason the sky is blue.

Problem 4.62: Scattering off a Conducting Sphere. Consider a conducting sphere of radius R experiencing an unpolarized beam of electromagnetic plane waves. Suppose that the radius of the sphere is much smaller than the wavelength of the incident waves. Show using the result of problem 4.29 that the scattering cross section off of the sphere is:

$$\frac{d\sigma}{d\Omega} = \left(\frac{\omega^2 R^3}{c^2} \right)^2 \left(\frac{5}{8}(1 + \cos^2 \theta) - \cos \theta \right)$$

Problem 4.63: Olber's Paradox. Suppose the universe is infinitely old and static (as in the shape and size of the universe does not change in time) and that the stars in the universe are distributed independently uniformly at random.

- Show that the intensity of light of a single star a distance r away is proportional to $\frac{1}{r^2}$.
- Show that the number of stars a distance r away from a point of interest is proportional to r^2 .
- Show that under these assumptions the night sky should be filled with light. Consequently, because the night is dark at least one of these assumptions must be false. This is the first hint that the assumptions we have made about the nature of space are potentially flawed.

Problem 4.64: The Relativistic Doppler Effect. Consider a source of electromagnetic waves which in its rest frame produces waves of frequency f_s . Consider a detector which is moving at velocity v (as measured in the rest frame of the source) in the direction of separation between the source and the detector. Show that the frequency of waves observed by the detector, f_d , is given by:

$$f_d = \sqrt{\frac{c-v}{c+v}} f_s.$$

Show in the low speed limit $|v| \ll c$ this reproduces the nonrelativistic Doppler formula.

4.7 Fixing Electromagnetism broke Gravity

While the Lorentz theory solves our problems with electricity and magnetism, it introduces a problem for gravity. Whereas in the Galilean theory we had the scalar potential theory and the vector potential theory to choose from, the two are united in the Lorentz case. And so, if we are to continue thinking about gravity in the same way we did in the Galilean theory, we would expect to keep our gravitational scalar potential ϕ and introduce a gravitational vector potential $\vec{\Omega}$. In the Galilean theory, gravity coupled to the mass density. Then, by our previous reasoning, the only possible Lagrangian of fields $\phi, \vec{\Omega}$ which reduces to the Galilean case (3.6.1) is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-\rho\phi + \vec{J} \cdot \vec{\Omega} - \frac{1}{8\pi G} \left(|\nabla\phi + \dot{\vec{\Omega}}|^2 - c^2 |\nabla \times \vec{\Omega}|^2 \right) \right) d\mathbb{S} \quad (4.7.1)$$

if we maintain that gravity should interact with the mass density ρ and mass current density $\vec{J}$. This theory is called gravitomagnetism.

Gravitomagnetism at a fundamental level makes many incorrect predictions. In particular, because we have persisted in thinking that gravity ought to couple to mass, this theory predicts that mass must be locally conserved by the continuity equation in the exact same way that charge must be locally conserved in Maxwell's equations. However, there are countless experiments in which mass is not conserved. It is an experimental fact that particles can be broken into pieces whose mass does not add up to the mass of the original particle. As well, because of the coupling to mass only and lack of terms involving $\vec{E}$ or $\vec{B}$, this theory predicts that gravity does not interact at all with electromagnetism. However, we observe a phenomenon known as gravitational lensing in which light is deflected when it passes by heavy objects. Experimentally, light is affected by gravity similarly to matter even though light is massless. Hence, it cannot be the case that gravity interacts with other things due to the mass, it must be through a different property. While mass is no longer believed to be conserved, energy and momentum still are. In fact, mass can be produced by energy and destroyed back into energy. In the Lorentz theory, **mass conservation is replaced by energy conservation**. We can see the energy contained in having mass by considering the Lorentz Hamiltonian for a free particle and looking at what happens when its momentum goes to 0:

$$\mathcal{H} = \sqrt{c^2 |\vec{p} - q\vec{A}|^2 + m^2 c^4} + q\phi \quad (4.7.2)$$

$$\text{Free} \implies \mathcal{H} = \sqrt{c^2 |\vec{p}|^2 + m^2 c^4} \quad (4.7.3)$$

$$\text{At } \vec{p} = 0 \implies \boxed{E = mc^2}. \quad (4.7.4)$$

This is the origin of Einstein's famous formula. It is the energy of a free particle just sitting there. You may remark "overall additive constants in the energy don't matter, they can just be removed by gauge transformation" and you would be correct in saying so. The only reason this term mc^2 matters is because when an object breaks into several objects that term is no longer a constant and so can't simply be removed. This is explored in detail in the homework.

Because energy conservation replaces mass conservation, we ought to just couple gravity to the energy right? Well, this is a good idea but unlike mass or charge, energy is not Lorentz invariant. From equation (4.3.32), energy and momentum mix into each other under a Lorentz transformation and so the only way to couple gravity to energy in a Lorentz invariant way is to also couple gravity to momentum. However, energy and momentum are each separately locally conserved and so we would have four charge densities (one for energy and three for momentum) which mix into each other under boost. This is not the same transformation law as the charge current density we have derived for coupling to a Lorentz field theory. Therefore, we have no such possibility open to us in the way we have studied so far to couple gravity to energy and momentum. We will need to do something more sophisticated in which gravity must couple to these four intermixing conserved currents in order to make a theory of gravity consistent with Lorentz symmetry. All of this is to say, it is not that gravity is inconsistent with Lorentz symmetry (it isn't). Instead, having a Lorentz symmetric theory of gravity will require us to develop a new theory rather than copying electromagnetism with a few terms changed the way we could for the Galilean case. The development of such a theory we will save for chapter 7. That is quite a long wait; we delay it for so long due to the high technical level of the resulting theory.

Exercises

Problem 4.65: Keeping or dropping mc^2 . Consider a particle of mass m_0 which is sitting at rest and

which then spontaneously decays into two particles of mass m_1 and m_2 .

- (a) Suppose that the correct Hamiltonian to use for a single free particle is $\mathcal{H} = \sqrt{c^2|\vec{p}|^2 + m^2c^4} + \varepsilon$ where ε is some constant parameter specific to the particle. For the decay process given, show that the magnitude of the final momenta for either of the two resulting particles is:

$$p = \frac{\sqrt{((m_0c^2 + \varepsilon_0 - \varepsilon_1 - \varepsilon_2)^2 - m_1^2c^4 - m_2^2c^4)^2 - 4m_1^2m_2^2c^8}}{2c(m_0c^2 + \varepsilon_0 - \varepsilon_1 - \varepsilon_2)}.$$

Explain then that measuring m_0, m_1, m_2 and the final velocities of the particles allows the determination of $\varepsilon_0 - \varepsilon_1 - \varepsilon_2$.

- (b) Show that under Lorentz transformation the only choice of ε for which the action is invariant (meaning the surface term which is added by the transformation is 0) is when $\varepsilon = 0$. Using this explain that if the energy and momentum results of a decay process in different reference frames are to be related by a Lorentz transformation the way we found in equation (4.3.32) then it must be the case that $\varepsilon = 0$ for all particles. Thus, conclude that one cannot just remove mc^2 as an additive constant from the energy as discussed in this section in a Lorentz symmetric theory in which particle decays are possible.

Problem 4.66: 1-to-2 Scattering. Consider a particle of mass m_0 which decays into a particle of mass m_1 and another of mass m_2 .

- (a) Show that for $m \neq 0$ we can go to a frame in which the initial particle is at rest. In that frame show that the magnitude of the final momenta for either of the two resulting particles is:

$$p = c \frac{\sqrt{(m_0^2 - m_1^2 - m_2^2)^2 - 4m_1^2m_2^2}}{2m_0}.$$

- (b) Show also that:

$$m_0 \geq m_1 + m_2$$

and thus that mass is not necessarily conserved in this process.

Problem 4.67: On-Shell Vacuum Pair production. Consider a particle of mass 0 and energy E which decays into two particles each of mass m . Show that this process is only possible (using energy and momentum conservation) if $m = 0$.

Problem 4.68: Radiation Kinematics. Consider a particle of mass m with energy E which emits a particle of mass 0 while maintaining its mass. Show using energy and momentum conservation that this requires the energy and momentum of the massless particle to be 0.

Problem 4.69: Relativistic Collision Kinematics. Consider two masses m_1 and m_2 , each moving freely for a while which then crash into each other and then again move freely afterward.

- (a) Given that the total energy and momentum of the two masses is conserved, write the momentum of particle 1 after the collision ($\vec{p}_{1f}$) in terms of its momentum before the collision ($\vec{p}_{10}$) as: $\vec{p}_{1f} = \vec{p}_{10} - \Delta p \hat{n}$ where Δp is the magnitude of momentum transferred from particle 1 to particle 2 and $\hat{n}$ is the unit vector pointing in the direction of the momentum transfer. Use this form to show that the momentum of particle 2 after the collision is related to its momentum before the collision as: $\vec{p}_{2f} = \vec{p}_{20} + \Delta p \hat{n}$ and show using the above expressions that if $\Delta p \neq 0$ (meaning a collision actually happens), then:

$$\Delta p = 2 \frac{E_1 E_2}{c(E_1 + E_2)} \frac{\hat{n} \cdot (\vec{v}_{10} - \vec{v}_{20})}{1 - \frac{(c(\vec{p}_{10} + \vec{p}_{20}) \cdot \hat{n})^2}{(E_1 + E_2)^2}}$$

where $E_1 = \sqrt{c^2|\vec{p}_{10}|^2 + m_1^2c^4}$ and $E_2 = \sqrt{c^2|\vec{p}_{20}|^2 + m_2^2c^4}$.

- (b) Show that the above formula reduces to the case of non-relativistic collision kinematics in the limit of small velocities.

Problem 4.70: Minimum process energy. Consider an interparticle interaction so that in the end there are N free particles of a variety of masses. Show that the minimum energy of the system necessary to make such a process happen requires that in the end all of the outgoing particles are moving at the same velocity and thus in the center of momentum frame they are all stationary. Show that in that center of momentum frame the minimum energy is simply the sum of all of the particle masses times c^2 .

Problem 4.71: ★ 2-to-2 Scattering. Consider two masses m_1 and m_2 , each moving freely for a while which then crash into each other and explode into two new particles of masses m_3 and m_4 . Let $\vec{p}_1$ be the incoming momentum of particle 1, $\vec{p}_2$ be the incoming momentum of particle 2, $\vec{p}_3$ be the outgoing momentum of particle 3, and $\vec{p}_4$ be the outgoing momentum of particle 4. Let $E_a = \sqrt{|\vec{p}_a|^2 + m_a^2}$ and use $c = 1$ units in this question.

- Let $g_{ab} = E_a E_b - \vec{p}_a \cdot \vec{p}_b$. Show that $g_{ba} = g_{ab}$ and thus that there are 10 independent components to g and that each g_{ab} is Lorentz invariant.
- Let $s = (E_1 + E_2)^2 - |\vec{p}_1 + \vec{p}_2|^2$ and $t = (E_1 - E_3)^2 - |\vec{p}_1 - \vec{p}_3|^2$. Show that s is the square of the energy of the system in the center of momentum frame and that s and t are Lorentz invariant.
- Show that $g_{aa} = m_a^2$ for each a and that:

$$\begin{aligned} g_{12} &= \frac{s - m_1^2 - m_2^2}{2}, & g_{13} &= \frac{m_1^2 + m_3^2 - t}{2}, & g_{14} &= \frac{s + t - m_2^2 - m_3^2}{2}, \\ g_{23} &= \frac{s + t - m_1^2 - m_4^2}{2}, & g_{24} &= \frac{m_2^2 + m_4^2 - t}{2}, & g_{34} &= \frac{s - m_3^2 - m_4^2}{2}. \end{aligned}$$

These g_{ab} are a complete set of Lorentz invariant quantities which can be defined for a 2-to-2 scattering process and in fact we can see that they are ultimately determined only by two variables: s and t .

- For some purposes it is useful to define a third quantity $u = (E_1 - E_4)^2 - |\vec{p}_1 - \vec{p}_4|^2$. Show that u is also Lorentz invariant and that:

$$s + t + u = m_1^2 + m_2^2 + m_3^2 + m_4^2.$$

These three quantities s , t , and u are called the Mandelstam variables for a 2-to-2 scattering process.

- Consider the special case that particle 3 is just a scattered particle 1 and particle 4 is just a scattered particle 2 (called elastic scattering) so that $m_3 = m_1$ and $m_4 = m_2$. Let γ be the Lorentz factor of particle 2 in the rest frame of particle 1 and q be the magnitude of the linear momentum transfer from particle 1 to particle 2 in the process in the center of mass frame. Show that $\gamma = \frac{g_{12}}{m_1 m_2}$, $t = -q^2$ and that in the center of momentum frame, $E_3 = E_1$ and $E_4 = E_2$. Finally then, show that for elastic scattering:

$$\begin{aligned} g_{12} &= \gamma m_1 m_2, & g_{13} &= m_1^2 + \frac{q^2}{2}, & g_{14} &= \gamma m_1 m_2 - \frac{q^2}{2}, \\ g_{23} &= \gamma m_1 m_2 - \frac{q^2}{2}, & g_{24} &= m_2^2 + \frac{q^2}{2}, & g_{34} &= \gamma m_1 m_2. \end{aligned}$$

Problem 4.72: Relativistic Rocket Equation. Consider a rocket. It propels itself forward by a chemical reaction in which mass is burned and expelled, of course conserving energy and momentum but not necessarily mass. Suppose that the fuel is emitted so that the relative velocity of the rocket to the fuel immediately after the fuel is emitted is $\vec{u}$. Let $m(t)$ be the mass of the rocket and its contents at time t , $\vec{v}(t)$ be the velocity of the rocket, γ be the Lorentz factor corresponding to that velocity and $\vec{l}(t)$ be the unit vector in the direction of the velocity.

- Show that the velocity of the rocket satisfies:

$$\gamma m \frac{d\vec{v}}{dt} = -\frac{dm}{dt} \left(\vec{u} + \left(\frac{1}{\gamma} - 1 \right) \vec{l} \cdot \vec{u} \right).$$

- Show that the above result in the low speed limit reproduces the non-relativistic rocket equation.
- Consider the special case of the rocket moving in 1 dimension. Show that the above equation becomes:

$$m \frac{dv}{dt} = - \left(1 - \frac{v^2}{c^2} \right) \frac{dm}{dt} u.$$

Solve this equation to show that the velocity of the rocket is given by:

$$v = c \frac{c + v_0 - (c - v_0) \left(\frac{m}{m_0} \right)^{\frac{2u}{c}}}{c + v_0 + (c - v_0) \left(\frac{m}{m_0} \right)^{\frac{2u}{c}}}$$

where v_0 is the initial velocity of the rocket and m_0 is its initial mass. Show that equivalently the rapidity defined in equation (4.3.25) satisfies:

$$\varphi = \varphi_0 + \frac{u}{c} \ln \frac{m_0}{m}.$$

- (d) Show that the power output of the rocket in its instantaneous rest frame through burning mass to accelerate is given by:

$$\mathcal{P} = c^2 \left(-\frac{dm}{dt} \right) \left(1 - \sqrt{1 - \frac{|\vec{u}|^2}{c^2}} \right)$$

4.8 The Failure of Point Particles

From this point forward in all relativistic theories we will use units of charge so that $\epsilon_0 = 1$ and no longer write ϵ_0 as a consequence. Now that we have a special designated speed, c appears repeatedly in our equations. Further, it reveals a previously unknown connection between measures of length and measures of time. It is very convenient and intelligent to define your units of length by the distance light would travel in your unit of time, thus making the speed of light 1 in those units. If you choose to measure time in seconds and measure distance in units of how far light travels in 1 second then the speed of light is automatically 1 lightsecond per second = 1. So, just like we can make $\epsilon_0 = 1$ by choice of unit of charge, we can make $c = 1$ by choice of unit of length. Because c is the unique special speed which is Lorentz invariant, in a relativistic theory it is the special natural speed to use to calibrate your unit of distance from your unit of time. It is bad form in relativistic theories to write c 's as they clutter the equations and obfuscate the fact that in relativistic theories time and space are interrelated. Because in relativistic theories durations and lengths mix with each other under the symmetry transformations of those theories, it is incongruous and artificial to use different units for them. The unit system in which $\epsilon_0 = c = 1$ so that the only independent units are mass and time is called Heaviside-Lorentz units or **Lorentz Natural Units (LNU)**. Later we will occasionally return to working with some non-relativistic theories and when doing so we may continue to use ϵ_0 and c for ease of comparing to SI unit sources. When working with relativistic theories, essentially no one uses SI units. You can always restore ϵ_0 and c factors if you have an attachment to historical unit systems and how to do so will be developed in the homework.

The initial analysis of this section is based on [52]. The more serious analysis in this section is based on [39], which goes much further and deeper than we will. It is recommended reading for interested readers but is at a higher technical level than this text.

4.8.1 The Liénard-Wiechert Potentials

Just as with the Galilean theory, we would like to compute the effective equations of motion for interacting charges. In order to do this, we need to understand what, if any, effect a charge's own field has on that charge. For this, it will be useful to compute the potentials due to a moving point charge. Consider a point charge at location $\vec{z}(t)$ (to avoid potentially ambiguous use of the symbol $\vec{x}$). Then,

$$\rho(t, \vec{x}) = q\delta(\vec{x} - \vec{z}(t)) \quad \vec{J}(t, \vec{x}) = q\dot{\vec{y}}(t)\delta(\vec{x} - \vec{z}(t)). \quad (4.8.1)$$

Using our solution to the wave equation:

$$\phi(t, \vec{x}) = \int_{\mathbb{S}} \frac{\rho(t - |\vec{x} - \vec{x}'|, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d\mathbb{S}' = \int_{\mathbb{S}} \frac{q\delta(\vec{x}' - \vec{z}(t - |\vec{x} - \vec{x}'|))}{4\pi|\vec{x} - \vec{x}'|} d\mathbb{S}'. \quad (4.8.2)$$

This is a quite nasty integral as it contains evaluation of the position of the charge at an earlier point in time. We can take care of the integral by adding an integral over t' , which is possible using a delta distribution.

$$\phi(t, \vec{x}) = \int_{-\infty}^t \int_{\mathbb{S}} \frac{q\delta(\vec{x}' - \vec{z}(t'))}{4\pi|\vec{x} - \vec{x}'|} \delta(t - |\vec{x} - \vec{x}'| - t') d\mathbb{S}' dt' \quad (4.8.3)$$

$$= \int_{-\infty}^t \frac{q\delta(t - t' - |\vec{x} - \vec{z}(t')|)}{4\pi|\vec{x} - \vec{z}(t')|} dt'. \quad (4.8.4)$$

The delta distribution for t' will pick out the specific moment when $t' = t - |\vec{x} - \vec{z}(t')|$. That is, it picks out the moment in the past so that the potential produced by the particle at that moment would just now be reaching the point at which we are evaluating the potential. This time is called the delayed time $T(t, \vec{x})$. While the integral will pick out this specific time as a delta does, we do need to treat the delta a little carefully. The delta in the integral is not simply of the form $\delta(t' - t_0)$ because the argument has a complicated dependence on t' . Let $f(x)$ be a differentiable function with zeros x_n . Then, by problem 3.2:

$$\delta(f(x)) = \sum_n \frac{\delta(x - x_n)}{|f'(x_n)|}. \quad (4.8.5)$$

Therefore,

$$\delta(t - t' - |\vec{x} - \vec{z}(t')|) = \sum_n \frac{\delta(t' - t_n)}{\left| \frac{\partial}{\partial t'} (t - t' - |\vec{x} - \vec{z}(t')|) \right|_{t'=t_n}}. \quad (4.8.6)$$

We see that in principle we need to sum over all the delayed times. So, let us verify that there is at most

(uniqueness) and at least (existence) one such time. Consider the function $f(t', t, \vec{x})$:

$$f(t', t, \vec{x}) = t - t' - |\vec{x} - \vec{z}(t')|. \quad (4.8.7)$$

Evaluating at $t' = t$:

$$f(t, t, \vec{x}) = 0 - |\vec{x} - \vec{z}(t)| \leq 0. \quad (4.8.8)$$

Now consider the derivative of f with respect to t' :

$$\frac{\partial f}{\partial t'} = -1 + \frac{\vec{x} - \vec{z}(t')}{|\vec{x} - \vec{z}(t')|} \cdot \dot{\vec{z}}(t') \leq -1 + \frac{|\vec{x} - \vec{z}(t')|}{|\vec{x} - \vec{z}(t')|} |\dot{\vec{z}}(t')| = -1 + |\dot{\vec{z}}(t')|. \quad (4.8.9)$$

If there is finite energy in the system then because as speed approaches 1 the particle energy diverges, there is a maximum speed less than 1 which the particle can reach given the energy available. Call this maximum speed u . Then, by the monotonicity of the integral:

$$\frac{\partial f}{\partial t'} \leq -1 + u < 0 \quad (4.8.10)$$

$$\implies \int_{t_0}^t \frac{\partial f}{\partial t'} dt' \leq \int_{t_0}^t (-1 + u) dt' \quad (4.8.11)$$

$$\implies f(t_0, t, \vec{x}) \geq f(t, t, \vec{x}) + (1 - u)(t - t_0). \quad (4.8.12)$$

Hence, picking a sufficiently early t_0 so that $f(t, t, \vec{x}) + (1 - u)(t - t_0) \geq 0$, we can guarantee that $f(t_0) \geq 0$. Because $f(t, t, \vec{x}) \leq 0$ and we can find t_0 such that $f(t_0, t, \vec{x}) \geq 0$, there exists a T between t_0 and t such that $f(T, t, \vec{x}) = 0$ by the intermediate value theorem and the continuity of f . Hence, a delayed time is guaranteed to exist in a system with finite energy in which the particle considered has always existed.

The easiest method to prove that the delayed time is unique is by contradiction. Consider two delayed times $t_1 < t_2$. Then, using the triangle inequality:

$$|\vec{z}(t_2) - \vec{z}(t_1)| \geq |\vec{z}(t_1) - \vec{x}| - |\vec{z}(t_2) - \vec{x}| = t - t_1 - (t - t_2) = t_2 - t_1 \implies \frac{|\vec{z}(t_2) - \vec{z}(t_1)|}{t_2 - t_1} \geq 1. \quad (4.8.13)$$

Hence the existence of two distinct delayed times implies that over the time interval between them the magnitude of the average velocity of the particle is greater than the speed of light which we know is impossible from our equations of motion.

Given the existence and uniqueness of the delayed time $T(t, \vec{x})$, we have:

$$\phi(t, \vec{x}) = \int_{-\infty}^t \frac{q \delta(t' - t_r)}{4\pi |\vec{x} - \vec{z}(t')| \left| \frac{\partial}{\partial t'} (t - t' - |\vec{x} - \vec{z}(t')|) \right|_{t'=T}} dt' \quad (4.8.14)$$

$$= \frac{q}{4\pi |\vec{x} - \vec{z}(T)| \left(1 - \frac{\vec{x} - \vec{z}(T)}{|\vec{x} - \vec{z}(T)|} \cdot \dot{\vec{z}}(T) \right)} \quad (4.8.15)$$

Just to keep the notation contained, it is useful to define $\vec{Z} = \vec{z}(T(t, \vec{x}))$ as the delayed position, $\dot{\vec{Z}} = \dot{\vec{z}}(T(t, \vec{x}))$ as the delayed velocity, $\ddot{\vec{Z}} = \ddot{\vec{z}}(T(t, \vec{x}))$ as the delayed acceleration, and $\vec{r}$ as the unit vector pointing from the delayed source to the evaluation point:

$$\vec{r} = \frac{\vec{x} - \vec{Z}}{|\vec{x} - \vec{Z}|} \quad (4.8.16)$$

$$\implies \phi(t, \vec{x}) = \frac{q}{4\pi |\vec{x} - \vec{Z}| (1 - \vec{r} \cdot \dot{\vec{Z}})}. \quad (4.8.17)$$

One ought to be careful here about notation, as the way I have defined $\dot{\vec{Z}}$, it is **NOT** equal to $\frac{d}{dt} \vec{Z}$ and similarly so for $\ddot{\vec{Z}}$. This calculation gives the vector potential as well:

$$\vec{A}(t, \vec{x}) = \int_{\mathbb{S}} \frac{\vec{J}(t - |\vec{x} - \vec{x}'|, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}' = \int_{\mathbb{S}} \frac{q \delta(\vec{x}' - \vec{z}(t - |\vec{x} - \vec{x}'|)) \dot{\vec{z}}(t - |\vec{x} - \vec{x}'|)}{4\pi |\vec{x} - \vec{x}'|} d\mathbb{S}' \quad (4.8.18)$$

$$\implies \vec{A}(t, \vec{x}) = \frac{q \dot{\vec{Z}}}{4\pi |\vec{x} - \vec{Z}| (1 - \vec{r} \cdot \dot{\vec{Z}})} = \dot{\vec{Z}} \phi(t, \vec{x}). \quad (4.8.19)$$

These potentials are called the Liénard-Wiechert potentials. It is now a direct but arduous task to

get the corresponding electric and magnetic fields. We find after significant labor:

$$\vec{E}(t, \vec{x}) = \frac{q(1 - |\dot{\vec{Z}}|^2)}{4\pi(1 - \vec{r} \cdot \dot{\vec{Z}})^3} \frac{\vec{r} - \dot{\vec{Z}}}{|\vec{x} - \dot{\vec{Z}}|^2} + \frac{q}{4\pi(1 - \vec{r} \cdot \dot{\vec{Z}})^3} \frac{\vec{r} \times ((\vec{r} - \dot{\vec{Z}}) \times \ddot{\vec{Z}})}{|\vec{x} - \dot{\vec{Z}}|} \quad (4.8.20)$$

$$\vec{B}(t, \vec{x}) = \vec{r} \times \vec{E}. \quad (4.8.21)$$

Naively trying to evaluate these fields at $\vec{z}(t)$, the present location of the particle, so that we can compute the right hand side of the equation of motion (4.3.36) leads to the same divergence problem as in the Galilean theory. Consider evaluating the delayed time at $(t, \vec{z}(t))$. Plainly $T(t, \vec{z}(t)) = t$ is a solution for the delayed time, and by the uniqueness property it is *the* solution. Immediately, $Z(t, \vec{z}(t)) = \vec{z}(T(t, \vec{z}(t))) = \vec{z}(t)$. Hence both $\vec{E}(t, \vec{z}(t))$ and $\vec{B}(t, \vec{z}(t))$ diverge as their denominator terms go to 0, just as in the Galilean theory. We will need to smoothen the charge distribution in order to make any sensible equations for a charge on itself.

4.8.2 Smoothened Equations of Motion

Let $f(t, \vec{x})$ be a smooth function which integrates to 1 when integrated over all space:

$$\int_{\mathbb{R}^3} f(t, \vec{x}) d^3 \vec{x} = 1. \quad (4.8.22)$$

Then, define the “nascent Dirac delta”:

$$F(\varepsilon, t, \vec{x}) = \frac{1}{\varepsilon^3} f\left(t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon}\right) \quad (4.8.23)$$

for $\varepsilon > 0$. F is called a “nascent Dirac delta” because of how it behaves when integrated against other smooth functions in the limit $\varepsilon \rightarrow 0^+$. Consider $g(t, \vec{x})$ another smooth function. Then:

$$\int_{\mathbb{R}^3} F(\varepsilon, t, \vec{x}) g(t, \vec{x}) d^3 \vec{x} = \int_{\mathbb{R}^3} \frac{1}{\varepsilon^3} f\left(t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon}\right) g(t, \vec{x}) d^3 \vec{x} = \int_{\mathbb{R}^3} f(t, \vec{x}) g(t, \vec{z} + \varepsilon \vec{x}) d^3 \vec{x}. \quad (4.8.24)$$

In the $\varepsilon \rightarrow 0^+$ limit:

$$\lim_{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^3} F(\varepsilon, t, \vec{x}) g(t, \vec{x}) d^3 \vec{x} = \int_{\mathbb{R}^3} f(t, \vec{x}) g(t, \vec{z}) d^d \vec{x} = g(t, \vec{z}) \quad (4.8.25)$$

$$\implies F(0, t, \vec{x}) = \delta(\vec{x} - \vec{z}(t)). \quad (4.8.26)$$

We want to consider a smooth charge distribution of finite size so that the associated potentials and electromagnetic fields are smooth and the corresponding forces and equations of motion are well defined. Then, we want to shrink that charge distribution down to a point and study the limit of the equations of motion, just as we did in the Galilean case. We can do so using this idea of a nascent Dirac delta. Let $\vec{z}(t)$ be the path in space we will shrink the distribution down to. Then, by the logic of our nascent Dirac delta, we take our charge distribution to be:

$$\rho(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon^3} \mathbf{r}\left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon}\right), \quad \vec{J}(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon^3} \vec{j}\left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon}\right) \quad (4.8.27)$$

for some functions $\mathbf{r}, \vec{j}$. Here we have explicitly factored out q , the total charge of the distribution defined by:

$$q = \int_{\mathbb{R}^3} \rho(\varepsilon, t, \vec{x}) d^3 \vec{x} \implies \int_{\mathbb{R}^3} \mathbf{r}(\varepsilon, t, \vec{x}) d^3 \vec{x} = 1. \quad (4.8.28)$$

As well, the functions $\mathbf{r}(\varepsilon, t, \vec{x})$ and $\vec{j}(\varepsilon, t, \vec{x})$ are required to be smooth and to be 0 for $\vec{x}$ sufficiently large so that the charge is contained in a finite size region. In order to shrink down to a point particle with position $\vec{z}(t)$ we will take the $\varepsilon \rightarrow 0^+$ limit.

It is necessary to allow $\mathbf{r}$ and $\vec{j}$ to be explicitly ε dependent in order for the charge distribution to satisfy the continuity equation. In particular, applying the continuity equation to (4.8.27) gives:

$$\varepsilon \frac{\partial \mathbf{r}}{\partial t}(\varepsilon, t, \vec{x}) - \dot{\vec{z}}(t) \cdot \nabla \mathbf{r}(\varepsilon, t, \vec{x}) + \nabla \cdot \vec{j}(\varepsilon, t, \vec{x}) = 0. \quad (4.8.29)$$

Now the explicit necessity of ε dependence is clear in the prefactor of $\frac{\partial \mathbf{r}}{\partial t}$.

Because $\mathbf{r}$ and $\vec{j}$ are smooth functions and we will be looking at small ε , it is useful to define the smooth functions corresponding to the Taylor series expansion of these quantities near $\varepsilon = 0$:

$$\mathbf{r}(\varepsilon, t, \vec{x}) = \mathbf{r}_{(0)}(t, \vec{x}) + \varepsilon \mathbf{r}_{(1)}(t, \vec{x}) + \varepsilon^2 \mathbf{r}_{(2)}(t, \vec{x}) + \mathcal{O}(\varepsilon^3) \quad (4.8.30)$$

and similarly so for $\vec{j}$, ρ , $\vec{J}$, or any other functions of ε . Integrating $\rho(\varepsilon, t, \vec{x})$ over all space against a smooth function $f(t, \vec{x})$ and taking the limit $\varepsilon \rightarrow 0^+$ produces:

$$\rho_{(0)}(t, \vec{x}) = q\delta(\vec{x} - \vec{z}(t)) \quad (4.8.31)$$

exactly like we would want for our point charge. Integrating $\vec{J}(\varepsilon, t, \vec{x})$ over all space against a smooth function $f(t, \vec{x})$ and taking the limit $\varepsilon \rightarrow 0^+$ produces:

$$\vec{J}_{(0)}(t, \vec{x}) = q\delta(\vec{x} - \vec{z}(t)) \int_{\mathbb{R}^3} \vec{j}_{(0)}(t, \vec{y}) d^3\vec{y}. \quad (4.8.32)$$

Integrating (4.8.29) over all space against x^a and taking the limit $\varepsilon \rightarrow 0^+$ produces:

$$\int_{\mathbb{R}^3} \vec{j}_{(0)}(t, \vec{x}) d^3\vec{x} = \dot{\vec{z}}(t). \quad (4.8.33)$$

Therefore, our current density also limits to the appropriate current density for a point charge:

$$\vec{J}_{(0)}(t, \vec{x}) = q\dot{\vec{z}}(t)\delta(\vec{x} - \vec{z}(t)). \quad (4.8.34)$$

The potentials ϕ and $\vec{A}$ can be divided into the potentials “due” to the charge distribution and the external potentials to the charge (meaning due to other electromagnetic sources than the specific distribution whose equations of motion we are looking at). Let ϕ_{self} and $\vec{A}_{\text{self}}$ correspond to the potentials due to the charge distribution and ϕ_{ext} and $\vec{A}_{\text{ext}}$ correspond to the externally produced potentials. Then, the electric and magnetic fields immediately decompose in the same way and the total force of the charge distribution is given by the Lorentz force law as:

$$\vec{F} = \int_{\mathbb{R}^3} (\rho\vec{E} + \vec{J} \times \vec{B}) d^3\vec{x} = \int_{\mathbb{R}^3} (\rho\vec{E}_{\text{self}} + \vec{J} \times \vec{B}_{\text{self}}) d^3\vec{x} + \int_{\mathbb{R}^3} (\rho\vec{E}_{\text{ext}} + \vec{J} \times \vec{B}_{\text{ext}}) d^3\vec{x} = \vec{F}_{\text{self}} + \vec{F}_{\text{ext}}. \quad (4.8.35)$$

The $\varepsilon \rightarrow 0^+$ behavior of the external force is exactly as expected using (4.8.31) and (4.8.34):

$$\lim_{\varepsilon \rightarrow 0^+} \vec{F}_{\text{ext}} = q\vec{E}_{(0)\text{ext}}(t, \vec{z}(t)) + q\dot{\vec{z}}(t) \times \vec{B}_{(0)\text{ext}}(t, \vec{z}(t)). \quad (4.8.36)$$

The $\varepsilon \rightarrow 0^+$ behavior of the “self-force” is of course the only point of difficulty.

Using the Lorenz gauge solution for the potentials, we immediately have for ϕ_{self} :

$$\phi_{\text{self}}(\varepsilon, t, \vec{x}) = \int_{\mathbb{R}^3} \frac{q}{\varepsilon^3} \frac{\mathbf{r} \left(\varepsilon, t - |\vec{x} - \vec{x}'|, \frac{\vec{x}' - \vec{z}(t - |\vec{x} - \vec{x}'|)}{\varepsilon} \right)}{4\pi|\vec{x} - \vec{x}'|} d^3\vec{x}' = \frac{q}{\varepsilon} \int_{\mathbb{R}^3} \frac{\mathbf{r} \left(\varepsilon, t - \varepsilon|\vec{y}|, \vec{y} + \frac{\vec{x} - \vec{z}(t - \varepsilon|\vec{y}|)}{\varepsilon} \right)}{4\pi|\vec{y}|} d^3\vec{y}. \quad (4.8.37)$$

Define then the function $\tilde{\phi}(\varepsilon, t, \vec{x})$:

$$\tilde{\phi}(\varepsilon, t, \vec{x}) = \int_{\mathbb{R}^3} \frac{\mathbf{r} \left(\varepsilon, t - \varepsilon|\vec{y}|, \vec{y} + \frac{\vec{x} - \vec{z}(t - \varepsilon|\vec{y}|)}{\varepsilon} \right)}{4\pi|\vec{y}|} d^3\vec{y} \quad (4.8.38)$$

which is automatically a smooth function. Then, ϕ_{self} is given by:

$$\phi_{\text{self}}(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon} \tilde{\phi} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right). \quad (4.8.39)$$

The same definitions and form are then given for the vector potential by repeating the analysis:

$$\vec{A}_{\text{self}}(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon} \tilde{\vec{A}} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) \quad (4.8.40)$$

where $\tilde{\vec{A}}$ is a smooth function. The definitions of $\vec{E}$ and $\vec{B}$ in terms of the potentials then give:

$$\vec{E}_{\text{self}}(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon^2} \tilde{\vec{E}} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right), \quad \vec{B}_{\text{self}}(\varepsilon, t, \vec{x}) = \frac{q}{\varepsilon^2} \tilde{\vec{B}} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) \quad (4.8.41)$$

where $\tilde{\vec{E}}$ and $\tilde{\vec{B}}$ are smooth functions given by:

$$\tilde{\vec{E}}(\varepsilon, t, \vec{x}) = -\nabla \tilde{\phi}(\varepsilon, t, \vec{x}) + \dot{\vec{z}}^a(t) \frac{\partial \tilde{\vec{A}}}{\partial x^a}(\varepsilon, t, \vec{x}) - \varepsilon \frac{\partial \tilde{\vec{A}}}{\partial t}(\varepsilon, t, \vec{x}), \quad \tilde{\vec{B}}(\varepsilon, t, \vec{x}) = \nabla \times \tilde{\vec{A}}(\varepsilon, t, \vec{x}). \quad (4.8.42)$$

Returning our expressions for the charge and current densities together with the self fields to the self

force, we have:

$$\vec{F}_{\text{self}} = \int_{\mathbb{R}^3} \left(\frac{q}{\varepsilon^3} \mathbf{r} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) \frac{q}{\varepsilon^2} \vec{E} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) + \frac{q}{\varepsilon^3} \vec{j} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) \times \frac{q}{\varepsilon^2} \vec{B} \left(\varepsilon, t, \frac{\vec{x} - \vec{z}(t)}{\varepsilon} \right) \right) d^3 \vec{x} \quad (4.8.43)$$

$$= \frac{q^2}{\varepsilon^2} \int_{\mathbb{R}^3} \left(\mathbf{r}(\varepsilon, t, \vec{x}) \vec{E}(\varepsilon, t, \vec{x}) + \vec{j}(\varepsilon, t, \vec{x}) \times \vec{B}(\varepsilon, t, \vec{x}) \right) d^3 \vec{x}. \quad (4.8.44)$$

We see that unless the integrand cancels in a very special way, the self force is divergent like $\frac{1}{\varepsilon^2}$. This is analogous to what we found in the Galilean case and in that case we did find a very special cancellation. Expanding the smooth functions here as a series in ε gives:

$$\vec{F}_{\text{self}} = \frac{q^2}{\varepsilon^2} \vec{F}_{-2} + \frac{q^2}{\varepsilon} \vec{F}_{-1} + q^2 \vec{F}_0 + \mathcal{O}(q^2 \varepsilon) \quad (4.8.45)$$

where:

$$\vec{F}_{-2} = \int_{\mathbb{R}^3} \left(\mathbf{r}_{(0)} \vec{E}_{(0)} + \vec{j}_{(0)} \times \vec{B}_{(0)} \right) d^3 \vec{x} \quad (4.8.46)$$

$$\vec{F}_{-1} = \int_{\mathbb{R}^3} \left(\mathbf{r}_{(0)} \vec{E}_{(1)} + \mathbf{r}_{(1)} \vec{E}_{(0)} + \vec{j}_{(0)} \times \vec{B}_{(1)} + \vec{j}_{(1)} \times \vec{B}_{(0)} \right) d^3 \vec{x} \quad (4.8.47)$$

$$\vec{F}_0 = \int_{\mathbb{R}^3} \left(\mathbf{r}_{(0)} \vec{E}_{(2)} + \mathbf{r}_{(1)} \vec{E}_{(1)} + \mathbf{r}_{(2)} \vec{E}_{(0)} + \vec{j}_{(0)} \times \vec{B}_{(2)} + \vec{j}_{(1)} \times \vec{B}_{(1)} + \vec{j}_{(2)} \times \vec{B}_{(0)} \right) d^3 \vec{x}. \quad (4.8.48)$$

Thus, we see in order for the Lorentz theory of point charges to make sense, both $\vec{F}_{-2}$ and $\vec{F}_{-1}$ have to be 0 (otherwise the point limit is divergent). Then, if both of those are 0, $\vec{F}_0$ gives the self force effect of the particle because in the $\varepsilon \rightarrow 0^+$ limit the $\mathcal{O}(\varepsilon)$ remainder will go to 0.

Before looking at $\vec{F}_0$, we need to see if $\vec{F}_{-2}$ and $\vec{F}_{-1}$ are both 0, because if they are not then there is no well defined point charge limit for the relativistic theory. To compute these, we will need the potentials at orders ε^0 and ε^1 . Using (4.8.38) gives:

$$\tilde{\phi}_{(0)}(t, \vec{x}) = \int_{\mathbb{R}^3} \frac{\mathbf{r}_{(0)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}(t))}{4\pi |\vec{y}|} d^3 \vec{y}, \quad \tilde{A}_{(0)}(t, \vec{x}) = \int_{\mathbb{R}^3} \frac{\vec{j}_{(0)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}(t))}{4\pi |\vec{y}|} d^3 \vec{y}, \quad (4.8.49)$$

$$\begin{aligned} \tilde{\phi}_{(1)}(t, \vec{x}) &= \int_{\mathbb{R}^3} \frac{\mathbf{r}_{(1)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}})}{4\pi |\vec{y}|} d^3 \vec{y} - \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\partial \mathbf{r}_{(0)}}{\partial t}(t, \vec{x}') \Big|_{\vec{x}' = \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}} d^3 \vec{y} \\ &\quad - \dot{z}^a \frac{\partial}{\partial x^a} \int_{\mathbb{R}^3} \frac{|\vec{y}|}{8\pi} \mathbf{r}_{(0)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}) d^3 \vec{y}, \end{aligned} \quad (4.8.50)$$

$$\begin{aligned} \tilde{A}_{(1)}(t, \vec{x}) &= \int_{\mathbb{R}^3} \frac{\vec{j}_{(1)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}})}{4\pi |\vec{y}|} d^3 \vec{y} - \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\partial \vec{j}_{(0)}}{\partial t}(t, \vec{x}') \Big|_{\vec{x}' = \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}} d^3 \vec{y} \\ &\quad - \dot{z}^a \frac{\partial}{\partial x^a} \int_{\mathbb{R}^3} \frac{|\vec{y}|}{8\pi} \vec{j}_{(0)}(t, \vec{y} + \vec{x} + |\vec{y}| \dot{\vec{z}}) d^3 \vec{y}. \end{aligned} \quad (4.8.51)$$

The use of (4.8.42) gives:

$$\vec{E}_{(0)} = -\nabla \tilde{\phi}_{(0)} + \dot{z}^a \frac{\partial \tilde{A}_{(0)}}{\partial x^a}, \quad \vec{B}_{(0)} = \nabla \times \tilde{A}_{(0)}, \quad (4.8.52)$$

$$\vec{E}_{(1)} = -\nabla \tilde{\phi}_{(1)} + \dot{z}^a \frac{\partial \tilde{A}_{(1)}}{\partial x^a} - \frac{\partial \tilde{A}_{(0)}}{\partial t}, \quad \vec{B}_{(1)} = \nabla \times \tilde{A}_{(1)}. \quad (4.8.53)$$

In order to evaluate the fields, it is easiest to assume that at the present time we are in the instantaneous rest frame (IRF) of the trajectory $\vec{z}(t)$. It is always possible to go to this frame at a particular moment in time using a Lorentz boost. Then, due to the Lorentz invariance of the theory, if we know the instantaneous force in this frame we can perform a Lorentz transformation to an arbitrary frame to get the equation of motion in that frame. In the IRF, by definition $\dot{\vec{z}}(t) = 0$ at the present value of t only. Evaluating the fields

in the IRF gives:

$$\tilde{E}_{(0)} \stackrel{\text{IRF}}{=} \int_{\mathbb{R}^3} \frac{\mathbf{r}_{(0)}(t, \vec{x}')}{4\pi} \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} d^3 \vec{x}', \quad \tilde{B}_{(0)} \stackrel{\text{IRF}}{=} \int_{\mathbb{R}^3} \frac{\vec{j}_{(0)}(t, \vec{x}')}{4\pi} \times \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} d^3 \vec{x}', \quad (4.8.54)$$

$$\tilde{E}_{(1)} \stackrel{\text{IRF}}{=} \int_{\mathbb{R}^3} \left(\frac{\mathbf{r}_{(1)}(t, \vec{x}')}{4\pi} \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} + \frac{\mathbf{r}_{(0)}(t, \vec{x}')}{8\pi|\vec{x} - \vec{x}'|} \left(\mathbb{1} - \frac{(\vec{x} - \vec{x}')(\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^2} \right) \cdot \ddot{\vec{z}}(t) - \frac{\partial_t \vec{j}_{(0)}(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} \right) d^3 \vec{x}' \quad (4.8.55)$$

$$\tilde{B}_{(1)} \stackrel{\text{IRF}}{=} \int_{\mathbb{R}^3} \left(\frac{\vec{j}_{(1)}(t, \vec{x}')}{4\pi} \times \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} + \frac{\vec{j}_{(0)}(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} \times \left(\left(\mathbb{1} - \frac{(\vec{x} - \vec{x}')(\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^2} \right) \cdot \ddot{\vec{z}} \right) \right) d^3 \vec{x}'. \quad (4.8.56)$$

With our expressions for the fields, we can now compute $\vec{F}_{-2}$ and $\vec{F}_{-1}$. Doing so we find for $\vec{F}_{-2}$ (after using the continuity equation):

$$\vec{F}_{-2} \stackrel{\text{IRF}}{=} \int_{\mathbb{R}^3 \mathbb{R}^3} \frac{\mathbf{r}_{(0)}(t, \vec{x}) \mathbf{r}_{(0)}(t, \vec{x}') - \vec{j}_{(0)}(t, \vec{x}) \cdot \vec{j}_{(0)}(t, \vec{x}')}{4\pi} \frac{\vec{x} - \vec{x}'}{|\vec{x} - \vec{x}'|^3} d^3 \vec{x} d^3 \vec{x}' = 0 \quad (4.8.57)$$

due to the integrand turning equal to its own negative under interchanging the names of the integration variables $\vec{x}$ and $\vec{x}'$. This cancellation is analogous to the cancellation which occurred for the Galilean particle. Simplifying for $\vec{F}_{-1}$ is significantly more effort, but after doing so we find:

$$\begin{aligned} \vec{F}_{-1} \stackrel{\text{IRF}}{=} & -\frac{d}{dt} \int_{\mathbb{R}^3 \mathbb{R}^3} \frac{\mathbf{r}_{(0)}(t, \vec{x}) \vec{j}_{(0)}(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' \\ & + \int_{\mathbb{R}^3 \mathbb{R}^3} \frac{\mathbf{r}_{(0)}(t, \vec{x}) \mathbf{r}_{(0)}(t, \vec{x}') - 2\vec{j}_{(0)}(t, \vec{x}) \cdot \vec{j}_{(0)}(t, \vec{x}')}{8\pi|\vec{x} - \vec{x}'|} \left(\mathbb{1} - \frac{(\vec{x} - \vec{x}')(\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^2} \right) \cdot \ddot{\vec{z}} d^3 \vec{x} d^3 \vec{x}'. \end{aligned} \quad (4.8.58)$$

Unfortunately, this is not automatically 0. While the Galilean particle universally had a well-defined point limit, the Lorentz theory has no such thing. One might hope that perhaps the time dependence of $\mathbf{r}_{(0)}$ and $\vec{j}_{(0)}$ can be rigged to make $\vec{F}_{-1}$ vanish. However, their time dependence is determined by ρ and $\vec{j}$ and their time evolution is determined by whatever the equations of motion for them are in the smoothened theory. Generically, even if $\vec{F}_{-1}$ vanishes at a particular time, its time derivative is nonzero and it will not vanish at later times. In fact, outside of the instantaneous rest frame, $\vec{F}_{-2}$ doesn't even vanish. Therefore the finite mass, finite charge point particle limit of the relativistic theory does not exist. This conclusion has nothing to do with the way we performed the limit. Many different attempts from many different perspectives have been attempted and consistently the same result has been concluded: **there is no well defined interaction of a point charge with $q \neq 0$ with Maxwell's equations.**

It is a disaster for the theory of point particles that there is no way to smoothen out the charge distribution to give self-consistent and finite equations of motion. This problem has caused much frustration among physicists for over a century. The lack of a well defined point limit for $q \neq 0$ tells us something very important: **point-particles are not real.** They do not correctly predict what is seen in experiment as they are either theoretically inconsistent or non-interacting. The best one can do while sticking to point particles is to consider further scaling q and m with ε so that the equation of motion becomes finite. The acceleration of a charge due to an external field is determined by the ratio $\frac{q}{m}$, and so for charges to respond as seen in experiment to external fields, $\frac{q}{m}$ must remain finite in the $\varepsilon \rightarrow 0^+$ limit. The lowest order force due to the self field is given proportional to $\frac{q^2}{\varepsilon}$ as we found and so the lowest order effect on the acceleration is proportional to $\frac{q^2}{\varepsilon m}$. For this to remain finite as $\varepsilon \rightarrow 0^+$ then we need q to be proportional to ε (and so m is proportional to ε as well). Instead of a point charge limit, this is known as the **test body limit**. A test body produces no effect on anything else because its interaction parameters (mass, charge) are vanishingly small. This can be useful for some effective theory purposes but is certainly only an approximation; we observe electromagnetic interactions and in this test body limit different charges simply do not interact with each other. This analysis is performed in full detail in [39] where they also compute the lowest order correction to the test body limit (meaning small bodies with small masses and charges). Because exact point particles cannot interact, we need continuous charge distributions of non-zero size to have well-defined interactions and to match experiment. For the purposes of treating point-particles in electromagnetism as an effective theory in the test body limit, the analysis of [39] reveals that the “self-force” and “radiation-reaction” effects of a charge on itself at least appear as higher order (in the size of the body) corrections to the equations of motion and that the lowest order behavior to consider is that a charge is unaffected by the fields it produces.

However unlike in the Galilean theory, vanishing self-force cannot be maintained exactly, only as the lowest order approximation. We have a fundamental result: **point-particles have failed**. We must abandon them for fundamental physics, though they remain useful as an effective theory for small bodies.

4.8.3 A Wave Theory of Matter?

Tragically, we are again at a point where two independently successful theories cannot coexist. Maxwell's equations produce an experimentally successful theory of electromagnetism. The Lorentz particle Hamiltonian/Lagrangian produces an often experimentally successful theory of matter. But, the interaction between the two leads to divergences which cannot be removed. Something has to be changed. We can either modify Maxwell's electromagnetism or Lorentz' point particles. It turns out that there are modifications of Maxwell which make point particles have finite energy and which may lead to a finite interaction between the two. One such example is explored in the homework. However, such modifications would necessarily have experimentally noticeable effects for sufficiently strong electric and magnetic fields and the corresponding deviations from Maxwell's equations have not been seen in experiment. As well, there are many other theoretical and experimental problems with point particles than just their failed electromagnetic interaction. In particular, as we found by Earnshaw's theorem in section 3.10, it may be impossible to have a stable theory of matter interacting with electromagnetism and it is not clear if this issue can be resolved by modifications of Maxwell's equations. More robustly, any modification of Maxwell's equations will generically produce some radiation reaction effect on a charge due to the fields that charge creates and as explored in the homework, the classical radiation reaction of a classical atom will cause the atom to collapse into itself almost immediately. A point-particle theory of matter cannot explain the stability of objects in the macroscopic world.

The alternative to modifying Maxwell's equations then is to try a theory of matter other than point particles as it is the point limit which has always caused us trouble. This would be compatible with the fact that Maxwell's equations are extremely successful experimentally and should still reproduce our point particle theory in the limit that our non-point matter was sufficiently localized as to appear point-like for experimental purposes. Because a discrete distribution of matter is precisely what failed us, we are then led to try a continuous distribution. In the Galilean theory, we developed a notion of a rigid body for continuous matter. This causes problems in the relativistic theory. Suppose a rigid body is pushed by something on one side in the relativistic theory and starts to move. Because it is rigid, instantaneously the other end also begins to move and thus the information that it was pushed propagates across a non-zero distance in zero time. Because these events are spacelike separated, one could go to a frame in which the opposite end of the rigid body moves before the first end of the body is pushed. That is, **finite size rigid bodies in relativity automatically violate causality**. To determine the time evolution of points on the body, one needs data from outside of its lightcone. This is not allowed by causality. So, there is no causally consistent notion of a relativistic perfectly rigid body. Elastic bodies (that is, deformable bodies) are allowed in relativity. Elastic bodies have internal speeds at which disturbances travel and the closest thing to a rigid body in relativity is actually an elastic body in which the inner disturbance travel speeds (called the speeds of sound of the body) are the same as the speed of light. However, at this point we are discussing a continuous theory of matter and thus would need to have a field to describe how much matter is at any given point at that time. That is, by abandoning our point matter we are immediately pushed into using a **field theory of matter**. A field theory of matter will be the successful avenue we explore to solve the problem with point particles.

Experimentally, there is a very clear way to distinguish between an ultimately point based and ultimately wave based theory of matter. Consider a screen which is impermeable to matter for our purposes and which has two parallel narrow slits cut through it. On one side of the slits at a distance d away is another screen, this one completely solid and which we are able to observe. Suppose we take a device which shoots out a beam of matter toward the narrow slits and ultimately toward the observation screen. What distribution of matter should we expect to see on the final screen? Let the axis normal to both screens and which is halfway between the slits be the z -axis. Our beam of matter would have for each particle in the beam a velocity distribution $f(\vec{v})$ which gives the probability density of any particle in the beam having velocity $\vec{v}$. Because the beam is traveling in the z direction, the average z velocity will be non-zero while the average x and y velocities will be zero. Consequently, on average a particle passing through either slit will go straight through with some distribution of particles around the straight path due to the probability distribution on velocity. As such, from point particles passing through the slit, one would expect a peak in intensity of number of particles directly on the other side of each slit with then a decaying tail all around those peaks as shown in Figure 4.1.

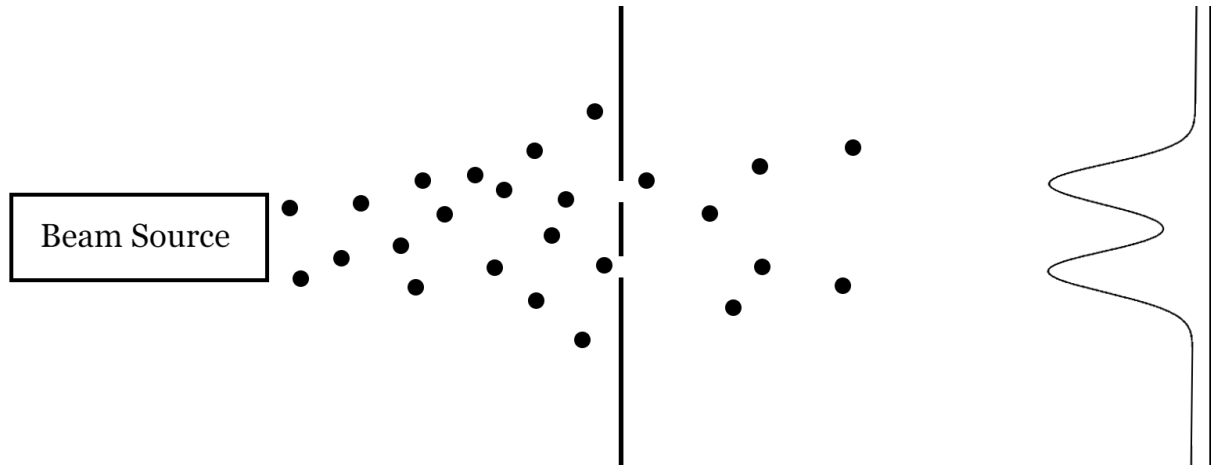


Figure 4.1: The point particle prediction for the intensity of incident particles through a double-slit apparatus. The plot given on the right hand screen is a graph of the predicted intensity versus position on the screen.

The prediction for the intensity pattern for point particles is quite different from the prediction for the intensity pattern if instead we were to consider a beam made of waves, for example using our theory of electromagnetism and considering light waves. If our beam were to consist of waves, then by linearity we can decompose the incoming beam in terms of plane waves and then for very narrow slits, we can approximate each of the slits as an oscillating point-like (approximately) source (oscillating due to the plane waves hitting it) in the wave equation. Using coordinates, place the upper slit at coordinates $\vec{x}_1 = (0, s/2, 0)$ and the lower slit at $\vec{x}_2 = (0, -s/2, 0)$. To the right ($z > 0$) of the slit screen, the system disturbance $\phi(t, \vec{x})$ satisfies the wave-equation with a speed v and source $\eta(t, \vec{x}) = A \cos(\omega t)(\delta(\vec{x} - \vec{x}_1) + \delta(\vec{x} - \vec{x}_2))$. If we are literally considering light waves, then $v = c$ and ϕ would correspond to any component of the electric or magnetic fields or to the scalar or vector potential in the Lorenz gauge. Using our Green's function solution to the wave equation in equation (3.9.36), we have then that:

$$\phi(t, \vec{x}) = \frac{A \cos\left(\omega \left(t - \frac{|\vec{x} - \vec{x}_1|}{v}\right)\right)}{4\pi|\vec{x} - \vec{x}_1|} + \frac{A \cos\left(\omega \left(t - \frac{|\vec{x} - \vec{x}_2|}{v}\right)\right)}{4\pi|\vec{x} - \vec{x}_2|}. \quad (4.8.59)$$

If we consider evaluating this solution at the screen located at $z = d$ and in particular for convenience in the plane shown in Figure 4.1 at $x = 0$:

$$\phi(t, 0, y, d) = \frac{A \cos\left(\omega \left(t - \frac{1}{v} \sqrt{d^2 + \frac{s^2}{4} - sy + y^2}\right)\right)}{4\pi \sqrt{d^2 + \frac{s^2}{4} - sy + y^2}} + \frac{A \cos\left(\omega \left(t - \frac{1}{v} \sqrt{d^2 + \frac{s^2}{4} + sy + y^2}\right)\right)}{4\pi \sqrt{d^2 + \frac{s^2}{4} + sy + y^2}} \quad (4.8.60)$$

Suppose the observation screen is very far from the slits and we are looking at y also much smaller than d . In that approximation (meaning to leading order in y/d):

$$\phi(t, 0, y, d) = \frac{A}{2\pi d} \cos\left(\omega \left(t - \frac{d}{v} - \frac{s^2}{8dv}\right)\right) \cos\left(\frac{\omega sy}{2dv}\right) + \text{Higher Order Terms} \quad (4.8.61)$$

where the higher order terms indicate terms which decay at order $1/d^2$ or faster meaning for a far away observation screen they become insignificant. Generically for a linear wave theory, the power intensity is proportional to the time average of the wave squared (as we found in particular for electromagnetism). Then, normalizing the wave so that proportionality constant is 1, we have that the intensity on the screen is:

$$\mathcal{I} = \mathbb{T}(|\phi|^2) = \frac{A^2}{8\pi^2 d^2} \cos^2\left(\frac{\omega sy}{2dv}\right) + \text{H.O.T.} \quad (4.8.62)$$

Thus, we see that for a wave source, the intensity on the screen is oscillatory rather than two simple peaks. The plot of the intensity due to (4.8.60) is given in Figure 4.2. It is no surprise that for electromagnetic waves the intensity pattern in Figure 4.2 is what is observed in experiment. However, quite surprisingly historically in the Davisson-Germer experiment when a beam of small particles (specifically electrons, though the phenomenon is more general) was used with small enough slits, the intensity pattern observed was that of Figure 4.2, not of Figure 4.1. That is, for elementary particles through sufficiently narrow slits we

find the wave intensity pattern, not the particle intensity pattern. This is one of many experiments which demonstrates that fixing point particle divergences is not enough, point particles are genuinely a fiction of our approximations thus far. **Fundamentally, matter must be described by a continuous theory, not a discrete one.** The development of that continuous theory will be the subject of Part II of this work.

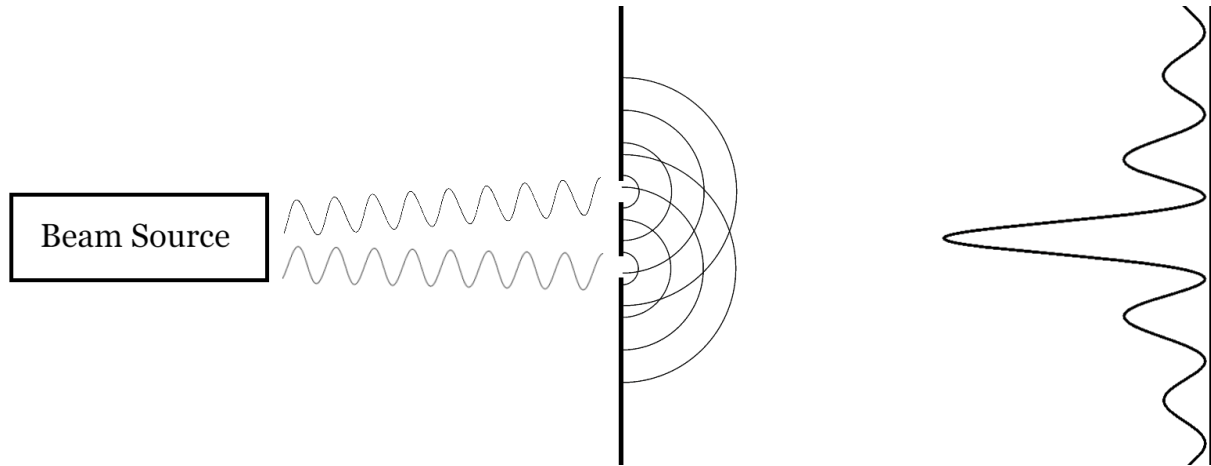


Figure 4.2: The wave theory prediction for the intensity of incident waves through a double-slit apparatus. The plot given on the right hand screen is a graph of the predicted intensity versus position on the screen.

Exercises

Problem 4.73: ★ Dimensional Analysis and Restoring factors of ϵ_0 and c . Occasionally, one needs to compare equations with someone who prefers to use historical unit systems in which c and ϵ_0 are not set to 1 by definition. Suppose one has a quantity of interest F whose units are known in Lorentz Natural Units (units in which $\epsilon_0 = c = 1$) to be $[F]_{\text{LNU}} = M^\alpha T^\beta$ where M indicates units of mass and T indicates units of time and known in your friend's unit system (for example SI units) to be $[F]_{\text{Friend}} = M^\gamma T^\lambda L^\mu Q^\nu$ where L indicates units of length and Q indicates units of charge. Show that:

$$\gamma + \frac{\nu}{2} = \alpha, \quad \mu + \lambda + \frac{\nu}{2} = \beta$$

and that F in your two unit systems are related by:

$$F_{\text{Friend}} = c^{\nu+\beta-\lambda} \epsilon_0^{\frac{\nu}{2}} F_{\text{LNU}}$$

with c and ϵ_0 being their respective values in your friend's unit system. Explain then that applying this to every quantity of interest in an equation allows one to restore powers of c and ϵ_0 in equations whenever one would like to and thus nothing is lost by choosing units which eliminate them.

Problem 4.74: ★ Collapse of the Classical Atom. Consider two charges interacting through electromagnetism. We will assume that the charges are moving very slowly compared to c so that we can neglect relativistic effects in their equations of motion on short time scales. Let one of the charges have charge $-q$ with $q > 0$ and mass m (think of it as an electron) and let the other charge be so heavy it basically doesn't move during the interaction with charge $Q > 0$ (think of it as a proton).

- (a) Show that due to the absence of nonrelativistic effects the resulting equation of motion for the electron's position $\vec{x}(t)$ is simply that of the Kepler problem:

$$m\ddot{\vec{x}} = -\frac{qQ}{4\pi\epsilon_0|\vec{x}|^3}\vec{x}.$$

Assume for simplicity that the orbit of the electron is circular with radius r . Show that the angular velocity and energy of the electron are given by:

$$\omega = \sqrt{\frac{qQ}{4\pi\epsilon_0 m r^3}}, \quad E = -\frac{qQ}{8\pi\epsilon_0 r}.$$

- (b) We know due to the Larmor formula that due to the electron accelerating, it will radiate electromagnetic

waves which carry energy. Show that in the nonrelativistic limit the Larmor formula becomes:

$$\frac{dE}{dt} = -\frac{q^2}{6\pi\epsilon_0 c^3} |\ddot{\vec{x}}|^2 + \mathcal{O}\left(\frac{1}{c^5}\right).$$

Thus, this gives the lowest order estimation for how energy is radiated away from the atom by electromagnetic fields.

- (c) Show using the relationship between the radius of the orbit and the energy that at lowest order in powers of $\frac{1}{c}$, the radius of the orbit will change due to radiation according to:

$$\frac{dr}{dt} \approx -\frac{q^3 Q}{12\pi^2 m^2 \epsilon_0^2 c^3 r^2}.$$

- (d) Solve the differential equation from the previous part. Let $R = r(0)$ and show that:

$$r(t) \approx \left(R^3 - \frac{q^3 Q}{4\pi^2 m^2 \epsilon_0^2 c^3} t \right)^{\frac{1}{3}}.$$

- (e) After a critical time T the above solution predicts that the radius will drop to 0 (the electron will inspiral into the proton and the atom will collapse). Show that that time is given by:

$$T \approx \frac{4\pi^2 m^2 \epsilon_0^2 c^3 R^3}{q^3 Q}.$$

Using our previously identified values of the electron mass, electron charge, proton charge (equal in magnitude to the electron charge but opposite in sign), ϵ_0 , c , and an estimate of $R = 10^{-10}\text{m}$, show that the collapse time T is on the order of 10^{-10}s . Thus, under this classical model, atoms should not be able to last any perceptible amount of time. Oops! This is a major issue with classical physics. Modeling the atomic constituents as point particles leads to fundamentally incorrect physical predictions about atomic behavior. (Improving this analysis by a more serious relativistic treatment does not resolve the issue of atomic stability.)

Problem 4.75: Born-Infeld Action. Consider the following non-linear modification of the Maxwell Lagrangian, called the Born-Infeld Lagrangian:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-b^2 \sqrt{1 - \frac{|\vec{E}|^2 - |\vec{B}|^2}{b^2}} - \frac{(\vec{E} \cdot \vec{B})^2}{b^4} + b^2 + \vec{J} \cdot \vec{A} - \rho\phi \right) d\mathbb{S}$$

This theory has a number of quite nice features which we will not explore fully.

- (a) Show that the modified Maxwell's equations for this theory are:

$$\nabla \cdot \vec{D} = \rho, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$$

where:

$$\vec{D} = \frac{\vec{E} + \frac{\vec{E} \cdot \vec{B}}{b^2} \vec{B}}{\sqrt{1 - \frac{|\vec{E}|^2 - |\vec{B}|^2}{b^2} - \frac{(\vec{E} \cdot \vec{B})^2}{b^4}}}, \quad \vec{H} = \frac{\vec{B} - \frac{\vec{E} \cdot \vec{B}}{b^2} \vec{E}}{\sqrt{1 - \frac{|\vec{E}|^2 - |\vec{B}|^2}{b^2} - \frac{(\vec{E} \cdot \vec{B})^2}{b^4}}}.$$

- (b) Show that for a stationary point charge q at the origin, this theory predicts:

$$\vec{B} = 0, \quad \vec{E} = \frac{q}{\sqrt{16\pi^2 |\vec{x}|^2 + \frac{q^2}{b^2}}} \frac{\vec{x}}{|\vec{x}|}$$

and that this solution has finite energy:

$$E = \sqrt{\frac{|q|^3 b}{4\pi}} C, \quad C \stackrel{\text{def}}{=} \int_0^\infty \left(\sqrt{1 + x^4} - x^2 \right) dx = \frac{8\Gamma\left(\frac{5}{4}\right)^2}{3\sqrt{\pi}}.$$

For additional challenge, prove the result of the integral defining C . It is suspected, though difficult to show due to the nonlinearity of these equations, that this theory produces finite radiation reaction corrections unlike Maxwell's equations. If this is true, it might seem like this theory or some other non-linear version of electromagnetism could make a well-defined theory of point particles. However, such a theory would still face all of the experimental issues we have mentioned with interference patterns and particle production.

4.9 Covariant Notation, Spacetime, and Tensors

It is time to make an enormous upgrade of our notation technology. This section will technically produce 0 new physics but it will give us the tools to proceed doing new physics more efficiently and to think about physics more clearly. While nothing will be fundamentally new, this new notation is such an advancement over our previous notation that previously difficult questions often become easy and calculations are generally much simpler. Because in the Lorentz theory time and space mix under a Lorentz boost and the theory has symmetry under such transformations, we really ought to think about time and space as being part of the same mathematical object. This thinking led us previously to define the spacetime event $X = (t, \vec{x})$. Further, it motivates actually including t in our index notation as $t = x^0$. This way, we write f^μ with a Greek letter index to refer to the components of a 4-vector (meaning a vector in the 4 dimensional spacetime) and f^a with a Latin letter index to refer to the components of a 3-vector (meaning a vector on space only). Because the Lorentz boosts and rotations matrices are given by 4x4 matrices acting on $(dt, d\vec{x})$, we can represent them both together as $L^\mu{}_\nu$ in components and call this a Lorentz transformation which now acts as:

$$dx'^\mu = L^\mu{}_\nu dx^\nu. \quad (4.9.1)$$

We know that Lorentz boost and rotations (and so Lorentz transformations) leave the proper time invariant. The proper time can be manipulated into being a quadratic form:

$$d\tau^2 = dt^2 - |d\vec{x}|^2 = - \begin{pmatrix} dt & dx & dy & dz \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix}. \quad (4.9.2)$$

This contains our 4-vector components dx^μ and a matrix which we call the **Minkowski metric** that has components $\eta_{\mu\nu}$:

$$\eta_{\mu\nu} \stackrel{\text{def}}{=} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{\mu\nu}. \quad (4.9.3)$$

Then, the proper time is written:

$$d\tau^2 = -\eta_{\mu\nu} dx^\mu dx^\nu. \quad (4.9.4)$$

Throughout this book so far I have not explained why sometimes I write indices as superscripts and sometimes I write them as subscripts. Until this point it did not matter. Now it does matter. By definition, the 4-vector components dx^μ are written with a superscript index. Under a Lorentz transformation they are transformed by equation (4.9.1). Any object that has components which transform by the same rule as dx^μ also is written with its index as a superscript and that object is also called a 4-vector. Note that the geometric object dX is not the same thing as its components dx^μ . As always, the vector dX is written in terms of not only its components but also its basis vectors. We call the vector space of 4-vectors Minkowski space and write it as $\mathbb{M}$. We call the standard basis vectors for Minkowski space $\vec{t}_\mu$. Then, we have:

$$dX = dx^\mu \vec{t}_\mu. \quad (4.9.5)$$

Here $\vec{t}_0 = (1, 0, 0, 0)$, $\vec{t}_1 = (0, 1, 0, 0)$, $\vec{t}_2 = (0, 0, 1, 0)$, and $\vec{t}_3 = (0, 0, 0, 1)$. The sum of products that the Einstein summation notation we have been using does is called a contraction. Now consider the derivative operators ∂_μ which by definition I have written with a lowered index. Then, by the chain rule under a Lorentz transformation:

$$\partial'_\mu = \frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial}{\partial x^\nu} = (L^{-1})^\nu{}_\mu \partial_\nu. \quad (4.9.6)$$

Hence the derivative operators transform inversely to the differentials. Anything which transforms inversely to the differentials (and so like the derivatives) is written with a lowered index. Now suppose that a^μ is something which transforms like the differentials and b_μ is something which transforms like the derivative operators. It immediately follows that $a^\mu b_\mu$ is Lorentz invariant:

$$a'^\mu b'_\mu = L^\mu{}_\nu a^\nu (L^{-1})^\rho{}_\mu b_\rho = (L^{-1})^\rho{}_\mu L^\mu{}_\nu a^\nu b_\rho = (L^{-1}L)^\rho{}_\nu a^\nu b_\rho = \delta^\rho{}_\nu a^\nu b_\rho = a^\nu b_\nu. \quad (4.9.7)$$

As you can see, this index notation is extremely efficient at managing matrix multiplication because for

matrices M and N , the components of the matrix MN are given by:

$$(MN)^\mu{}_\nu = M^\mu{}_\alpha N^\alpha{}_\nu. \quad (4.9.8)$$

As well, the identity matrix has 1 along the diagonal $\mu = \nu$ and 0 everywhere else which is precisely the definition of the Kronecker delta:

$$\mathbb{1}^\mu{}_\nu = \delta^\mu{}_\nu. \quad (4.9.9)$$

The components of a matrix transpose are also easily given in this notation. The transpose of a matrix just swaps the rows and columns and therefore just swaps the two indices of its components:

$$(M^T)^{\mu\nu} = M^{\nu\mu}. \quad (4.9.10)$$

There is not currently a universal notation for the inverse of a matrix. I personally put a negative sign next to an index to indicate the inverse which for our purposes (because all indices will be positive) is not ambiguous. If there is a risk of being ambiguous, it is best to be explicit.

$$(L^{-1})^\mu{}_\nu = L^{-\mu}{}_\nu. \quad (4.9.11)$$

Because the proper time is invariant under Lorentz transformations, it follows that:

$$d\tau'^2 = -\eta_{\mu\nu} dx'^\mu dx'^\nu = -\eta_{\mu\nu} L^\mu{}_\alpha L^\nu{}_\beta dx^\alpha dx^\beta \stackrel{!}{=} d\tau^2 = -\eta_{\alpha\beta} dx^\alpha dx^\beta \quad (4.9.12)$$

$$\implies \boxed{\eta_{\alpha\beta} = \eta_{\mu\nu} L^\mu{}_\alpha L^\nu{}_\beta}. \quad (4.9.13)$$

By multiplying by two powers of the inverse matrix of the Lorentz transformation, we get that each index of the Minkowski metric transforms like the derivatives:

$$L^{-\alpha}{}_\rho L^{-\beta}{}_\sigma \eta_{\alpha\beta} = \eta_{\mu\nu} L^\mu{}_\alpha L^\nu{}_\beta L^{-\alpha}{}_\rho L^{-\beta}{}_\sigma \quad (4.9.14)$$

$$\implies \eta_{\rho\sigma} = L^{-\alpha}{}_\rho L^{-\beta}{}_\sigma \eta_{\alpha\beta}. \quad (4.9.15)$$

From equation (4.9.13), if we only multiply by one power of the inverse matrix of the Lorentz transformation we get an interesting relationship between the Lorentz transformation matrix and its inverse:

$$L^{-\alpha}{}_\rho \eta_{\alpha\beta} = \eta_{\mu\nu} L^\mu{}_\alpha L^\nu{}_\beta L^{-\alpha}{}_\rho \quad (4.9.16)$$

$$\implies L^{-\alpha}{}_\rho \eta_{\alpha\beta} = \eta_{\rho\nu} L^\nu{}_\beta. \quad (4.9.17)$$

Using this identity, now consider the transformation of $\eta_{\alpha\beta} dx^\beta$:

$$\eta_{\alpha\beta} dx'^\beta = \eta_{\alpha\beta} L^\beta{}_\gamma dx^\gamma = L^{-\lambda}{}_\alpha \eta_{\lambda\gamma} dx^\gamma. \quad (4.9.18)$$

Hence, the object $\eta_{\alpha\beta} dx^\beta$ transforms like the coordinate derivatives. This motivates the definition of lowering an index. dx^μ with an upper index is already defined. We define dx_μ as this contraction of the metric and dx^μ :

$$dx_\mu \stackrel{\text{def}}{=} \eta_{\mu\nu} dx^\nu. \quad (4.9.19)$$

As we see in equation (4.9.18), dx_μ properly transforms like the derivatives ∂_μ . Now we can see why whether indices are up or down is important. Upstairs indices and downstairs indices have different transformation properties under a change of coordinates! Further, by direct calculation:

$$dx_\mu = \eta_{\mu\nu} dx^\nu = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} dt \\ dx \\ dy \\ dz \end{pmatrix}_\mu = \begin{pmatrix} -dt \\ dx \\ dy \\ dz \end{pmatrix}_\mu. \quad (4.9.20)$$

Hence $dx_\mu \neq dx^\mu$. The two only differ in the time component which is why when we were working with 3-vectors it did not matter whether we put the indices up or down because the 3-vector part is unchanged by lowering the index.

We define $\eta^{\mu\nu}$ as the matrix inverse of the Minkowski metric. It is a special fact of the matrix in equation (4.9.3) that the Minkowski metric is actually its own inverse:

$$\eta^{\mu\nu} \stackrel{\text{def}}{=} (\eta^{-1})^{\mu\nu} = \eta_{\mu\nu}. \quad (4.9.21)$$

While it is the case that the Minkowski metric with upper indices is numerically equal to the Minkowski metric with lower indices, it is not typically a good idea to replace the lowered version with the upper version or vice versa in a calculation. This is because expressions with opposing indices contracted into each other are automatically Lorentz invariant, as shown by equation (4.9.7), and so by misplacing indices you lose clarity

of thought about the Lorentz transformation properties of what you are looking at. Using the inverse metric, you can raise indices:

$$dx^\mu = \eta^{\mu\nu} dx_\nu. \quad (4.9.22)$$

It immediately follows that if f_ν transforms like the derivatives then f^ν transforms like the differentials. Hence the Minkowski metric gives us a way to raise and lower the indices of any quantity at will while keeping the transformation properties consistent with the placement of the indices.

Using index raising and lowering gives a nice relation between a Lorentz transformation and its inverse from equation (4.9.17):

$$L^{-\alpha}{}_{\rho} \eta_{\alpha\beta} = \eta_{\rho\nu} L^{\nu}{}_{\beta} \implies L^{-1}_{\beta\rho} = L_{\rho\beta}. \quad (4.9.23)$$

If we define the basis vectors $\vec{t}_\mu$ to transform under the Lorentz transformation as:

$$\vec{t}'_\mu \stackrel{\text{def}}{=} L^{-\nu}{}_{\mu} \vec{t}'_\nu \quad (4.9.24)$$

then any 4-vector a actually remains unchanged under Lorentz transformation:

$$a' = a'^\mu \vec{t}'_\mu = (L^\mu{}_\nu a^\nu)(L^{-\rho}{}_{\mu} \vec{t}'_\rho) = \delta^\rho_\nu a^\nu \vec{t}'_\rho = a^\nu \vec{t}'_\nu = a. \quad (4.9.25)$$

In this way, we can simply view Lorentz transformations as a change of basis transformation for $\mathbb{M}$. When one changes basis the basis vectors change and the components of any vector change accordingly so that whatever vector is being represented in components is the same geometric object in either basis, exactly as seen here. This transformation property happens to be the usual one for a quantity written with a lowered index. We can also raise the index of our basis vectors:

$$\vec{t}^\mu = \eta^{\mu\nu} \vec{t}_\nu. \quad (4.9.26)$$

One should be careful about what this means. $\vec{t}_\mu$ is itself a vector, not a component. The list of these for different μ produces a list of 4 vectors. The raised vectors $\vec{t}^\mu$ with a raised index form another basis of vectors related to our original basis by the change of basis matrix with components $\eta^{\mu\nu}$. The raised index vectors give us a way to put the derivative operators into a 4-vector:

$$\implies \nabla = \vec{t}^\mu \partial_\mu. \quad (4.9.27)$$

One should be careful to note that in this relativistic notation, ∇ as given by equation (4.9.27) is not the same ∇ used before in the notation in which space and time were written separately. This new ∇ is a 4-vector operator and includes the spatial derivatives of the previous ∇ (which was a 3-vector operator) as well as a time derivative.

Let us take our expression for the vector dX in (4.9.5) and formally take the “dot product” of it with itself:

$$dX \cdot dX = dx^\mu \vec{t}_\mu \cdot dx^\nu \vec{t}_\nu = dx^\mu dx^\nu \vec{t}_\mu \cdot \vec{t}_\nu. \quad (4.9.28)$$

If we define the dot product on our basis vectors so that they give the Minkowski metric, then this gives us an expression for our proper time:

$$\boxed{\vec{t}_\mu \cdot \vec{t}_\nu \stackrel{\text{def}}{=} \eta_{\mu\nu}} \quad (4.9.29)$$

$$\implies dX \cdot dX = dx^\mu dx^\nu \eta_{\mu\nu} = -d\tau^2. \quad (4.9.30)$$

Being careful, this is not actually an inner product in the math sense as an inner product must be positive definite ($u \cdot u \geq 0$ and only 0 for $u = 0$) by definition. This construction is bilinear and symmetric (the other two properties of an inner product) but is not positive definite. Instead, it does satisfy a weaker condition in that it is non-degenerate. That is, there is no vector $u \neq 0$ so that $v \cdot u = 0$ for all vectors v . Because this $\cdot$ operation is bilinear, symmetric, and non-degenerate it is called a pseudo-inner product. For pseudo-inner products, many but not all of the results of regular inner products hold. This pseudo-inner product is a very useful construction for us as it gives a map from two 4-vectors into a Lorentz invariant scalar quantity following equation (4.9.7).

4.9.1 Tensors, a New Friend You Already Knew

Just about every quantity we have been interested in so far and very many of the quantities we will be interested in going forward are examples of **tensors**. Before we define a tensor precisely we must first define the notion of a tensor product. A tensor product is a specific operation between two vector spaces which

produces a new vector space. If we have a vector space $\mathbb{U}$ with basis $\vec{l}_\mu$ then a general vector u in that vector space has some components u^μ so that:

$$u = u^\mu \vec{l}_\mu. \quad (4.9.31)$$

If we then have another vector space $\mathbb{V}$ with basis $\vec{j}_\nu$ a general vector v in that vector space has some components v^ν so that:

$$v = v^\nu \vec{j}_\nu. \quad (4.9.32)$$

The tensor product $\mathbb{W} = \mathbb{U} \otimes \mathbb{V}$ is a vector space where we take each basis vector $\vec{l}_\mu$ of $\mathbb{U}$ and for each basis vector $\vec{j}_\nu$ in $\mathbb{V}$ we define a new vector written $\vec{l}_\mu \otimes \vec{j}_\nu$ and we take this set of pairs of vectors as the basis of our new vector space in $\mathbb{W}$. So, a general vector w in the tensor product space has components $w^{\mu\nu}$ and can be written as:

$$w = w^{\mu\nu} \vec{l}_\mu \otimes \vec{j}_\nu. \quad (4.9.33)$$

The tensor product $\otimes$ between elements of two vector spaces is defined to be linear and associative (here a and b are scalars):

$$u \otimes (av_1 + bv_2) = au \otimes v_1 + bu \otimes v_2 \quad (4.9.34)$$

$$(au_1 + bu_2) \otimes v = au_1 \otimes v + bu_2 \otimes v \quad (4.9.35)$$

$$(u \otimes v) \otimes w = u \otimes (v \otimes w). \quad (4.9.36)$$

These properties are necessary to make the tensor product space independent of the bases used to construct it and of the order in which tensor products are taken (order in the sense of equation (4.9.36); the tensor product is not commutative, that is $u \otimes v \neq v \otimes u$). This definition may seem very abstract right now but it will become concrete as we see examples of this structure appear naturally very shortly.

Now that we have defined the tensor product, let us define a tensor. A rank N tensor T over $\mathbb{M}$ is an element of the vector space $\mathbb{M} \otimes \mathbb{M} \otimes \dots \otimes \mathbb{M}$ where N factors of $\mathbb{M}$ have been taken. By the definition of the tensor product then, T can be written with some components $T^{\mu_1 \dots \mu_N}$ as:

$$T = T^{\mu_1 \dots \mu_N} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_N}. \quad (4.9.37)$$

Under a Lorentz transformation, the basis vectors $\vec{l}_\mu$ and the components of T will change but the geometric object that is the tensor is defined to stay the same object, analogously to vectors. Then: we have:

$$T'^{\mu_1 \dots \mu_N} \vec{l}'_{\mu_1} \otimes \dots \otimes \vec{l}'_{\mu_N} = T^{\mu_1 \dots \mu_N} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_N} \quad (4.9.38)$$

$$\implies T'^{\mu_1 \dots \mu_N} (L^{-\nu_1}_{\mu_1} \vec{l}_{\nu_1}) \otimes \dots \otimes (L^{-\nu_N}_{\mu_N} \vec{l}_{\nu_N}) = T^{\mu_1 \dots \mu_N} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_N} \quad (4.9.39)$$

$$\implies L^{-\mu_1}_{\nu_1} \dots L^{-\mu_N}_{\nu_N} T'^{\nu_1 \dots \nu_N} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_N} = T^{\mu_1 \dots \mu_N} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_N} \quad (4.9.40)$$

$$\implies L^{-\mu_1}_{\nu_1} \dots L^{-\mu_N}_{\nu_N} T'^{\nu_1 \dots \nu_N} = T^{\mu_1 \dots \mu_N} \quad (4.9.41)$$

$$\implies \boxed{T'^{\mu_1 \dots \mu_N} = L^{\mu_1}_{\nu_1} \dots L^{\mu_N}_{\nu_N} T^{\nu_1 \dots \nu_N}}. \quad (4.9.42)$$

Thus, each upper index of the components of a tensor transforms under a Lorentz transformation exactly the way the coordinate displacements do. Using the metric, we can raise or lower any of the components of a tensor and automatically then each upper index will transform as the displacements and each lower index will transform as the derivatives. In this way, we can equivalently write a tensor as:

$$T = T^{\mu_1 \dots \mu_n}_{\nu_1 \dots \nu_m} \vec{l}_{\mu_1} \otimes \dots \otimes \vec{l}_{\mu_n} \otimes \vec{l}^{\nu_1} \otimes \dots \otimes \vec{l}^{\nu_m}. \quad (4.9.43)$$

where here I have kept the first n indices raised and lowered the remaining $m = N - n$. We can keep raised or lower any combination of the indices of the tensor and the transformation rules for its components follow directly from the final positions of its indices (upper like the displacements, lower like the derivatives). So, we can see that the Minkowski metric is a rank 2 tensor, 4-vector is just another word for a rank 1 tensor, and a rank 0 tensor (an object with no components which does not transform at all when the coordinates transform) is just a scalar.

Essentially all of the important quantities we have discussed previously are actually tensors of some kind. For example, consider the energy and momentum which we found transform under a Lorentz boost as:

$$E' = \gamma (E + \vec{v} \cdot \vec{p}), \quad \vec{p}' = (\mathbb{1} + (\gamma - 1) \vec{l}_v \vec{l}_v) \cdot \vec{p} + \gamma E \vec{v}. \quad (4.9.44)$$

This is the exact same transformation property as the coordinate differentials and so $p^\mu = (E, \vec{p})^\mu$ makes the

momentum 4-vector (rank 1 tensor). As well, the charge density and current density make a 4-vector:

$$\rho' = \gamma\rho + \gamma\vec{v} \cdot \vec{J}, \quad \vec{J}' = (\mathbb{1} + (\gamma - 1)\vec{v}\vec{v}) \cdot \vec{J} + \gamma\rho\vec{v} \quad (4.9.45)$$

$$\implies \boxed{J^\mu = (\rho, \vec{J})^\mu}. \quad (4.9.46)$$

Because the charge and current densities are fields, they are then a rank 1 tensor field (or 4-vector field). The continuity equation can be written very nicely in this notation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = \partial_0 J^0 + \partial_a J^a = \boxed{\partial_\mu J^\mu = 0}. \quad (4.9.47)$$

The scalar and vector potential together make a 4-vector field:

$$\phi' = \gamma(\phi + \vec{v} \cdot \vec{A}), \quad \vec{A}' = (\mathbb{1} + (\gamma - 1)\vec{v}\vec{v}) \cdot \vec{A} + \vec{v}\phi \quad (4.9.48)$$

$$\implies \boxed{A^\mu = (\phi, \vec{A})^\mu}. \quad (4.9.49)$$

The gauge transformation is expressed extremely nicely in this notation:

$$\phi' = \phi - \frac{\partial f}{\partial t}, \quad \vec{A}' = \vec{A} + \nabla f \implies A'^0 = A^0 - \partial_0 f, \quad A'^a = A^a + \partial_a f \quad (4.9.50)$$

$$\implies \boxed{A'_\mu = A_\mu + \partial_\mu f}. \quad (4.9.51)$$

Notice that the electric and magnetic fields make nothing like a 4-vector:

$$\vec{E}' = \gamma\vec{E} - (\gamma - 1)\vec{v}\vec{v} \cdot \vec{E} - \gamma\vec{v} \times \vec{B}, \quad \vec{B}' = \gamma\vec{B} - (\gamma - 1)\vec{v}\vec{v} \cdot \vec{B} + \gamma\vec{v} \times \vec{E}. \quad (4.9.52)$$

We can make sense of these by looking at their components and expressions in terms of the potentials. Start with the magnetic field:

$$\vec{B} = \vec{v}^a B_a = \nabla \times \vec{A} \implies B_a = \epsilon_a^{bc} \partial_b A_c. \quad (4.9.53)$$

So, the magnetic field is made out of an anti-symmetric combination of derivatives of A . Now do the same with the electric field:

$$\vec{E} = \vec{v}^a E_a = -\nabla\phi - \frac{\partial \vec{A}}{\partial t} \implies E_a = \partial_a A_0 - \partial_0 A_a. \quad (4.9.54)$$

Hence the electric field can also be made out of an anti-symmetric combination of derivatives of A . This motivates us to define $\mathcal{F}$ called the field strength which has components:

$$\boxed{\mathcal{F}_{\mu\nu} \stackrel{\text{def}}{=} \partial_\mu A_\nu - \partial_\nu A_\mu} \quad (4.9.55)$$

$$\implies \mathcal{F}_{00} = 0, \quad \mathcal{F}_{0a} = -E_a, \quad \mathcal{F}_{a0} = E_a, \quad \mathcal{F}_{ab} = \epsilon_{ab}^c B_c. \quad (4.9.56)$$

So, the electric and magnetic fields can both be put together into this single object. Written as a matrix, (4.9.55) reads:

$$\boxed{\mathcal{F}_{\mu\nu} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_x \\ E_z & B_y & -B_x & 0 \end{pmatrix}_{\mu\nu}}. \quad (4.9.57)$$

Further, by direct calculation, the field strength is actually a tensor:

$$\mathcal{F}'_{\mu\nu} = \partial'_\mu A'_\nu - \partial'_\nu A'_\mu = L^{-\alpha}_\mu \partial_\alpha (L^{-\beta}_\nu A_\beta) - L^{-\beta}_\nu \partial_\beta (L^{-\alpha}_\mu A_\alpha) = L^{-\alpha}_\mu L^{-\beta}_\nu (\partial_\alpha A_\beta - \partial_\beta A_\alpha) \quad (4.9.58)$$

$$= L^{-\alpha}_\mu L^{-\beta}_\nu \mathcal{F}_{\alpha\beta}. \quad (4.9.59)$$

The electric and magnetic fields actually make the anti-symmetric rank 2 field strength tensor in the relativistic notation. One can check that putting equation (4.9.59) into components reproduces the transformation rules given for the electric and magnetic fields in equation (4.9.52). We can also see that $\mathcal{F}_{\mu\nu}$ is like the “4-curl” (in the sense of anti-symmetric combination of derivatives) of the 4-vector potential and that the gauge transformation corresponds to adding a 4-gradient to the potential. This makes the field strength automatically gauge invariant because the curl of a gradient is always 0.

4.9.2 Covariant Equations of Motion

The Euler-Lagrange equations of motion can also be rewritten in an equivalent but compact way in the relativistic notation. To see some use of our upgraded notation, the Lagrangian for a massive particle in the Lorentz theory is:

$$\mathcal{L} = -m\sqrt{1 - |\dot{\vec{x}}|^2} + q\vec{x} \cdot \vec{A} - q\phi = -m\frac{\sqrt{dt^2 - |d\vec{x}|^2}}{dt} + q\frac{d\vec{x}}{dt} \cdot \vec{A} - q(A_0)\frac{dt}{dt} \quad (4.9.60)$$

$$= -m\frac{d\tau}{dt} + q\frac{dx^a}{dt}A_a + qA_0\frac{dx^0}{dt} = -m\frac{d\tau}{dt} + q\frac{dx^\mu}{dt}A_\mu. \quad (4.9.61)$$

This makes the action for the massive particle:

$$S = \int_{t_0}^{t_f} \mathcal{L} dt = \int_{t=t_0}^{t=t_f} (-md\tau + qA_\mu dx^\mu). \quad (4.9.62)$$

The form of this action sheds light on the true usefulness of the covariant index notation. We can see plainly by looking at each term in the expression for the action that it is Lorentz invariant because the proper time is Lorentz invariant and the $A_\mu dx^\mu$ term is the contraction of two 4-vectors and thus Lorentz invariant. **The covariant index notation makes it possible to know exactly how an equation transforms by glancing at it.** We say an expression is Lorentz *covariant* if the form of that expression is unchanged by any Lorentz transformation. This is distinct from saying invariant; we say an expression is Lorentz *invariant* if its value is unchanged by any Lorentz transformation.

To this point, when we considered a particle's position, we always parameterized its position $\vec{x}$ as a function of time t . Because position and time mix under a Lorentz boost, this kind of formulation is pretty inconvenient for relativity. So, let us consider some parameter λ which is invertibly related to t : $t = t(\lambda)$ or $\lambda = \lambda(t)$ but not necessarily t itself. Then, we can write $X(\lambda) = (t(\lambda), \vec{x}(\lambda))$ (written this way, the curve $X(\lambda)$ in spacetime is called the worldline of the particle). Then, because the particle's path is now written as a function of λ , we can rewrite our action as an integral over it as:

$$S = \int_{\lambda_0}^{\lambda_f} \left(-m\frac{d\tau}{d\lambda} + qA_\mu \frac{dx^\mu}{d\lambda} \right) d\lambda = \int_{\lambda_0}^{\lambda_f} \left(-m\sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} + qA_\mu \frac{dx^\mu}{d\lambda} \right) d\lambda. \quad (4.9.63)$$

Viewing this λ parameter as our effective “time” parameter in the sense of the variable which parameterizes the path, we can then define the λ -Lagrangian as:

$$\mathcal{L}_\lambda = \frac{dS}{d\lambda} = -m\sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} + qA_\mu \frac{dx^\mu}{d\lambda}. \quad (4.9.64)$$

The λ -Lagrangian is a function of x^μ and $\frac{dx^\mu}{d\lambda}$ (which we shall call $\dot{x}^\mu$). The action is invariant under how we define λ in the sense that if we define a new parameter $\lambda' = \lambda'(\lambda)$ and rewrite all λ s in terms of λ' using the chain rule, we arrive at the same form of the action:

$$S = \int_{\lambda'_0}^{\lambda'_f} \left(-m\sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{d\lambda'} \frac{dx^\nu}{d\lambda'}} + qA_\mu \frac{dx^\mu}{d\lambda'} \right) d\lambda'. \quad (4.9.65)$$

In doing so we can see that the λ -Lagrangian transforms as:

$$\mathcal{L}_\lambda(x, \dot{x}') = \mathcal{L}_\lambda(x, \dot{x}) \frac{d\lambda}{d\lambda'} \quad (4.9.66)$$

where:

$$\dot{x}'^\mu = \frac{dx^\mu}{d\lambda'} = \frac{d\lambda}{d\lambda'} \frac{dx^\mu}{d\lambda} = \frac{d\lambda}{d\lambda'} \dot{x}^\mu. \quad (4.9.67)$$

Letting $\alpha = \frac{d\lambda}{d\lambda'}$ we have:

$$\mathcal{L}_\lambda(x, \alpha\dot{x}) = \alpha\mathcal{L}_\lambda(x, \dot{x}). \quad (4.9.68)$$

Because this is true for all reparameterizations and thus all α , differentiate with respect to α and evaluate at $\alpha = 1$:

$$\implies \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \dot{x}^\mu = \mathcal{L}_\lambda(x, \dot{x}). \quad (4.9.69)$$

The λ -Lagrangian looks like it is a function of 4 canonical coordinates: x^μ and the velocities of each of the coordinates with respect to λ . Thus, when computing the Euler-Lagrange equations, we will get 4

equations. This is quite surprising because in our original notation we only had the 3 canonical coordinates for $\vec{x}(t)$ and their velocities and thus only got 3 equations of motion. It is not obvious that varying all 4 canonical coordinates with result in equivalent equations of motion. Let us compute the variation of our action with 4 coordinates and see how it compares to the variation with 3 coordinates:

$$\frac{\delta S}{\delta x^\mu(\lambda)} = \frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} - \frac{d}{d\lambda} \left(\frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \right) \stackrel{?}{=} 0. \quad (4.9.70)$$

In the specific case that we now choose our λ parameter to simply be $t = x^0$, we then have that the λ -Lagrangian is the ordinary Lagrangian:

$$\mathcal{L}_t = \left. \frac{dS}{d\lambda} \right|_{\lambda=t} = \frac{dS}{dt} = \mathcal{L} \quad (4.9.71)$$

and consequently the variations for $\mu \neq 0$ simply become our old Euler-Lagrange equations for the 3 coordinates:

$$\left. \frac{dx^\mu}{d\lambda} \right|_{\lambda=t} = \frac{dx^\mu}{dt} \implies \frac{\partial \mathcal{L}_\lambda}{\partial x^a} - \frac{d}{d\lambda} \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^a} = \frac{\partial \mathcal{L}}{\partial x^a} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}^a} = 0. \quad (4.9.72)$$

Thus, certainly for this choice of parameter and $\mu \neq 0$ equation (4.9.70) holds. For $\lambda = t$, equation (4.9.69) also becomes quite interesting:

$$\frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \dot{x}^\mu = \mathcal{L}_\lambda \quad (4.9.73)$$

$$\implies \frac{\partial \mathcal{L}}{\partial \dot{x}^0} = \mathcal{L} - \frac{\partial \mathcal{L}}{\partial \dot{x}^a} \dot{x}^a = -\mathcal{H}. \quad (4.9.74)$$

Then, the $\mu = 0$ variation becomes:

$$\frac{\partial \mathcal{L}_\lambda}{\partial x^0} - \frac{d}{d\lambda} \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^0} = \frac{\partial \mathcal{L}}{\partial t} - \frac{d}{dt} (-\mathcal{H}) = \frac{d\mathcal{H}}{dt} + \frac{\partial \mathcal{L}}{\partial t} = 0 \quad (4.9.75)$$

by equation (2.2.11). Thus, for $\lambda = t$, all four equations of motion in equation (4.9.70) are in fact true (and the only restriction we needed on $\mathcal{L}_\lambda$ to prove it was equation (4.9.69)) for all 4 coordinates whenever the corresponding equations of motion are true for the original 3 spatial coordinates. Now let us reparameterize equation (4.9.70):

$$\frac{\delta S}{\delta x^\mu(\lambda')} = \frac{\partial \mathcal{L}_\lambda(x, \dot{x}')}{\partial x^\mu} - \frac{d}{d\lambda'} \frac{\partial \mathcal{L}_\lambda(x, \dot{x}')}{\partial \dot{x}^\mu} \quad (4.9.76)$$

$$= \frac{\partial}{\partial x^\mu} \left(\frac{d\lambda}{d\lambda'} \mathcal{L}_\lambda(x, \dot{x}) \right) - \frac{d\lambda}{d\lambda'} \frac{d}{d\lambda} \left(\frac{d\lambda}{d\lambda'} \frac{\partial \mathcal{L}_\lambda(x, \dot{x})}{\partial \dot{x}^\nu} \frac{\partial \dot{x}^\nu}{\partial \dot{x}^\mu} \right) \quad (4.9.77)$$

$$= \frac{d\lambda}{d\lambda'} \frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} - \frac{d\lambda}{d\lambda'} \frac{d}{d\lambda} \left(\frac{d\lambda}{d\lambda'} \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\nu} \delta_\mu^\nu \frac{d\lambda'}{d\lambda} \right) \quad (4.9.78)$$

$$= \frac{d\lambda}{d\lambda'} \left(\frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} - \frac{d}{d\lambda} \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \right) = \frac{d\lambda}{d\lambda'} \frac{\delta S}{\delta x^\mu(\lambda)}. \quad (4.9.79)$$

Hence, if the variation of the action vanishes in 1 parameterization, it vanishes in all parameterizations. Because the variation (as we found) vanishes for $\lambda = t$, it follows that we can use equation (4.9.63) as the action for all 4 coordinates x^μ for any parameterization $x^\mu(\lambda)$.

Now let us actually compute the equations of motion:

$$\frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} = q \frac{\partial A_\nu}{\partial x^\mu} \frac{dx^\nu}{d\lambda} \quad (4.9.80)$$

$$\frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} = \frac{m\eta_{\mu\nu}\dot{x}^\nu}{\sqrt{-\eta_{\alpha\beta}\dot{x}^\alpha\dot{x}^\beta}} + qA_\mu = m \frac{\left(\frac{dx_\mu}{d\lambda} \right)}{\left(\frac{d\tau}{d\lambda} \right)} + qA_\mu = m \frac{dx_\mu}{d\tau} + qA_\mu \quad (4.9.81)$$

where here we have used the proper time τ . Then, we have:

$$\frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} - \frac{d}{d\lambda} \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} = q\partial_\mu A_\nu \frac{dx^\nu}{d\lambda} - \frac{d}{d\lambda} \left(m \frac{dx_\mu}{d\tau} + qA_\mu \right) \quad (4.9.82)$$

$$= q\mathcal{F}_{\mu\nu} \frac{dx^\nu}{d\lambda} - m \frac{d\tau}{d\lambda} \frac{d^2 x_\mu}{d\tau^2} = \frac{d\tau}{d\lambda} \left(q\mathcal{F}_{\mu\nu} \frac{dx^\nu}{d\tau} - m \frac{d^2 x_\mu}{d\tau^2} \right) \stackrel{!}{=} 0 \quad (4.9.83)$$

$$\implies m \frac{d^2 x_\mu}{d\tau^2} = q\mathcal{F}_{\mu\nu} \frac{dx^\nu}{d\tau} \quad (4.9.84)$$

Or, after raising an index using the metric $\eta^{\mu\nu}$:

$$\boxed{\frac{d^2 x^\mu}{d\tau^2} = q \mathcal{F}^\mu{}_\nu \frac{dx^\nu}{d\tau}}. \quad (4.9.85)$$

We can see explicitly that our particular choice of λ drops out in the final equation of motion. This equation of motion is identical to the standard Lorentz force equation of motion we had previously, just now written so that the Lorentz transformation properties of the theory are much clearer. If one breaks this equation of motion into components and returns everything to our old notation, it just becomes the equation of motion in equation (4.3.36).

The quantity $\frac{dx^\mu}{d\tau}$ is called the 4-velocity u^μ of the particle; we will see it often and because $d\tau$ is Lorentz invariant, the 4-velocity is automatically a 4-vector. We can see that its components are related to the traditional 3-velocity $v^a = \frac{dx^a}{dt}$ by:

$$u^0 = \frac{dx^0}{d\tau} = \frac{dt}{d\tau} = \frac{1}{\sqrt{1 - |\dot{\vec{x}}|^2}} = \gamma \quad (4.9.86)$$

$$u^a = \frac{dx^a}{d\tau} = \frac{dx^a}{dt} \frac{dt}{d\tau} = \gamma v^a. \quad (4.9.87)$$

Because the λ -Lagrangian has 4 canonical coordinates, it produces 4 conjugate momenta. The spatial components of the conjugate momenta match the result from before we used this notation:

$$\frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^a} = m \frac{dx_a}{d\tau} + q A_a = m \gamma \frac{dx_a}{dt} + q A_a = p_a. \quad (4.9.88)$$

The time component then gives the time component of the momentum 4-vector, which is we found is simply the energy (for a raised index, the negative of the energy for a lowered index):

$$\frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^0} = m \frac{dx_0}{d\tau} + q A_0 = -m\gamma - q\phi = -\mathcal{H}. \quad (4.9.89)$$

Thus, we can write:

$$p_\mu = \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \quad (4.9.90)$$

and understand that this p_μ is genuinely the momentum 4-vector we had identified previously. From equation (4.9.69) it follows that the Legendre transformed “ λ -Hamiltonian” is automatically 0:

$$p_\mu \dot{x}^\mu - \mathcal{L}_\lambda = \frac{\partial \mathcal{L}_\lambda}{\partial \dot{x}^\mu} \dot{x}^\mu - \mathcal{L}_\lambda = 0. \quad (4.9.91)$$

This is not so surprising as we know that the canonical coordinates and momenta in the Hamiltonian all have to be independent variables for the canonical Poisson brackets to hold and among these $4 + 4 = 8$ variables there are only $3 + 3 = 6$ genuinely independent ones. Neither the standard Lagrangian (meaning $\lambda = t$) nor the Hamiltonian are Lorentz invariant and so for relativity it is very common to usually work with the action (which is Lorentz invariant) or something like this λ -Lagrangian which is Lorentz invariant whenever λ is chosen to be Lorentz invariant. Of course, both the standard Lagrangian and Hamiltonian have well defined Lorentz transformation laws and can always be used in relativity just as we have done before however doing so is sometimes less computationally simple than performing the same analysis with the action. The λ parameterization also provides a nice covariant expression for the current 4-vector by combining equations (4.4.6) and (4.4.9) we have immediately that for a single point charge with worldline $Z(\lambda)$:

$$J^\mu(X) = q \int_{-\infty}^{\infty} \frac{dz^\mu}{d\lambda} \delta(X - Z(\lambda)) d\lambda. \quad (4.9.92)$$

The Euler-Lagrange equations for fields are also nicely recast in the index notation. By writing the action as the integral over time of the Lagrangian which is then the integral over space of the Lagrangian density, we have that the action is the integral over spacetime of the Lagrangian density:

$$S = \int_{t_0}^{t_f} \mathcal{L} dt = \int_{t_0}^{t_f} \int_{\mathbb{S}} \mathfrak{L} d\mathbb{S} dt = \int_{\mathbb{T}} \mathfrak{L} d\mathbb{T}. \quad (4.9.93)$$

In Minkowskian coordinates t, x, y, z , $d\mathbb{T} = dt dx dy dz = d^4x$. If we have fields ϕ^a and a Lagrangian density which depends only on those fields and their first derivatives then it is straightforward to compute the

Euler-Lagrange equations (as always, one could generalize to higher derivatives by performing the same steps):

$$S = \int_{\mathbb{T}} \mathfrak{L} d^4x \implies \delta S = \int_{\mathbb{T}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} \delta \phi^a + \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \delta \partial_\mu \phi^a \right) d^4x \quad (4.9.94)$$

$$\implies \delta S = \int_{\mathbb{T}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} \delta \phi^a + \partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \delta \phi^a \right) - \partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \right) \delta \phi^a \right) d^4x. \quad (4.9.95)$$

The total derivative term becomes a boundary term by the divergence theorem and then becomes 0 as always because we don't vary the fields at the boundary of the integration region. Hence we have the equation of motion:

$$\delta S = \int_{\mathbb{T}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} - \partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \right) \right) \delta \phi^a d^4x \quad (4.9.96)$$

$$\implies \boxed{\frac{\delta S}{\delta \phi^a} = \frac{\partial \mathfrak{L}}{\partial \phi^a} - \partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \right) \stackrel{!}{=} 0.} \quad (4.9.97)$$

We can verify that this produces the equation of motion we derived without the covariant notation by breaking up the sum into the time and spatial components:

$$\partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \right) = \partial_0 \frac{\partial \mathfrak{L}}{\partial \partial_0 \phi^a} + \partial_b \frac{\partial \mathfrak{L}}{\partial \partial_b \phi^a} = \partial_t \frac{\partial \mathfrak{L}}{\partial \dot{\phi}^a} + \nabla \cdot \frac{\partial \mathfrak{L}}{\partial \nabla \phi^a} \quad (4.9.98)$$

$$\implies \partial_t \frac{\partial \mathfrak{L}}{\partial \dot{\phi}^a} = \frac{\partial \mathfrak{L}}{\partial \phi^a} - \nabla \cdot \frac{\partial \mathfrak{L}}{\partial \nabla \phi^a}. \quad (4.9.99)$$

This exactly as before. Another nice fact about the Lagrangian density is that it inherits the Lorentz invariance of the action. Because by theorem 4.1 Lorentz boosts do not change $d\mathbb{T}$ and because rotations also do not change $d\mathbb{T}$ (as they change neither dt nor dS due to having determinant 1), $d\mathbb{T}$ is Lorentz invariant and so because the Lorentz invariant action is the integral with respect to this Lorentz invariant measure $d\mathbb{T}$ of the Lagrangian density, it follows that the Lagrangian density is Lorentz invariant. Of course, this is up to adding total divergences to the Lagrangian density as those become surface terms on the integral. One should not forget that the Lagrangian density is only defined up to such terms, as always. In fact, the surface terms one can add also take a nice form in the relativistic notation. From equation (3.2.62), two Lagrangian densities are equivalent if and only if:

$$\mathfrak{L}' = \mathfrak{L} + \nabla \cdot \vec{F} + \frac{df}{dt} \quad (4.9.100)$$

for some functions of the coordinates and fields f and $\vec{F}$. If we then define $f^0 = f$ and $f^a = F^a$ we can reexpress this as:

$$\boxed{\mathfrak{L}' = \mathfrak{L} + \partial_\mu f^\mu} \quad (4.9.101)$$

and so two Lagrangian densities are equivalent if and only if they differ by a 4-divergence. Of course, as we have done before, we could always use the regular Lagrangian or Hamiltonian for relativity but because they are not Lorentz invariant and thus don't easily reflect the symmetries of our theory, it is often (but not always) easier to see what is going on through the Lagrangian density or the action than the Hamiltonian or Lagrangian. It is absolutely the case though that both the regular Hamiltonian and Lagrangian have their place and usefulness within relativistic theories as well, as we will see through examples.

As an example of our covariant field equations of motion, consider the action for Maxwell's equations:

$$S = \int_{\mathbb{T}} \left(\frac{1}{2} (|\vec{E}|^2 - |\vec{B}|^2) + \vec{J} \cdot \vec{A} - \rho \phi \right) d\mathbb{T}. \quad (4.9.102)$$

Using the definition of the 4-potential A and the 4-current J :

$$J \cdot A = J^\mu A_\mu = J^0 A_0 + J^a A_a = \vec{J} \cdot \vec{A} - \rho \phi. \quad (4.9.103)$$

As well, using the definition of the field strength tensor $\mathcal{F}_{\mu\nu}$:

$$E_a = \mathcal{F}_{a0}, \quad \mathcal{F}_{ab} = \epsilon_{ab}{}^c B_c \implies B_a = \frac{1}{2} \epsilon_a{}^{bc} \mathcal{F}_{bc}. \quad (4.9.104)$$

Then:

$$|\vec{E}|^2 - |\vec{B}|^2 = \mathcal{F}_{a0} \mathcal{F}^a{}_0 - \frac{1}{4} \epsilon_a{}^{bc} \mathcal{F}_{bc} \epsilon^{ade} \mathcal{F}_{de} \quad (4.9.105)$$

$$= -\frac{1}{2} \left(2\mathcal{F}^{a0}\mathcal{F}_{a0} + \frac{1}{2}(\delta^{bd}\delta^{ce} - \delta^{be}\delta^{cd})\mathcal{F}_{bc}\mathcal{F}_{de} \right) \quad (4.9.106)$$

$$= -\frac{1}{2} (\mathcal{F}^{00}\mathcal{F}_{00} + \mathcal{F}^{a0}\mathcal{F}_{a0} + \mathcal{F}^{0a}\mathcal{F}_{0a} + \mathcal{F}^{ab}\mathcal{F}_{ab}) \quad (4.9.107)$$

$$= -\frac{1}{2} \mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu}. \quad (4.9.108)$$

Thus, in the covariant notation the action becomes:

$$S = \int_{\mathbb{T}} \left(-\frac{1}{4} \mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu} + J^\mu A_\mu \right) d\mathbb{T}. \quad (4.9.109)$$

Then, the equations of motion become:

$$\frac{\partial \mathcal{L}}{\partial A_\mu} - \partial_\nu \frac{\partial \mathcal{L}}{\partial \partial_\nu A_\mu} \stackrel{!}{=} 0 \quad (4.9.110)$$

$$\frac{\partial \mathcal{L}}{\partial A_\mu} = J^\mu \quad (4.9.111)$$

$$\frac{\partial \mathcal{L}}{\partial \partial_\nu A_\mu} = \frac{\partial}{\partial \partial_\nu A_\mu} \left(-\frac{1}{4} \mathcal{F}^{\alpha\beta}\mathcal{F}_{\alpha\beta} \right) = -\frac{1}{2} \mathcal{F}^{\alpha\beta} \frac{\partial}{\partial \partial_\nu A_\mu} (\partial_\alpha A_\beta - \partial_\beta A_\alpha) = -\frac{1}{2} \mathcal{F}^{\alpha\beta} (\delta_\alpha^\nu \delta_\beta^\mu - \delta_\beta^\nu \delta_\alpha^\mu) = \mathcal{F}^{\mu\nu} \quad (4.9.112)$$

$$\implies \boxed{\partial_\nu \mathcal{F}^{\mu\nu} = J^\mu}. \quad (4.9.113)$$

This equation gives both Gauss' law (as the 0-component) and the Maxwell-Ampere law (as the spatial components). The other two of Maxwell's equations, the Solenoid law and Faraday's law follow automatically from the expression for $\vec{E}$ and $\vec{B}$ in terms of the potentials. We can though express the Solenoid law and Faraday's law in terms of the field strength given that they can be expressed in terms of $\vec{E}$ and $\vec{B}$:

$$\nabla \cdot \vec{B} = 0 \implies \partial_a B^a = \frac{1}{2} \epsilon^{abc} \partial_a \mathcal{F}_{bc} = 0 \implies \epsilon^{abc} \partial_a \mathcal{F}_{bc} = 0 \quad (4.9.114)$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \implies \partial_0 B^a + \epsilon^{abc} \partial_b E_c = \frac{1}{2} \epsilon^{abc} \partial_0 \mathcal{F}_{bc} + \epsilon^{abc} \partial_b \mathcal{F}_{c0} = 0. \quad (4.9.115)$$

If we now define the 4-dimensional Levi-Civita symbol $\epsilon_{\mu\nu\rho\sigma}$ so that $\epsilon_{0123} = 1$ and so that it is anti-symmetric under the interchange of any pair of indices, we immediately have that $\epsilon_{0abc} = \epsilon_{abc}$. It is very important to note that with how we have defined $\epsilon_{\mu\nu\rho\sigma}$ so that $\epsilon_{0123} = 1$, if one raises each of its indices with the Minkowski metric then the fully raised $\epsilon^{\mu\nu\rho\sigma}$ satisfies $\epsilon^{0123} = -1$ due to the -1 in η^{00} . This leads to $\epsilon^{0abc} = -\epsilon^{abc}$ and so:

$$\epsilon^{0\nu\rho\sigma} \partial_\nu \mathcal{F}_{\rho\sigma} = -\epsilon^{abc} \partial_a \mathcal{F}_{bc} = 0 \quad (4.9.116)$$

$$\epsilon^{a\nu\rho\sigma} \partial_\nu \mathcal{F}_{\rho\sigma} = -\epsilon^{a0bc} \partial_0 \mathcal{F}_{bc} - \epsilon^{ab0c} \partial_b \mathcal{F}_{0c} - \epsilon^{abc0} \partial_c \mathcal{F}_{c0} \quad (4.9.117)$$

$$= \epsilon^{abc} \partial_0 \mathcal{F}_{bc} + 2\epsilon^{abc} \partial_b \mathcal{F}_{c0} = 0. \quad (4.9.118)$$

Thus, we have:

$$\epsilon^{\mu\nu\rho\sigma} \partial_\nu \mathcal{F}_{\rho\sigma} = 0 \quad (4.9.119)$$

as the covariant way of expressing the Solenoid law and Faraday's law together. There is a 4 dimensional analogue of the double Levi-Civita identity in problem 2.6 which will be useful. In particular:

$$\epsilon^{\mu\nu\rho\sigma} \epsilon_{\mu\alpha\beta\gamma} = -\delta_\alpha^\nu \delta_\beta^\rho \delta_\gamma^\sigma + \delta_\beta^\nu \delta_\alpha^\rho \delta_\gamma^\sigma - \delta_\beta^\nu \delta_\gamma^\rho \delta_\alpha^\sigma + \delta_\gamma^\nu \delta_\beta^\rho \delta_\alpha^\sigma - \delta_\gamma^\nu \delta_\alpha^\rho \delta_\beta^\sigma + \delta_\alpha^\nu \delta_\gamma^\rho \delta_\beta^\sigma. \quad (4.9.120)$$

Using this, by contracting $\epsilon_{\mu\alpha\beta\gamma}$ onto equation (4.9.119) we may rewrite it equivalently as:

$$\boxed{\partial_\alpha \mathcal{F}_{\beta\gamma} + \partial_\beta \mathcal{F}_{\gamma\alpha} + \partial_\gamma \mathcal{F}_{\alpha\beta} = 0}. \quad (4.9.121)$$

Either of equations (4.9.119) or (4.9.121) are generally called the Bianchi identity for electromagnetism.

Exercises

Problem 4.76: ★ Tensor Product Practice. The tensor product can be difficult to get a hold of at first, so let us do an example. Consider a two dimensional real vector space $\mathbb{U}$ with basis vectors $\vec{i}_1 = (1, 0)$ and $\vec{i}_2 = (0, 1)$ and a three dimensional real vector space $\mathbb{V}$ with basis vectors $\vec{j}_1 = (1, 0, 0)$, $\vec{j}_2 = (0, 1, 0)$,

and $\vec{j}_3 = (0, 0, 1)$. Let the six basis vectors of the tensor product vector space $\mathbb{W} = \mathbb{U} \otimes \mathbb{V}$ be called $\vec{k}_1 = (1, 0, 0, 0, 0, 0)$, $\vec{k}_2 = (0, 1, 0, 0, 0, 0)$, $\vec{k}_3 = (0, 0, 1, 0, 0, 0)$, $\vec{k}_4 = (0, 0, 0, 1, 0, 0)$, $\vec{k}_5 = (0, 0, 0, 0, 1, 0)$, and $\vec{k}_6 = (0, 0, 0, 0, 0, 1)$ and define them by:

$$\begin{aligned}\vec{k}_1 &= \vec{i}_1 \otimes \vec{j}_1, & \vec{k}_2 &= \vec{i}_1 \otimes \vec{j}_2, & \vec{k}_3 &= \vec{i}_1 \otimes \vec{j}_3 \\ \vec{k}_4 &= \vec{i}_2 \otimes \vec{j}_1, & \vec{k}_5 &= \vec{i}_2 \otimes \vec{j}_2, & \vec{k}_6 &= \vec{i}_2 \otimes \vec{j}_3.\end{aligned}$$

- (a) Consider $\vec{u} = (u_1, u_2)$ a general vector in $\mathbb{U}$ and $\vec{v} = (v_1, v_2, v_3)$ a general vector in $\mathbb{V}$. Show that $\vec{u} \otimes \vec{v}$ has components given by:

$$\vec{u} \otimes \vec{v} = (u_1 v_1, u_1 v_2, u_1 v_3, u_2 v_1, u_2 v_2, u_2 v_3).$$

- (b) Explain why the dimension of the tensor product space of two vector space will always be the product of the dimensions of the individual vector spaces.
- (c) Let $\hat{A}$ be a 2x2 matrix which acts as a linear transformation from $\mathbb{U}$ into $\mathbb{U}$ and $\hat{B}$ be a 3x3 matrix which acts as a linear transformation from $\mathbb{V}$ into $\mathbb{V}$. Let $\hat{C}$ be the 6x6 matrix which acts as a linear transformation from $\mathbb{W}$ into $\mathbb{W}$ and is defined to satisfy:

$$\hat{C}(\vec{u} \otimes \vec{v}) = (\hat{A}\vec{u}) \otimes (\hat{B}\vec{v})$$

for all vectors $\vec{u}$ and $\vec{v}$. It is a common abuse of notation to write $\hat{C} = \hat{A} \otimes \hat{B}$. If $\hat{A}$ and $\hat{B}$ have component expressions:

$$\hat{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}$$

show that $\hat{C}$ has the component expression:

$$\hat{C} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{11}b_{13} & a_{12}b_{11} & a_{12}b_{12} & a_{12}b_{13} \\ a_{11}b_{21} & a_{11}b_{22} & a_{11}b_{23} & a_{12}b_{21} & a_{12}b_{22} & a_{12}b_{23} \\ a_{11}b_{31} & a_{11}b_{32} & a_{11}b_{33} & a_{12}b_{31} & a_{12}b_{32} & a_{12}b_{33} \\ a_{21}b_{11} & a_{21}b_{12} & a_{21}b_{13} & a_{22}b_{11} & a_{22}b_{12} & a_{22}b_{13} \\ a_{21}b_{21} & a_{21}b_{22} & a_{21}b_{23} & a_{22}b_{21} & a_{22}b_{22} & a_{22}b_{23} \\ a_{21}b_{31} & a_{21}b_{32} & a_{21}b_{33} & a_{22}b_{31} & a_{22}b_{32} & a_{22}b_{33} \end{pmatrix} = \begin{pmatrix} a_{11}\hat{B} & a_{12}\hat{B} \\ a_{21}\hat{B} & a_{22}\hat{B} \end{pmatrix}$$

where we have used block matrix notation in this last expression.

- (d) Consider the vectors $\vec{u}_1 = (1, 0)$, $\vec{u}_2 = (0, 1)$, $\vec{v}_1 = (1, 0, 0)$, $\vec{v}_2 = (0, 1, 0)$, $\vec{v}_3 = (0, 0, 1)$. Compute the components of the vector:

$$\vec{w} = \vec{u}_1 \otimes \vec{v}_1 + \vec{u}_2 \otimes \vec{v}_2.$$

Show that there does not exist a pair of vectors $\vec{u}_3 \in \mathbb{U}$, $\vec{v}_3 \in \mathbb{V}$ so that $\vec{u}_3 \otimes \vec{v}_3 = \vec{w}$. Because the vector $\vec{w}$ cannot be written as a tensor product of vectors in the spaces $\mathbb{U}$, $\mathbb{V}$, $\vec{w}$ is said to be “entangled”. The property of being entangled is completely basis independent. So, while vectors in $\mathbb{W}$ which are a tensor product of individual vectors in $\mathbb{U}$ and $\mathbb{V}$ are enough to make a basis for the space $\mathbb{W}$, not every vector in the tensor product space $\mathbb{W}$ is itself a tensor product of individual vectors.

Problem 4.77: 4-Dimensional Levi-Civita Properties.

- (a) Using the definition of $\epsilon_{\mu\nu\rho\sigma}$ and the operation of raising and lowering indices, show that $\epsilon^{0123} = -1$.
- (b) Show that $\epsilon_{0abc} = \epsilon_{abc}$ (the 3-dimensional Levi-Civita) and that $\epsilon^{0abc} = -\epsilon^{abc}$.
- (c) Consider the product $\epsilon^{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\gamma\lambda}$. Explain that this is 0 unless μ, ν, ρ, σ are all distinct, $\alpha, \beta, \gamma, \lambda$ are all distinct and that in 4-dimensions this implies that both sets each contain 0, 1, 2, 3 exactly once each. Then, explain that this forces the list $(\alpha, \beta, \gamma, \lambda)$ to be a reordering of (μ, ν, ρ, σ) and show that this product is 1 if that reordering requires an even number of swaps of list elements and -1 if it requires an odd number of swaps of list elements.
- (d) Use the results of the previous part to show:

$$\begin{aligned}\epsilon^{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\gamma\lambda} &= -\eta^{\mu\alpha}\eta^{\nu\beta}\eta^{\rho\gamma}\eta^{\sigma\lambda} + \eta^{\mu\alpha}\eta^{\nu\beta}\eta^{\rho\lambda}\eta^{\sigma\gamma} - \eta^{\mu\alpha}\eta^{\nu\gamma}\eta^{\rho\lambda}\eta^{\sigma\beta} + \eta^{\mu\alpha}\eta^{\nu\gamma}\eta^{\rho\beta}\eta^{\sigma\lambda} \\ &\quad - \eta^{\mu\alpha}\eta^{\nu\lambda}\eta^{\rho\beta}\eta^{\sigma\gamma} + \eta^{\mu\alpha}\eta^{\nu\lambda}\eta^{\rho\gamma}\eta^{\sigma\beta} + \eta^{\mu\beta}\eta^{\nu\alpha}\eta^{\rho\gamma}\eta^{\sigma\lambda} - \eta^{\mu\beta}\eta^{\nu\alpha}\eta^{\rho\lambda}\eta^{\sigma\gamma} \\ &\quad + \eta^{\mu\beta}\eta^{\nu\gamma}\eta^{\rho\lambda}\eta^{\sigma\alpha} - \eta^{\mu\beta}\eta^{\nu\gamma}\eta^{\rho\alpha}\eta^{\sigma\lambda} + \eta^{\mu\beta}\eta^{\nu\lambda}\eta^{\rho\alpha}\eta^{\sigma\gamma} - \eta^{\mu\beta}\eta^{\nu\lambda}\eta^{\rho\gamma}\eta^{\sigma\alpha} \\ &\quad - \eta^{\mu\gamma}\eta^{\nu\alpha}\eta^{\rho\beta}\eta^{\sigma\lambda} + \eta^{\mu\gamma}\eta^{\nu\alpha}\eta^{\rho\lambda}\eta^{\sigma\beta} - \eta^{\mu\gamma}\eta^{\nu\beta}\eta^{\rho\lambda}\eta^{\sigma\alpha} + \eta^{\mu\gamma}\eta^{\nu\beta}\eta^{\rho\alpha}\eta^{\sigma\lambda}\end{aligned}$$

$$\begin{aligned}
& -\eta^{\mu\gamma}\eta^{\nu\lambda}\eta^{\rho\alpha}\eta^{\sigma\beta} + \eta^{\mu\gamma}\eta^{\nu\lambda}\eta^{\rho\beta}\eta^{\sigma\alpha} + \eta^{\mu\lambda}\eta^{\nu\alpha}\eta^{\rho\beta}\eta^{\sigma\gamma} - \eta^{\mu\lambda}\eta^{\nu\alpha}\eta^{\rho\gamma}\eta^{\sigma\beta} \\
& + \eta^{\mu\lambda}\eta^{\nu\beta}\eta^{\rho\gamma}\eta^{\sigma\alpha} - \eta^{\mu\lambda}\eta^{\nu\beta}\eta^{\rho\alpha}\eta^{\sigma\gamma} + \eta^{\mu\lambda}\eta^{\nu\gamma}\eta^{\rho\alpha}\eta^{\sigma\beta} - \eta^{\mu\lambda}\eta^{\nu\gamma}\eta^{\rho\beta}\eta^{\sigma\alpha}.
\end{aligned}$$

- (e) Show that lowering $\alpha, \beta, \gamma, \lambda$ in the previous part and then contracting $\alpha = \mu$ gives equation (4.9.121).
(f) Show that any four index object $A^{\mu\nu\rho\sigma}$ which is anti-symmetric under the interchange of all pairs of two indices is proportional to $\epsilon^{\mu\nu\rho\sigma}$
(g) Use the result of part (d) and the definition of the determinant of a 4x4 matrix to show that for a matrix $A^\mu{}_\nu$:

$$\det A = -\frac{1}{24}\epsilon_{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\gamma\lambda}A^\mu{}_\alpha A^\nu{}_\beta A^\rho{}_\gamma A^\sigma{}_\lambda.$$

- (h) $\epsilon^{\mu\nu\rho\sigma}$ due to its index placement looks like a rank 4 tensor. Show using the results of the previous parts that under a Lorentz transformation:

$$L^\mu{}_\alpha L^\nu{}_\beta L^\rho{}_\gamma L^\sigma{}_\lambda \epsilon^{\alpha\beta\gamma\lambda} = (\det L) \epsilon^{\mu\nu\rho\sigma}.$$

(To understand the following analysis, read the next section.) So, $\epsilon^{\mu\nu\rho\sigma}$ can be treated as a constant unchanged rank 4 tensor by all Lorentz transformations in the connected Lorentz group (as they all have determinant 1) but it is inverted by either a parity or time reversal transformation. Because of this it is called a rank 4 pseudotensor (tensor means it has same behavior under the connected Lorentz group as a tensor product of vectors but pseudo means its sign behaves opposite under parity to the way a tensor product of vectors would).

Problem 4.78: Playing with covariant expressions.

- (a) Consider a point charge q sitting stationary at the origin. Let u^μ be its 4-velocity. Show that the 4-vector potential produced by this charge can be written as:

$$A_\mu(x) = \frac{qu_\mu}{4\pi\sqrt{x^2 + (x \cdot u)^2}}.$$

(For a 4-vector v^μ , $v^2 = v \cdot v$; this can be ambiguous with the y component of v unfortunately. I will always mean $v^2 = v \cdot v = v^\mu v_\mu$ unless we are working explicitly in numbered components rather than abstract indices such as μ .) Explain that because this form is manifestly covariant, it is valid as well for a point charge moving at constant velocity. This is the covariant form of Coulomb's law.

- (b) Define the dual field strength tensor ${}^*\mathcal{F}_{\mu\nu}$ by:

$${}^*\mathcal{F}_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}\mathcal{F}^{\rho\sigma}.$$

Show that the full set of Maxwell's equations can be expressed as:

$$\partial_\nu \mathcal{F}^{\mu\nu} = J^\mu, \quad \partial_\nu {}^*\mathcal{F}^{\mu\nu} = 0.$$

As well, show that $\mathcal{F}_{\mu\nu}$ can be recovered from its dual by:

$$\mathcal{F}_{\mu\nu} = -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}{}^*\mathcal{F}^{\rho\sigma}.$$

- (c) Show that the Lorentz gauge condition is $\partial^\mu A_\mu = 0$ and that in this gauge the equation of motion for the vector potential is:

$$-\partial^2 A^\mu = J^\mu$$

- (d) Let $n^\mu = (1, 0, 0, 0)^\mu$ be the time direction vector in some reference frame. Using the expression in equation (4.9.57), show that E_μ and B_μ defined here satisfy:

$$E_\mu \stackrel{\text{def}}{=} \mathcal{F}_{\mu\nu}n^\nu = (0, E_x, E_y, E_z)_\mu, \quad B_\mu \stackrel{\text{def}}{=} -{}^*\mathcal{F}_{\mu\nu}n^\nu = (0, B_x, B_y, B_z)_\mu$$

where the explicit components written here are those of the usual electric and magnetic fields. Thus, these E_μ and B_μ look like 4-vector versions of the electric and magnetic fields. However, E_μ and B_μ only transform like 4-vectors if in the transformation one transforms both $\mathcal{F}_{\mu\nu}$ and the reference frame time direction n^μ . Show that the field strength can be written as:

$$\mathcal{F}_{\mu\nu} = n_\mu E_\nu - n_\nu E_\mu + \epsilon_{\mu\nu\rho\sigma}n^\rho B^\sigma.$$

- (e) Show that in terms of the E_μ and B_μ vectors the point charge equation of motion becomes:

$$m \frac{d^2 x_\mu}{d\tau^2} = q \dot{x}^\nu E_\nu n_\mu - q \dot{x}^\nu n_\nu E_\mu + q \epsilon_{\mu\nu\rho\sigma} \dot{x}^\nu n^\rho B^\sigma.$$

- Explain how this can easily be seen to match the Lorentz force law in non-covariant 3-vector notation.
- (f) We can now easily solve the motion of a relativistic particle in uniform fields. Show that if $\vec{E}$ and $\vec{B}$ are uniform and constant, then $\mathcal{F}_{\mu\nu}$ is uniform and constant and that the motion of a charged particle in such fields is solved by:

$$x^\mu(\tau) = x^\mu(0) + \frac{m}{q} \left(\frac{e^{\frac{q\tau}{m}\mathcal{F}} - 1}{\mathcal{F}} \right)^\mu{}_\nu \frac{dx^\nu}{d\tau}(0)$$

where the expression above in terms of $\mathcal{F}$ is defined by series expansion:

$$\frac{e^x - 1}{x} = \sum_{n=0}^{\infty} \frac{x^n}{(n+1)!} \implies \frac{m}{q} \left(\frac{e^{\frac{q\tau}{m}\mathcal{F}} - 1}{\mathcal{F}} \right)^\mu{}_\nu = \sum_{n=0}^{\infty} \frac{q^n \tau^{n+1}}{m^n (n+1)!} \mathcal{F}^\mu{}_{\rho_1} \mathcal{F}^{\rho_1}{}_{\rho_2} \dots \mathcal{F}^{\rho_{n-1}}{}_\nu.$$

Explain how using standard techniques from linear algebra this matrix formula can be explicitly computed for a given $\mathcal{F}_{\mu\nu}$, allowing a fully explicit solution for $x^\mu(\tau)$.

4.10 The Structure of the Lorentz Group

We identified that because all Lorentz boosts and rotations preserve the proper time that they also satisfy (4.9.13):

$$\eta_{\alpha\beta} = \eta_{\mu\nu} L^\mu{}_\alpha L^\nu{}_\beta. \quad (4.10.1)$$

As well, this is the only property we used to derive the transformation features of the previous section. However, it is not clear at this point that only Lorentz boosts and rotations have this property. So, we ought to find the set all of the matrices L which satisfy this relationship with the Minkowski metric. (4.10.1) can be written in matrix form as:

$$\eta = L\eta L^T. \quad (4.10.2)$$

It immediately follows from this that the set of such matrices L is closed under matrix multiplication (if both L and L' are in the set then LL' is in the set):

$$\eta = L\eta L^T, \quad \eta = L'\eta L'^T \implies (LL')\eta(LL')^T = LL'\eta L'^T L^T = L\eta L^T = \eta. \quad (4.10.3)$$

By taking the determinant of both sides we find that L must have determinant of ± 1 and thus is invertible:

$$\det \eta = \det L \det \eta \det L \implies (\det L)^2 = 1 \implies \det L = \pm 1. \quad (4.10.4)$$

Now that we know L is invertible we can see also that L^{-1} is in the set:

$$\eta = L\eta L^T \implies L^{-1}\eta L^{-T} = \eta. \quad (4.10.5)$$

Trivially as well the identity is contained in the set:

$$\mathbb{1}\eta\mathbb{1}^T = \eta. \quad (4.10.6)$$

Hence the set satisfies all of the properties of a group. The group of all matrices L satisfying equation (4.10.2) is called the **improper Lorentz group**.

We defined orthogonal matrices $\hat{O}$ as matrices which satisfy $\hat{O}\mathbb{1}\hat{O}^T = \mathbb{1}$. We see in (4.10.2) that the matrices in the Lorentz group satisfy a very similar equation in the orthogonal matrices, simply with $\mathbb{1}$ replaced by η . The identity matrix is just a diagonal matrix of 1's, while the Minkowski metric is just a diagonal matrix of 1's with a single -1. So, another name for the improper Lorentz group is $O(3,1)$, the group of orthogonal matrices where the orthogonality condition has a metric on both sides which is diagonal with 3 copies of 1 and 1 copy of -1.

4.10.1 Components of the Improper Lorentz Group

The improper Lorentz group does include more matrices than just rotation, boosts, and their composition. From the definition of the proper time:

$$d\tau^2 = dt^2 - |d\vec{x}|^2 \quad (4.10.7)$$

it is clear that the proper time is agnostic to taking $dt \rightarrow -dt$ or $dx \rightarrow -dx$ or $dy \rightarrow -dy$ or $dz \rightarrow -dz$. We have already encountered these transformations. As defined in 1.9, the transformation $t' = -t$ keeping everything else fixed is known as time reversal. As a matrix on the coordinate displacements we see it is given by:

$$\mathcal{T} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4.10.8)$$

and it is plainly in the group. While we could put a reversal matrix for each of the x, y, z axes, a rotation about any axis by 180° inverts the other two so we only need to include the operation of inverting all three and then through the composition of that transformation and rotation we can make the inversion of any axis of our choice. The transformation of inverting all spatial coordinates we already defined in 3.3; it is the parity transformation. As a matrix on the coordinate displacements we see it is given by:

$$\mathcal{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (4.10.9)$$

and it is also plainly in the group. So, at the very least the improper Lorentz group contains the composition of boosts, rotations, parity, and time reversal. We will now show that this is all it contains.

It will be useful to consider the explicit form of the boost matrix. We found that for a general Lorentz boost:

$$dt' = \gamma(dt + \vec{v} \cdot d\vec{x}), \quad d\vec{x}' = \left(1 + (\gamma - 1)\frac{\vec{v}\vec{v}}{|\vec{v}|^2}\right) \cdot d\vec{x} + \gamma\vec{v}dt. \quad (4.10.10)$$

Now write everything in components in terms of the boost 4-velocity:

$$u^0 = \gamma, \quad u^a = \gamma v^a \quad (4.10.11)$$

$$\implies dx'^0 = u^0 dx^0 + u_a dx^a, \quad dx'^a = dx^a + (u^0 - 1)\frac{u^a u_b}{u^c u_c} dx^b + u^a dx^0. \quad (4.10.12)$$

By the definition of the 4-velocity, this can be simplified a bit:

$$u^\mu u_\mu = \frac{dx^\mu}{d\tau} \frac{dx_\mu}{d\tau} = -1 \quad (4.10.13)$$

$$\implies -(u^0)^2 + u^a u_a = -1 \implies u^a u_a = (u^0)^2 - 1 \quad (4.10.14)$$

$$\implies \frac{u^0 - 1}{u^a u_a} = \frac{1}{u^0 + 1}. \quad (4.10.15)$$

Thus we have that the Lorentz boost matrix is given by:

$$dx'^\mu = B^\mu{}_\nu dx^\nu \quad (4.10.16)$$

$$B^0{}_0 = u^0, \quad B^0{}_a = u_a, \quad B^a{}_0 = u^a, \quad B^a{}_b = \delta^a_b + \frac{u^a u_b}{1 + u^0}. \quad (4.10.17)$$

Now consider L an arbitrary element of our group. By definition:

$$\eta_{\mu\nu} = L^\alpha{}_\mu \eta_{\alpha\beta} L^\beta{}_\nu \quad (4.10.18)$$

$$\implies \eta_{00} = L^\alpha{}_0 \eta_{\alpha\beta} L^\beta{}_0 \implies -1 = -(L^0{}_0)^2 + L^a{}_0 L^a{}_0 \implies L^0{}_0 = \pm \sqrt{1 + L^a{}_0 L^a{}_0}. \quad (4.10.19)$$

Suppose $L^0{}_0 < 0$. Then, $(\mathcal{T}L)^0{}_0 > 0$ automatically. Hence we can consider only the L with positive 00 component and get all of the L with negative 00 component by composing them with $\mathcal{T}$. (We can recover the negative 00 L because $\mathcal{T}$ is invertible.) So, without loss of generality we can now assume that $L^0{}_0 > 0$. Now continue applying the conditions implied by (4.10.18):

$$\eta_{0a} = L^\alpha{}_0 \eta_{\alpha\beta} L^\beta{}_a \implies 0 = -L^0{}_0 L^0{}_a + L^b{}_0 L^b{}_a \implies L^0{}_a = \frac{L^b{}_0 L^b{}_a}{L^0{}_0}. \quad (4.10.20)$$

Now consider the composition of L with a boost. This will produce a new L' but because the boost is invertible, the set of all L' is the same as the set of all L . In particular look at the components $L'^a{}_0$:

$$L'^\mu{}_\nu = B^\mu{}_\lambda L^\lambda{}_\nu \quad (4.10.21)$$

$$\implies L'^a{}_0 = B^a{}_\mu L^\mu{}_0 = B^a{}_0 L^0{}_0 + B^a{}_b L^b{}_0 = u^a L^0{}_0 + \left(\delta^a_b + \frac{u^a u_b}{1 + u^0}\right) L^b{}_0. \quad (4.10.22)$$

Now choose the boost velocity as $u^a = -L^a{}_0$:

$$u^0 = \sqrt{1 + u^a u_a} = \sqrt{1 + L^a{}_0 L^a{}_0} = L^0{}_0 \quad (4.10.23)$$

$$\implies L'^a{}_0 = 0. \quad (4.10.24)$$

Hence we can always boost so that $L'^a{}_0 = 0$ and so without loss of generality can consider L such that this condition holds. Then, from (4.10.19) and (4.10.20) we have that after doing so:

$$L^0{}_0 = 1, \quad L^a{}_0 = 0, \quad L^0{}_a = 0. \quad (4.10.25)$$

Now we can consider the final conditions implied by (4.10.18):

$$\eta_{ab} = L^\alpha{}_a \eta_{\alpha\beta} L^\beta{}_b \implies \delta_{ab} = L^c{}_a L^c{}_b. \quad (4.10.26)$$

At this point we have reduced the problem to restrictions on 3x3 matrices so it is useful to define the 3x3 matrix m :

$$m^a{}_b = L^a{}_b \implies \delta_{ab} = m^c{}_a m^c{}_b \implies m^T m = \mathbb{1}. \quad (4.10.27)$$

By the results of problem 2.8 this means that m is a composition of parity transformations and rotations. If m has determinant 1 no parity transformation is necessary. If m has determinant -1 a parity transformation

is necessary. So, a general element of the improper Lorentz group can be written as some composition of time reversal, boost, parity, and rotation. This construction also shows us that there are 4 disconnected components of the improper Lorentz group. There is the component which has L^0_0 positive and the 3x3 matrix L^a_b has positive determinant which is exactly the connected Lorentz group (or just the Lorentz group). It is also written as $SO_+(3,1)$. The S is for Special, meaning determinant 1, and the + is because L^0_0 is positive. This component consists only of compositions of boosts and rotations. There is also the component which has L^0_0 negative and the 3x3 matrix L^a_b has positive determinant. This is just the time reversed version of the connected Lorentz group. There is the component which has L^0_0 positive and the 3x3 matrix L^a_b has negative determinant which is just the parity reversed version of the connected Lorentz group. Finally then there is the component which has L^0_0 negative and the 3x3 matrix L^a_b has negative determinant which is the fully reversed (both time and parity) version of the connected Lorentz group, which can be written as $SO_-(3,1)$.

In our relativistic theories so far we have only assumed symmetry under the connected Lorentz group $SO_+(3,1)$ and have been silent on whether we should expect parity symmetry or time reversal symmetry. It is a genuine physics question whether we should expect symmetry under the full improper Lorentz group, the connected Lorentz group with time reversal, the connected Lorentz group with parity, or simply only the connected Lorentz group. Peculiarly, so far only assuming symmetry under the connected Lorentz group we have actually gotten theories which additionally have symmetry under time reversal and parity and thus the full improper Lorentz group. To see this, consider a system of N charges interacting with the potentials. It will be easiest to use the non-covariant formulation to study parity and time reversal as they act on the time and space components separately.

$$S = \sum_{n=1}^N \int_{t_0}^{t_f} \left(-m_n \sqrt{1 - |\dot{\vec{x}}|^2} + q_n \vec{A}(t, \vec{x}_n) \cdot \dot{\vec{x}}_n - q_n \phi(t, \vec{x}_n) \right) dt + \int_{\mathbb{T}} \frac{|\vec{E}|^2 - |\vec{B}|^2}{2} d\mathbb{T}. \quad (4.10.28)$$

Under a parity transformation, we have that: $\vec{x}'_n = \mathcal{P}(\vec{x}_n) = -\vec{x}_n$. Then, the first term is automatically unchanged by parity. To complete the parity transformation we have to define how the scalar and vector potentials transform under it. In order for the second and third terms to be unchanged by parity though we need:

$$\mathcal{P}(\vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x})) \stackrel{!}{=} \vec{A}'(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x}) \quad (4.10.29)$$

$$\implies \vec{A}'(t, -\vec{x}) \cdot (-\dot{\vec{x}}) - \phi'(t, -\vec{x}) = \vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x}) \quad (4.10.30)$$

$$\implies \vec{A}'(t, \vec{x}) = -\vec{A}(t, -\vec{x}), \quad \phi'(t, \vec{x}) = \phi(t, -\vec{x}). \quad (4.10.31)$$

So, we take these as the definitions of how the potentials transform under parity. Hence, under parity the scalar potential does not change sign (ϕ is parity even) and the vector potential does ($\vec{A}$ is parity odd). Consequently, the electric and magnetic fields change as:

$$\vec{E}'(t, \vec{x}) = -\nabla \phi'(t, \vec{x}) - \frac{\partial \vec{A}'}{\partial t}(t, \vec{x}) = -\nabla \phi(t, -\vec{x}) - \frac{\partial}{\partial t}(-\vec{A}(t, -\vec{x})) \quad (4.10.32)$$

$$= - \left(-\nabla' \phi(t, \vec{x}') - \frac{\partial \vec{A}}{\partial t}(t, \vec{x}') \right) \Big|_{\vec{x}' = -\vec{x}} = -\vec{E}(t, -\vec{x}) \quad (4.10.33)$$

$$\vec{B}'(t, \vec{x}) = \nabla \times \vec{A}'(t, \vec{x}) = \nabla \times (-\vec{A}(t, -\vec{x})) = \left(\nabla' \times \vec{A}(t, \vec{x}') \right) \Big|_{\vec{x}' = -\vec{x}} = \vec{B}(t, -\vec{x}). \quad (4.10.34)$$

Hence $\vec{E}$ is parity odd and $\vec{B}$ is parity even. It immediately follows that the $|\vec{E}|^2 - |\vec{B}|^2$ term in equation (4.10.28) is parity even. The volume measure changes as $dt' d^3 \vec{x}' = |\det \mathcal{P}| dt d^3 \vec{x} = dt d^3 \vec{x}$ and thus the entire action in equation (4.10.28) is invariant under parity. So even though we did not need to assume parity symmetry to arrive at that action, we incidentally acquired it anyway. In components, we see that under parity transformation the 4-potential transforms as:

$$A'_\mu(X') = (\mathcal{P}A)_\mu(X) \quad (4.10.35)$$

using the component expression for $\mathcal{P}$ given in equation (4.10.9). By definition, coordinates under parity transform as $x'^\mu = (\mathcal{P}x)^\mu$ and so the derivative operators transform inversely as $\partial'_\mu = (\mathcal{P}\partial)_\mu$ because $\mathcal{P}$ is its own inverse matrix. Consequently, the field strength tensor transforms as:

$$\mathcal{F}'_{\mu\nu}(X') = (\mathcal{P}\mathcal{F}\mathcal{P})_{\mu\nu}(X). \quad (4.10.36)$$

Under time reversal, we have that $t' = -t$. So, the time measure dt satisfies $dt' = -dt$. As well, the

initial and final times on the action reverse order so that $t'_f = -t_0$ and $t'_0 = -t_f$ because $t'_f > t'_0$ by definition. Thus, interchanging the order of the integration bounds and the integral measure gives that the signs cancel out:

$$\int_{t_0}^{t_f} f(t)dt = \int_{-t'_f}^{-t'_0} f(t)dt = \int_{t'_f}^{t'_0} f(-t')(-dt') = \int_{t'_0}^{t'_f} f(-t')dt'. \quad (4.10.37)$$

Because of this, the Lagrangian is even under time reversal. Time reversal is a symmetry whenever the time reversed Lagrangian and the original Lagrangian differ only by a surface term.

Under time reversal, the velocities become: $\dot{x}'_n(t') = \frac{d\vec{x}_n}{dt'} = -\dot{x}_n(-t)$. Then, again the first term in equation (4.10.28) is automatically unchanged by time reversal. We now need to define how the potentials change under time reversal. Requiring the second and third terms to be unchanged:

$$\mathcal{T}(\vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x})) \stackrel{!}{=} \vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x}) \quad (4.10.38)$$

$$\implies \vec{A}'(-t, \vec{x}) \cdot (-\dot{\vec{x}}) - \phi'(-t, \vec{x}) \stackrel{!}{=} \vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - \phi(t, \vec{x}) \quad (4.10.39)$$

$$\implies \vec{A}'(t, \vec{x}) = -\vec{A}(-t, \vec{x}), \quad \phi'(t, \vec{x}) = \phi(-t, \vec{x}). \quad (4.10.40)$$

We see that the vector potential is time reversal odd and the scalar potential is time reversal even. Consequently, the electric and magnetic fields change as:

$$\vec{E}'(t, \vec{x}) = -\nabla\phi'(t, \vec{x}) - \frac{\partial \vec{A}'}{\partial t}(t, \vec{x}) = -\nabla\phi(-t, \vec{x}) - \frac{\partial}{\partial t}(-\vec{A}(-t, -\vec{x})) \quad (4.10.41)$$

$$= \left(-\nabla\phi(t', \vec{x}) - \frac{\partial \vec{A}}{\partial t'}(t', \vec{x}) \right) \Big|_{t'=-t} = \vec{E}(-t, \vec{x}) \quad (4.10.42)$$

$$\vec{B}'(t, \vec{x}) = \nabla \times \vec{A}'(t, \vec{x}) = \nabla \times (-\vec{A}(-t, \vec{x})) = -\vec{B}(-t, \vec{x}). \quad (4.10.43)$$

Hence $\vec{E}$ is time reversal even and $\vec{B}$ is time reversal odd. It immediately follows that the $|\vec{E}|^2 - |\vec{B}|^2$ term in equation (4.10.28) is time reversal even and thus the entire action is invariant under time reversal and we again have incidentally acquired a symmetry we never assumed. Under time reversal, the 4-potential transforms as:

$$A'_\mu(X') = -(\mathcal{T}A)_\mu(X). \quad (4.10.44)$$

Consequently, the field strength tensor transforms as:

$$\mathcal{F}'_{\mu\nu}(X') = -(\mathcal{T}\mathcal{F}\mathcal{T})_{\mu\nu}(X). \quad (4.10.45)$$

We have gotten lucky in finding that parity and time reversal symmetries are automatic for relativistic electromagnetism. Requiring symmetry under the connected Lorentz group incidentally made the theory symmetry under the improper Lorentz group. Typically this does not happen. That is, there may be terms in a connected Lorentz symmetric theory which do not have parity and/or time reversal symmetry. So, should we expect parity symmetry? Should we expect time reversal symmetry? These questions can only be settled by experiment. For now, we will wait to make a determination because it doesn't yet affect us but we will return to this issue in chapter 12.

4.10.2 Generators of the Lorentz Group

Now that we have related every part of the improper Lorentz group to some discrete transformation of the connected Lorentz group, we will study the connected Lorentz group. As we established, the connected Lorentz group consists of only boosts and rotations and is connected to the identity. Therefore, if we find the Lie algebra of the connected Lorentz group we can exponentiate the Lie algebra to recover the full group. As always, we can find the Lie algebra by differentiating the group about the identity. So, take the defining property of the group:

$$\eta_{\mu\nu} = L^\alpha{}_\mu L^\beta{}_\nu \eta_{\alpha\beta} \quad (4.10.46)$$

and differentiate and evaluate the result at the identity:

$$\implies 0 = \frac{dL^\alpha{}_\mu}{d\varepsilon} L^\beta{}_\nu \eta_{\alpha\beta} + L^\alpha{}_\mu \frac{dL^\beta{}_\nu}{d\varepsilon} \eta_{\alpha\beta} \quad (4.10.47)$$

$$\implies 0 = \frac{dL^\alpha{}_\mu}{d\varepsilon} \Big|_0 \delta^\beta_\nu \eta_{\alpha\beta} + \delta^\alpha_\mu \frac{dL^\beta{}_\nu}{d\varepsilon} \Big|_0 \eta_{\alpha\beta} \quad (4.10.48)$$

$$\Rightarrow 0 = \left. \frac{dL_{\nu\mu}}{d\varepsilon} \right|_0 + \left. \frac{dL_{\mu\nu}}{d\varepsilon} \right|_0. \quad (4.10.49)$$

Hence the derivative of $L_{\mu\nu}$ at the identity must be anti-symmetric and this is the only requirement. Any anti-symmetric matrix can be written as a linear combination of anti-symmetric matrices which have exactly 1 positive component and exactly 1 negative component. We can expand the derivative of $L_{\mu\nu}$ about the identity in terms of these matrices. Let $(J_{\mu\nu})^\alpha_\beta$ denote the $\alpha\beta$ component of the matrix $J_{\mu\nu}$ with components explicitly given by:

$$(J_{\mu\nu})^\alpha_\beta \stackrel{\text{def}}{=} \delta^\alpha_\nu \eta_{\mu\beta} - \delta^\alpha_\mu \eta_{\nu\beta}. \quad (4.10.50)$$

The lowered index quantity $(J_{\mu\nu})_{\alpha\beta}$ is automatically antisymmetric under exchanging α, β and it has exactly one positive component and one corresponding negative component. The list of these automatically form a basis for all 4×4 anti-symmetric matrices. Therefore, there exist coefficients $c^{\mu\nu}$ so that our anti-symmetric matrix that is the derivative of $L_{\alpha\beta}$ about the identity can be expanded in terms of these matrices:

$$\left. \frac{dL^\alpha_\beta}{d\varepsilon} \right|_0 = c^{\mu\nu} (J_{\mu\nu})^\alpha_\beta. \quad (4.10.51)$$

Now by exponentiating the Lie algebra we know we can recover the Lie group:

$$L^\alpha_\beta = (e^{\varepsilon L'(0)})^\alpha_\beta = (e^{\varepsilon c^{\mu\nu} J_{\mu\nu}})^\alpha_\beta. \quad (4.10.52)$$

Renaming these coefficients with the factor of ε as $\theta^{\mu\nu} = \varepsilon c^{\mu\nu}$, we have:

$$L = e^{\theta^{\mu\nu} J_{\mu\nu}} \quad (4.10.53)$$

for some parameters $\theta^{\mu\nu} = -\theta^{\nu\mu}$ for any element of the connected Lorentz group. We can also check that our choice of basis matrices J in fact corresponds to the basis of rotations and boosts. Taking equation (4.10.50) and letting $J_{\mu\nu}$ be the matrix with components $(J_{\mu\nu})^\alpha_\beta$, we find the resulting matrices:

$$J_{01} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -K_1, \quad J_{02} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -K_2, \quad J_{03} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} = -K_3, \quad (4.10.54)$$

$$J_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = J_3, \quad J_{23} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = J_1, \quad J_{31} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = J_2 \quad (4.10.55)$$

where J_1, J_2, J_3 as matrices generate rotations of the coordinates (compare them to (2.4.25)) and the K_1, K_2, K_3 as matrices generate Lorentz boosts of the coordinates (compare them to the φ derivatives at 0 of (4.3.26)). Hence the 6 independent $J_{\mu\nu}$ exactly map to our generators of boosts and of rotations. Because the Lorentz transformations are linear point transformations, we know we can compute their Poisson brackets very easily simply by computing their matrix commutators. By Theorem 1.11, the matrices $J_{\mu\nu}$ are a matrix representation of the Lorentz algebra with the matrix commutator acting as the bracket. Now let us compute the commutator:

$$[J_{\mu\nu}, J_{\rho\sigma}]^\alpha_\beta = (\delta^\alpha_\nu \eta_{\mu\gamma} - \delta^\alpha_\mu \eta_{\nu\gamma})(\delta^\gamma_\sigma \eta_{\rho\beta} - \delta^\gamma_\rho \eta_{\sigma\beta}) - (\delta^\alpha_\sigma \eta_{\rho\gamma} - \delta^\alpha_\rho \eta_{\sigma\gamma})(\delta^\gamma_\nu \eta_{\mu\beta} - \delta^\gamma_\mu \eta_{\nu\beta}) \quad (4.10.56)$$

$$= \eta_{\mu\sigma}(\delta^\alpha_\nu \eta_{\rho\beta} - \delta^\alpha_\rho \eta_{\nu\beta}) - \eta_{\mu\rho}(\delta^\alpha_\nu \eta_{\sigma\beta} - \delta^\alpha_\sigma \eta_{\nu\beta}) - \eta_{\nu\sigma}(\delta^\alpha_\mu \eta_{\rho\beta} - \delta^\alpha_\rho \eta_{\mu\beta}) + \eta_{\nu\rho}(\delta^\alpha_\mu \eta_{\sigma\beta} - \delta^\alpha_\sigma \eta_{\mu\beta}) \quad (4.10.57)$$

$$= \eta_{\mu\sigma}(J_{\rho\nu})^\alpha_\beta - \eta_{\mu\rho}(J_{\sigma\nu})^\alpha_\beta - \eta_{\nu\sigma}(J_{\rho\mu})^\alpha_\beta + \eta_{\nu\rho}(J_{\sigma\mu})^\alpha_\beta. \quad (4.10.58)$$

Therefore we have the Lie algebra of the Lorentz group:

$$J_{\mu\nu} \angle J_{\rho\sigma} = \eta_{\nu\sigma} J_{\mu\rho} - \eta_{\mu\sigma} J_{\nu\rho} - \eta_{\nu\rho} J_{\mu\sigma} + \eta_{\mu\rho} J_{\nu\sigma}. \quad (4.10.59)$$

Note that by definition $J_{\mu\nu} = -J_{\nu\mu}$ and so you actually only need to remember the first of these 4 terms and the others can be produced by just anti-symmetrizing the two pairs of indices μ, ν and ρ, σ .

It is sometimes useful to rewrite the relationship between the generators in this covariant form to the generators in the non-covariant form. By equations (4.10.54) and (4.10.55):

$$J_{0a} = -K_a, \quad J_{ab} = \epsilon_{ab}^c J_c \Rightarrow J_c = \frac{1}{2} \epsilon^{ab}_c J_{ab}. \quad (4.10.60)$$

We can also relate the parameters $\theta^{\mu\nu}$ to the rapidity and angle parameters of the boosts and rotations:

$$\theta^{\mu\nu} J_{\mu\nu} = -2\theta^{0a} K_a + \theta^{ab} \epsilon_{ab}{}^c J_c \stackrel{!}{=} \varphi^a K_a + \theta^a J_a \quad (4.10.61)$$

$$\Rightarrow \varphi^a = -2\theta^{0a}, \quad \theta^c = \epsilon_{ab}{}^c \theta^{ab} \quad (4.10.62)$$

$$\Rightarrow \theta^{0a} = -\frac{1}{2}\varphi^a, \quad \theta^{ab} = \frac{1}{2}\epsilon^{ab}{}_c \theta^c. \quad (4.10.63)$$

As well we can write down the Lie algebra (4.10.59) in non-covariant notation by simply rewriting the components in terms of K_a and J_a . Doing so yields:

$$K_a \angle K_b = -\epsilon_{ab}{}^c J_c, \quad J_a \angle K_b = \epsilon_{ab}{}^c K_c, \quad J_a \angle J_b = \epsilon_{ab}{}^c J_c. \quad (4.10.64)$$

Hence, we have:

Theorem 4.5: Lorentz Group Theorem

The improper Lorentz group $O(3,1)$ of all matrices L which satisfy:

$$L\eta L^T = \eta \quad (4.10.65)$$

is exactly the group of transformations so that $dX' = LdX$ preserves the proper time of dX . This group consists of compositions of rotations, Lorentz boosts, parity, and time reversal and decomposes into four disconnected components characterized by the signs of $L^0{}_0$ and $\det L$. The component connected to the identity, the connected Lorentz group $SO_+(3,1)$, is a connected Lie group with 6 generators, 3 J_a for the rotations and 3 K_a for the boosts, that satisfy:

$$K_a \angle K_b = -\epsilon_{ab}{}^c J_c, \quad J_a \angle K_b = \epsilon_{ab}{}^c K_c, \quad J_a \angle J_b = \epsilon_{ab}{}^c J_c. \quad (4.10.66)$$

Equivalently, these generators can be put into an antisymmetric tensor $J_{\mu\nu}$ by $J_{a0} = K_a$ and $J_{ab} = \epsilon_{ab}{}^c J_c$. The algebra for these generators is:

$$J_{\mu\nu} \angle J_{\rho\sigma} = \eta_{\nu\sigma} J_{\mu\rho} - \eta_{\mu\sigma} J_{\nu\rho} - \eta_{\nu\rho} J_{\mu\sigma} + \eta_{\mu\rho} J_{\nu\sigma}. \quad (4.10.67)$$

When acting on coordinates these generators have the matrix representation:

$$(J_{\mu\nu})^\alpha{}_\beta = \delta^\alpha_\nu \eta_{\mu\beta} - \delta^\alpha_\mu \eta_{\nu\beta}. \quad (4.10.68)$$

Exercises

Problem 4.79: ★ Parity Transformations of common quantities. By definition, under a parity transformation the position of an object is inverted and the time is unchanged:

$$\vec{x}'(t') = -\vec{x}(t), \quad t' = t$$

Show that if we are in a theory with a parity invariant action the Lagrangian, Hamiltonian, angular momentum vector, scalar potential, and magnetic field are parity even (unchanged by a parity transformation) and the velocity, linear momentum, dynamical energy moment vector, vector potential, and electric field are parity odd (their signs are changed by a parity transformation).

Problem 4.80: ★ Time Reversal Transformations of common quantities. By definition, under a time reversal transformation the position of an object is unchanged but the time is inverted:

$$\vec{x}'(t') = \vec{x}(t), \quad t' = -t.$$

Show that if we are in a theory with a time reversal invariant action the Lagrangian, Hamiltonian, dynamical energy moment vector, scalar potential, and electric field are time reversal even and the velocity, linear momentum, angular momentum vector, vector potential, and magnetic field are time reversal odd.

Problem 4.81: ★ Covariantizing the Poincare algebra.

- Show that the total energy, linear momentum, angular momentum, and dynamic energy moment found in problems 4.31, 4.32, 4.33, and 4.34 satisfy the Poincare algebra in problem 4.10.
- Let $J_{\mu\nu}$ be the antisymmetric rank 2 angular momentum tensor formed as in equation (4.10.60) from the angular momentum vector and dynamical energy moment vector. Show that in covariant form the Poincare algebra is:

$$\{p_\mu, p_\nu\} = 0$$

$$\begin{aligned}\{p_\mu, J_{\rho\sigma}\} &= p_\rho \eta_{\mu\sigma} - p_\sigma \eta_{\mu\rho} \\ \{J_{\mu\nu}, J_{\rho\sigma}\} &= \eta_{\nu\sigma} J_{\mu\rho} - \eta_{\mu\sigma} J_{\nu\rho} - \eta_{\nu\rho} J_{\mu\sigma} + \eta_{\mu\rho} J_{\nu\sigma}.\end{aligned}$$

Problem 4.82: ★ Covariant Conservation Laws and the Energy-Momentum Tensor.

- (a) Take the electromagnetic energy density $\mathcal{E}$ found in problem 4.31 and linear momentum density $\vec{\wp}$ and stress tensor $\hat{\sigma}$ found in problem 4.32. Show, using the Lorentz transformation properties of the electric and magnetic fields that these have the Lorentz transformation properties:

$$\begin{aligned}\mathcal{E}' &= \gamma^2 \mathcal{E} - (\gamma^2 - 1) \vec{l} \cdot \hat{\sigma} \cdot \vec{l} + 2\gamma^2 \vec{v} \cdot \vec{\wp} \\ \vec{\wp}' &= \gamma \vec{\wp} + (2\gamma + 1)(\gamma - 1) \vec{l} \vec{l} \cdot \vec{\wp} + \gamma^2 \mathcal{E} \vec{v} - \gamma \hat{\sigma} \cdot \vec{v} - \gamma(\gamma - 1) \vec{l} \cdot \hat{\sigma} \cdot \vec{l} \vec{v} \\ \hat{\sigma}' &= \hat{\sigma} + (\gamma - 1)(\vec{l} \vec{l}^T \hat{\sigma} + \hat{\sigma} \vec{l} \vec{l}^T) + (\gamma - 1)^2 (\vec{l} \cdot \hat{\sigma} \cdot \vec{l}) \vec{l} \vec{l}^T - \gamma \vec{\wp} \vec{v}^T - \gamma \vec{v} \vec{\wp}^T - 2\gamma(\gamma - 1)(\vec{v} \cdot \vec{\wp}) \vec{l} \vec{l}^T - \gamma^2 \mathcal{E} \vec{v} \vec{v}^T.\end{aligned}$$

Thus, these quantities all mix under Lorentz transformation and so should be thought of as part of one larger quantity in the relativistic theory.

- (b) Define the Energy-Momentum tensor $T^{\mu\nu}$ as having the components:

$$T^{00} = \mathcal{E}, \quad T^{0a} = T^{a0} = \wp^a, \quad T^{ab} = -\sigma^{ab}.$$

Equivalently, in block matrix form $T^{\mu\nu}$ is:

$$T^{\mu\nu} = \begin{pmatrix} \mathcal{E} & \vec{\wp} \\ \vec{\wp} & -\hat{\sigma} \end{pmatrix}^{\mu\nu}.$$

Show using the results of the previous part that this $T^{\mu\nu}$ in fact correctly transforms as a rank 2 tensor under Lorentz transformation and thus it is actually a tensor and the appropriate object that energy density, linear momentum density, and the stress tensor all belong to in the relativistic theory. The energy-momentum tensor in different sources is variously called the energy tensor, the stress-energy tensor, the stress-energy-momentum tensor, or even just the stress tensor (even though that name is already in use for $\hat{\sigma}$). We may sometimes call the energy-momentum tensor simply the “energy tensor” as our preferred shortening.

- (c) Show from the particular expressions for $\mathcal{E}, \vec{\wp}, \hat{\sigma}$ in terms of $\vec{E}$ and $\vec{B}$ that the electromagnetic energy-momentum tensor can be expressed covariantly as:

$$T^{\mu\nu} = -\mathcal{F}^{\mu\rho} \mathcal{F}_\rho{}^\nu - \eta^{\mu\nu} \frac{1}{4} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma}.$$

Show that this energy-momentum tensor is symmetric ($T^{\nu\mu} = T^{\mu\nu}$). Once we have some more mathematical tools, we will show that Lorentz invariance of a theory guarantees that it has a symmetric energy-momentum tensor.

- (d) Show that the continuity equations for energy and momentum from problems 4.31 and 4.32 can be expressed in terms of the electromagnetic energy-momentum tensor as:

$$\partial_\nu T^{\mu\nu} = -\mathcal{F}^{\mu\nu} J_\nu.$$

- (e) Show that the electromagnetic total energy and total linear momentum gotten by integrating their respective densities have the correct Lorentz transformation properties to form a 4-vector as expected for energy and momentum. To do so you will have to Lorentz transform a volume integral over all space.
- (f) Show by the same method used in this question to derive the energy-momentum tensor that the angular momentum density and dynamic mass moment density found in problems 4.33 and 4.34 and their associated conservation laws can be organized into a rank 3 “angular momentum current density tensor” $\mathcal{J}^\mu_{\alpha\beta}$ defined by:

$$\mathcal{J}^\mu_{\alpha\beta} = x_\alpha T^\mu{}_\beta - x_\beta T^\mu{}_\alpha$$

which satisfies:

$$\partial_\mu \mathcal{J}^\mu_{\alpha\beta} = (x_\alpha \mathcal{F}_{\mu\beta} - x_\beta \mathcal{F}_{\mu\alpha}) J^\mu.$$

and has the correct transformation properties for a rank 3 tensor.

4.11 Noether's Theorem (Version 2)

Electromagnetism is described by a local classical field theory. We found that our point particle theory of matter is sick, and we will find in part II that a single particle of matter is actually described by a local classical field theory. As well, later on in this part we will find that macroscopic matter (such as gases, fluids, solids) and gravity are also all well described by local classical field theory. Classical field theory is extremely important! The most important result in classical field theory is its generalization of Noether's theorem. In 1.10 we proved Noether's theorem version 1: any system with a continuous symmetry conserves the generator of that symmetry in time, and any conserved quantity of a system generates a continuous symmetry of that system. In this section we will repeat the logic of the argument used to prove the general Noether's theorem but apply it to the additional structure of a local classical field theory and find an even more powerful result. Although we will use the covariant notation in this section, the resulting theorem will not depend at all on relativity.

4.11.1 Field Canonical Transformations

First we need to understand the transformation properties of classical fields. Suppose we have a local classical field theory with fields $\phi^a(x)$ which has Lagrangian density $\mathcal{L}(x, \phi, \partial\phi)$. Here we have allowed the Lagrangian density to retain explicit dependence on $(t, \vec{x})$, even though if it does have such dependence it will break time and space translational symmetries. We have also only included terms in the Lagrangian density containing 1 or fewer derivatives on the fields. This is simply done to make the calculations shorter in this section and because it is typically all that is needed. If one needs higher derivative dependence in their theory, the arguments of this section can be completely generalized to accommodate that. As well, we will be agnostic as to whether this Lagrangian density is written in terms of only the canonical coordinate fields (meaning $\phi(x) = Q(x)$) of theory or is written in terms of both the canonical coordinate fields and their conjugate momenta fields (meaning $\phi(x) = (Q(x), P(x))$). Let $\mathbb{M}$ be a region of spacetime which consists of a volume of space $\mathbb{V}$ at each time between t_0 and t_f , so that the action of the theory on $\mathbb{M}$ is:

$$S_{\mathbb{M}}[\phi] = \int_{\mathbb{M}} \mathcal{L}(x, \phi, \partial\phi) d^4x. \quad (4.11.1)$$

If the integrand is written in terms of canonical coordinate fields only then this action is in the Lagrangian action form, as described in section 1.7, whereas if it is in terms of canonical coordinate and conjugate momenta fields then it is in the Hamiltonian action form. Much like in the arguments of section 1.8, which form is used will not matter here.

Suppose we have a local canonical transformation from our fields $\phi^a(x)$ into new fields $\phi'^a(x')$, generically transforming the coordinates as well. That is, we have some functions $x'(x, \phi)$ and $\phi'(x, \phi)$ so that:

$$x'^{\mu} = x'^{\mu}(x, \phi), \quad \phi'^a(x') = \phi'^a(x, \phi). \quad (4.11.2)$$

It is perfectly legal to include derivatives of ϕ in the functions defining x' and ϕ' , though doing so will generally add higher derivatives to the Lagrangian density under the transformation. Under this canonical transformation, $\phi'^a(x')$ will now be a field theory on a new region $\mathbb{M}'$ with some new action $S'_{\mathbb{M}'}[\phi']$. That action will be the integral of some new Lagrangian density $\mathcal{L}'(x', \phi', \partial\phi')$:

$$S'_{\mathbb{M}'}[\phi'] = \int_{\mathbb{M}'} \mathcal{L}'(x', \phi', \partial\phi') d^4x'. \quad (4.11.3)$$

Requiring that this is a canonical transformation, as explained in section 1.9, means that if $S'_{\mathbb{M}'}[\phi']$ were to be reexpressed as a functional of ϕ , then it would produce the same equations of motion as $S_{\mathbb{M}}[\phi]$. In order for it to do so, the two can only differ by a functional of the boundary conditions on ϕ , so that their functional derivatives on the interior of $\mathbb{M}$ agree. Thus, there must exist a functional $F_{\partial\mathbb{M}}[\phi]$ depending on ϕ only through its values on the boundary $\partial\mathbb{M}$ of the region $\mathbb{M}$ so that:

$$S'_{\mathbb{M}'}[\phi'] = S_{\mathbb{M}}[\phi] + F_{\partial\mathbb{M}}[\phi]. \quad (4.11.4)$$

A generic local functional $F_{\partial\mathbb{M}}[\phi]$ as described can be written as an integral over $\partial\mathbb{M}$ of some integrand vector field $f^{\mu}(x, \phi)$:

$$F_{\partial\mathbb{M}}[\phi] = \int_{\partial\mathbb{M}} f^{\mu}(x, \phi(x)) d\partial\mathbb{M}_{\mu} \quad (4.11.5)$$

where $d\partial\mathbb{M}_{\mu}$ is the outward pointing normal vector on $\partial\mathbb{M}$ which has magnitude given by the surface area

element of $\partial\mathbb{M}$. Equation (4.11.5) just states that $F_{\partial\mathbb{M}}$ depends in some generic way on the boundary data. Importantly, the vector field $f^\mu(x, \phi)$ is not unique, even for a given $F_{\partial\mathbb{M}}$. Consider two vector fields f'^μ and f^μ which differ by a divergence free vector field J^μ (meaning $f'^\mu = f^\mu + J^\mu$ and $\partial_\mu J^\mu = 0$). Then, using Stokes' theorem:

$$\int_{\partial\mathbb{M}} f'^\mu d\mathbb{M}_\mu = \int_{\partial\mathbb{M}} f^\mu d\mathbb{M}_\mu + \int_{\partial\mathbb{M}} J^\mu d\mathbb{M}_\mu = \int_{\partial\mathbb{M}} f^\mu d\mathbb{M}_\mu + \int_{\mathbb{M}} \partial_\mu J^\mu d^4x = \int_{\partial\mathbb{M}} f^\mu d\mathbb{M}_\mu. \quad (4.11.6)$$

Therefore, f^μ and f'^μ produce the same functional $F_{\partial\mathbb{M}}$. This argument also shows that if f'^μ and f^μ produce the same $F_{\partial\mathbb{M}}$ then their difference must be divergence free.

Every divergence free vector field J^μ (meaning $\partial_\mu J^\mu = 0$) can be expressed in the form:

$$J^\mu = \partial_\nu \chi^{\mu\nu} \quad (4.11.7)$$

for an antisymmetric tensor $\chi^{\mu\nu}$. To see this, consider a vector field A^μ which satisfies $-\partial^2 A^\mu = J^\mu$ with some divergence free initial conditions. We know such an A^μ exists because this is just the d'Alembert wave equation, which we can explicitly solve. Because $\partial_\mu J^\mu = 0$, it follows that $\partial_\mu A^\mu = 0$. From that A^μ , define $\chi^\mu = \partial^\mu A^\nu - \partial^\nu A^\mu$. Automatically this $\chi^{\mu\nu}$ is antisymmetric and satisfies $\partial_\nu \chi^{\mu\nu} = J^\mu$. It is no coincidence how closely this argument mirrors Maxwell's equations. Conversely, the vector field $\partial_\nu \chi^{\mu\nu}$ is automatically divergence free: $\partial_{\mu\nu}^2 \chi^{\mu\nu} = 0$, because $\chi^{\mu\nu}$ is antisymmetric. Therefore, for two vector fields f'^μ and f^μ which produce the same $F_{\partial\mathbb{M}}$, there must exist a tensor field $\chi^{\mu\nu}$ so that:

$$f'^\mu = f^\mu + \partial_\nu \chi^{\mu\nu}, \quad \chi^{\mu\nu} = -\chi^{\nu\mu}. \quad (4.11.8)$$

When the transformed action is reexpressed in terms of ϕ , it becomes:

$$S'_{\mathbb{M}'}[\phi'] = \int_{\mathbb{M}} \mathfrak{L}'(x', \phi', \partial\phi') \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| d^4x \quad (4.11.9)$$

by using the Jacobian transformation property of the integration measure d^4x . Returning this to (4.11.4) and using Stokes theorem gives:

$$\int_{\mathbb{M}} \mathfrak{L}'(x', \phi', \partial\phi') \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| = \int_{\mathbb{M}} (\mathfrak{L}(x, \phi, \partial\phi) + \partial_\mu f^\mu(x, \phi)) d^4x. \quad (4.11.10)$$

Because the field theory is local, this construction can be made for arbitrary region $\mathbb{M}$ and so we may equate the integrands themselves:

$$\mathfrak{L}'(x', \phi', \partial\phi') \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| = \mathfrak{L}(x, \phi, \partial\phi) + \partial_\mu f^\mu(x, \phi). \quad (4.11.11)$$

This is true whether the transformation of interest is to be a symmetry of our system or not. By the same argument given immediately before theorem 1.8, a transformation is a symmetry if and only if the transformed and untransformed fields have the same equation of motion functions. If this is so, we can take the Hamiltonian function is unchanged by the transformation and so the resulting Lagrangian and Lagrangian density are also unchanged through the Legendre transformation. Therefore, we have:

Theorem 4.6: Field Canonical Transformations

In a local classical field theory, the transformation:

$$x'^\mu = x'^\mu(x, \phi(x)), \quad \phi'^a(x') = \phi'^a(x, \phi(x)) \quad (4.11.12)$$

is canonical if and only if there exists a vector field $f^\mu(x, \phi)$ so that:

$$\mathfrak{L}'(x', \phi', \partial\phi') \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| = \mathfrak{L}(x, \phi, \partial\phi) + \partial_\mu f^\mu(x, \phi). \quad (4.11.13)$$

If such a vector field exists, it is not unique. Any two such vector fields f'^μ and f^μ must be related by:

$$f'^\mu = f^\mu + \partial_\nu \chi^{\mu\nu} \quad (4.11.14)$$

for some antisymmetric tensor field $\chi^{\mu\nu}$.

The transformation is a symmetry if and only if the transformed ($\mathfrak{L}'$) and untransformed ($\mathfrak{L}$) Lagrangian densities are the same function.

4.11.2 Noether's Current

Suppose now that we have a continuous 1-parameter family of local canonical transformations depending on the parameter ε so that $\varepsilon = 0$ corresponds to the identity transformation. That is, we have some functions $x'(\varepsilon, x, \phi)$ and $\phi'(\varepsilon, x, \phi)$ so that:

$$x'^\mu = x'^\mu(\varepsilon, x, \phi), \quad \phi'^a(x') = \phi'^a(\varepsilon, x, \phi). \quad (4.11.15)$$

We define the functions $\mathcal{D}x^\mu$ and $\mathcal{D}\phi^a$ by the ε derivative of this quantities at the identity:

$$\mathcal{D}x^\mu(x, \phi) \stackrel{\text{def}}{=} \left. \frac{\partial x'^\mu(\varepsilon, x, \phi)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}\phi^a(x, \phi) \stackrel{\text{def}}{=} \left. \frac{\partial \phi'^a(\varepsilon, x, \phi)}{\partial \varepsilon} \right|_{\varepsilon=0}. \quad (4.11.16)$$

For a generic quantity which depends on x' and $\phi'(x')$ we define $\mathcal{D}$ as its total ε derivative at fixed x and $\phi(x)$, evaluated at $\varepsilon = 0$.

The transformed Lagrangian density $\mathcal{L}'$ depends on ε in a nontrivial way in general in that $\mathcal{L}'(x', \phi', \partial\phi')$ will generally change its form as a function as ε is changed. So, we write $\mathcal{L}'(\varepsilon, x', \phi', \partial\phi')$ to explicitly indicate that $\mathcal{L}'$ changes directly with ε (as its functional form changes) and indirectly with ε (through the ε dependence of $x', \phi', \partial\phi'$). We will use the notation $\delta\mathcal{L}$ to indicate the change in the form of $\mathcal{L}'$ as a function as ε is changed near the identity. That is, we define:

$$\delta\mathcal{L} \stackrel{\text{def}}{=} \frac{\partial}{\partial \varepsilon} \mathcal{L}'(\varepsilon, x', \phi', \partial\phi')|_{\varepsilon=0} \quad (4.11.17)$$

where the partial derivative is taken at fixed $x', \phi', \partial\phi'$.

To avoid ambiguity with explicit x^μ dependence in $\mathcal{L}$ and implicit x^μ dependence through the fields, define the derivative:

$$\tilde{\partial}_\mu \mathcal{L}(x, \phi, \partial\phi) \stackrel{\text{def}}{=} \lim_{h \rightarrow 0} \frac{\mathcal{L}(x + h\vec{e}_\mu, \phi, \partial\phi) - \mathcal{L}(x, \phi, \partial\phi)}{h} \quad (4.11.18)$$

to be only the explicit x^μ derivative of $\mathcal{L}$. Then, the total x^μ derivative of the Lagrangian density is:

$$\partial_\mu \mathcal{L} = \tilde{\partial}_\mu \mathcal{L} + \frac{\partial \mathcal{L}}{\partial \phi^a} \partial_\mu \phi^a + \frac{\partial \mathcal{L}}{\partial \partial_\nu \phi^a} \partial_{\mu\nu}^2 \phi^a. \quad (4.11.19)$$

It is also useful to define the ε derivative at fixed x for the fields:

$$\mathcal{D}\phi^a|_x \stackrel{\text{def}}{=} \frac{\partial}{\partial \varepsilon} \phi'^a(x)|_{\varepsilon=0}. \quad (4.11.20)$$

Using the chain rule:

$$\frac{\partial}{\partial \varepsilon} \phi'^a(x')|_{\varepsilon=0} = \frac{\partial}{\partial \varepsilon} \phi'^a(x)|_{\varepsilon=0} + \frac{\partial \phi^a}{\partial x^\mu} \frac{\partial x'^\mu}{\partial \varepsilon} \Big|_{\varepsilon=0} \quad (4.11.21)$$

$$\implies \mathcal{D}\phi^a = \mathcal{D}\phi^a|_x + \partial_\mu \phi^a \mathcal{D}x^\mu. \quad (4.11.22)$$

The ε derivative at fixed x automatically commutes with x^μ derivatives because it doesn't change x . So:

$$\partial_\mu \mathcal{D}\phi^a|_x = \mathcal{D} \partial_\mu \phi^a|_x. \quad (4.11.23)$$

With these pieces together, the the total ε derivative of $\mathcal{L}'$ evaluated at $\varepsilon = 0$ gives:

$$\mathcal{D}\mathcal{L} = \delta\mathcal{L} + \tilde{\partial}_\mu \mathcal{L} \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \partial_\mu \phi^a \quad (4.11.24)$$

$$= \delta\mathcal{L} + \left(\partial_\mu \mathcal{L} - \frac{\partial \mathcal{L}}{\partial \phi^a} \partial_\mu \phi^a - \frac{\partial \mathcal{L}}{\partial \partial_\nu \phi^a} \partial_{\mu\nu}^2 \phi^a \right) \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \partial_\mu \phi^a \quad (4.11.25)$$

$$= \delta\mathcal{L} + \partial_\mu \mathcal{L} \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a|_x + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \partial_\mu \phi^a|_x \quad (4.11.26)$$

$$= \delta\mathcal{L} + \left(\frac{\partial \mathcal{L}}{\partial \phi^a} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \right) \mathcal{D}\phi^a|_x + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \mathcal{D}\phi^a|_x + \mathcal{L} \mathcal{D}x^\mu \right) - \mathcal{L} \partial_\mu \mathcal{D}x^\mu. \quad (4.11.27)$$

Because the transformation is canonical for each ε , by theorem 4.6 there will exist a vector field $f^\mu(\varepsilon, x, \phi(x))$ so that:

$$\mathcal{L}'(\varepsilon, x', \phi', \partial\phi') \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) = \mathcal{L}(x, \phi, \partial\phi) + \partial_\mu f^\mu(\varepsilon, x, \phi). \quad (4.11.28)$$

The Jacobian determinant will necessarily be positive in the neighborhood of $\varepsilon = 0$ because at $\varepsilon = 0$ it is equal to 1, therefore we can drop the absolute value around it. Now we would like to take the derivative

of this expression at $\varepsilon = 0$. Doing so requires that we know how to differentiate the coordinate Jacobian determinant, which is inconvenient. In section 5.2, specifically in equation (5.2.30), we will prove that for a matrix $M(\varepsilon)$ dependent on a parameter ε :

$$\frac{d}{d\varepsilon} \det(M) = \text{Tr} \left(M^{-1} \frac{dM}{d\varepsilon} \right) \det M. \quad (4.11.29)$$

Here we will just take this result for granted. Then, taking our matrix to have components:

$$M^\mu{}_\nu = \frac{\partial x'^\mu(\varepsilon, x, \phi(x))}{\partial x^\nu} \quad (4.11.30)$$

we have:

$$\frac{\partial}{\partial \varepsilon} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) = \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial^2 x'^\mu(\varepsilon, x, \phi(x))}{\partial \varepsilon \partial x^\nu} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \quad (4.11.31)$$

$$\Rightarrow \frac{\partial}{\partial \varepsilon} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \Big|_{\varepsilon=0} = \partial_\mu \mathcal{D} x^\mu. \quad (4.11.32)$$

Now taking the ε derivative of (4.11.28) at fixed $x, \phi(x)$:

$$\mathcal{D} \mathfrak{L} \det \left(\frac{\partial x'}{\partial x} \right) \Big|_{\varepsilon=0} + \mathfrak{L} \frac{\partial}{\partial \varepsilon} \det \left(\frac{\partial x'}{\partial x} \right) \Big|_{\varepsilon=0} = \partial_\mu \mathcal{D} f^\mu \quad (4.11.33)$$

$$\Rightarrow \mathcal{D} \mathfrak{L} = \partial_\mu \mathcal{D} f^\mu - \mathfrak{L} \partial_\mu \mathcal{D} x^\mu. \quad (4.11.34)$$

Then, combining this with (4.11.27):

$$\delta \mathfrak{L} + \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} - \partial_\mu \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \right) \mathcal{D} \phi^a|_x + \partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \phi^a|_x + \mathfrak{L} \mathcal{D} x^\mu - \mathcal{D} f^\mu \right) = 0. \quad (4.11.35)$$

Equation (4.11.35) is true for all field configurations (we have not assumed that the equations of motion are satisfied) and is true whether the transformation of interest is a symmetry or not. Under the actual dynamics of the system (meaning applying the equations of motion), if the transformation is a symmetry (and thus $\delta \mathfrak{L} = 0$) we have:

$$\partial_\mu \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \phi^a|_x + \mathfrak{L} \mathcal{D} x^\mu - \mathcal{D} f^\mu \right) = 0. \quad (4.11.36)$$

Therefore, the current density J^μ , called the Noether current for this transformation, defined by:

$$J^\mu = \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \phi^a|_x + \mathfrak{L} \mathcal{D} x^\mu - \mathcal{D} f^\mu \quad (4.11.37)$$

is divergence free under the equations of motion if and only if the transformation is a symmetry of the action. Generally $\mathcal{D} \phi^a$ is simpler than the fixed x variation, and so it is useful to express the Noether current in terms of it rather than $\mathcal{D} \phi^a|_x$. Doing so:

$$J^\mu = \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D} \phi^a + \left(\mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a \right) \mathcal{D} x^\nu - \mathcal{D} f^\mu \quad (4.11.38)$$

Recall that the vanishing 4-divergence of a vector field is actually just the continuity equation for its time component:

$$\partial_\mu J^\mu = \frac{\partial J^0}{\partial t} + \nabla \cdot \vec{J} = 0. \quad (4.11.39)$$

Therefore, if J^μ is divergence free, the integral of J^0 over all space is conserved. J^0 only depends on $\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a}$ through its time component $\frac{\partial \mathfrak{L}}{\partial \phi^a}$. For a field in the list of ϕ which is a canonical coordinate field Q^a , this combination is simply its conjugate momentum field P_a . For a field in the list of ϕ which is a canonical momentum field P_a , the Lagrangian density does not depend on $\dot{P}_a$ by the definition of the Lagrangian density. Therefore:

$$\frac{\partial \mathfrak{L}}{\partial \partial_0 \phi^a} \mathcal{D} \phi^a = P_a \mathcal{D} Q^a, \quad \frac{\partial \mathfrak{L}}{\partial \partial_0 \phi^a} \partial_\nu \phi^a = P_a \partial_\nu Q^a. \quad (4.11.40)$$

Integrating J^0 over all space:

$$\int_{\mathbb{S}} J^0 d\mathbb{S} = \int_{\mathbb{S}} \left(P_a (\mathcal{D} Q^a - \nabla Q^a \cdot \mathcal{D} \vec{x}) - \left(\frac{\partial \mathfrak{L}}{\partial \dot{Q}^a} \dot{Q}^a - \mathfrak{L} \right) \mathcal{D} t - \mathcal{D} f^0 \right) d\mathbb{S} \quad (4.11.41)$$

$$= \int_{\mathbb{S}} \left(P_a \frac{\partial Q'^a(t', \vec{x})}{\partial \varepsilon} \right) \Big|_{\varepsilon=0} - H \mathcal{D}t - \mathcal{D}f^0 \Big) d\mathbb{S} \quad (4.11.42)$$

where H is the Hamiltonian density. This last expression is precisely the original formula we had for the generator G of the transformation in the original version of Noether's theorem! Thus:

$$G = \int_{\mathbb{S}} \mathcal{J}^0 d\mathbb{S} \quad (4.11.43)$$

is the generator of the continuous transformation. Because the theory is local, the generator is not only globally conserved as found in the original Noether's theorem, but locally conserved in the sense that its density satisfies a continuity equation. When an equation is valid only when the equations of motion are applied, that equation is said to hold **on-shell**. An equation which is true independent of the equations of motion holding is said to be **off-shell**. Because our interest in the Noether current is through its conservation law, which is only valid on-shell, two Noether currents which are equal on-shell are considered equivalent.

If the transformation is a symmetry of the action then we can replace the function $\mathcal{L}'$ with the function $\mathcal{L}$ in equation (4.11.28). Then, the ε derivative near the identity of that equation becomes:

$$\frac{\partial}{\partial \varepsilon} \left(\mathcal{L}(x', \phi', \partial \phi') \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right) \Big|_{\varepsilon=0} = \partial_\mu \mathcal{D}f^\mu(x, \phi). \quad (4.11.44)$$

Conversely, if a $\mathcal{D}f^\mu(x, \phi)$ can be identified so that this is true, then the transformation is a symmetry of the action. Altogether we have:

Theorem 4.7: Noether's Theorem – Local Conservation

For a continuous transformation $x' = x'(\varepsilon, x, \phi)$, $\phi'(x') = \phi'(\varepsilon, x, \phi)$ (with parameter ε so that $\varepsilon = 0$ corresponds to the identity transformation) so that:

$$S'_{\mathbb{M}'}[\phi'] - S_{\mathbb{M}}[\phi] = \int_{\partial \mathbb{M}} f^\mu(\varepsilon, x, \phi(x)) d\partial \mathbb{M}_\mu \quad (4.11.45)$$

over any region of spacetime $\mathbb{M}$, the Noether current of that transformation is given by:

$$J^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \mathcal{D}\phi^a + \left(\mathcal{L} \delta_\nu^\mu - \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a \right) \mathcal{D}x^\nu - \mathcal{D}f^\mu \quad (4.11.46)$$

where:

$$\mathcal{D}x^\mu(x, \phi) = \frac{\partial x'^\mu(\varepsilon, x, \phi)}{\partial \varepsilon} \Big|_{\varepsilon=0}, \quad \mathcal{D}\phi^a(x, \phi) = \frac{\partial \phi'^a(\varepsilon, x, \phi)}{\partial \varepsilon} \Big|_{\varepsilon=0}, \quad \mathcal{D}f^\mu = \frac{\partial f^\mu(\varepsilon, x, \phi)}{\partial \varepsilon} \Big|_{\varepsilon=0}. \quad (4.11.47)$$

The definition of $\mathcal{D}f^\mu$ is not unique and may be modified by:

$$\mathcal{D}f'^\mu = \mathcal{D}f^\mu + \partial_\nu \chi^{\mu\nu} \quad (4.11.48)$$

for any antisymmetric tensor field $\chi^{\mu\nu}$. The phase space generator of the transformation is given by:

$$G = \int_{\mathbb{S}} J^0 d\mathbb{S}. \quad (4.11.49)$$

The on-shell divergence of the Noether current is given by:

$$\partial_\mu J^\mu = -\delta \mathcal{L} \quad (4.11.50)$$

where $\delta \mathcal{L}$ is the rate of change of the functional form of the Lagrangian density under the transformation. Hence, the Noether current is locally conserved if and only if the transformation is a symmetry of the action.

The symmetry condition is equivalent to requiring the existence of a function $\mathcal{D}f^\mu(x, \phi)$ so that:

$$\frac{\partial}{\partial \varepsilon} \left(\mathcal{L}(x', \phi', \partial \phi') \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right) \Big|_{\varepsilon=0} = \partial_\mu \mathcal{D}f^\mu(x, \phi). \quad (4.11.51)$$

Equivalently, a continuous transformation is a symmetry if and only if when the untransformed action is evaluated at the transformed fields the result differs from the untransformed action evaluated at the untransformed fields only by a functional of the boundary conditions.

4.11.3 Existence of a Poincare Invariant Action

Suppose we have a local classical field theory with fields ϕ^a which are all tensor fields. Suppose that the field theory has symmetry under the connected Poincare group (spacetime translations, Lorentz boosts, and rotations). Let $F_a(\phi, \partial\phi, \partial^2\phi)$ be the equation of motion functions for our fields:

$$F_a(\phi, \partial\phi, \partial^2\phi) = \frac{\delta S}{\delta \phi^a}. \quad (4.11.52)$$

We have omitted possible explicit x dependence in F_a because of spacetime translational symmetry. A Lorentz transformation is a local change of configuration coordinates of our fields. For a tensor of any rank, the Lorentz transformation property of that tensor is linear. Therefore, by assuming all of our fields are tensors, we have that under a Lorentz transformation for some matrix U^a_b which does not depend on x or ϕ :

$$x'^\mu = L^\mu_\nu x^\nu, \quad \phi'^a(x') = U^a_b \phi^b(x). \quad (4.11.53)$$

Because of the functional chain rule, under such a local change of fields we have:

$$\delta S = \int F_a(\phi, \partial\phi, \partial^2\phi) \delta \phi^a(x) d^4x = \int F'_a(\phi', \partial'\phi', \partial'^2\phi') \delta \phi'^a(x') d^4x' \quad (4.11.54)$$

$$\implies F_a(\phi, \partial\phi, \partial^2\phi) = F'_b(\phi', \partial'\phi', \partial'^2\phi') U^b_a \quad (4.11.55)$$

where we have used that $d^4x' = d^4x$ because $\det L = 1$. Evaluating this with $\phi(x)$ replaced by $\lambda\phi(x)$ for a constant λ and then contracting this with $\phi^a(x)$, we find:

$$F_a(\lambda\phi, \lambda\partial\phi, \lambda\partial^2\phi) \phi^a = F'_a(\lambda\phi', \lambda\partial'\phi', \lambda\partial'^2\phi') \phi'^a. \quad (4.11.56)$$

If we now field this into (3.2.30), we have that:

$$\mathfrak{L} = \int_0^1 \phi^a F_a(\lambda\phi, \lambda\partial\phi, \lambda\partial^2\phi) d\lambda \quad (4.11.57)$$

is a valid Lagrangian density for this theory (meaning it produces the correct equation of motion functions) and this Lagrangian density is invariant under the entire connected Poincare group. Therefore, we see:

Theorem 4.8: Poincare Invariance of the Lagrangian Density

Suppose a local classical field theory has fields $\phi^a(x)$ which are all tensor fields and that the theory has symmetry under the connected Poincare group. Then, there exists a gauge of the action so that the Lagrangian density of the theory is invariant under spacetime translations, rotations, and Lorentz boosts.

4.11.4 Energy-Momentum Tensor

There are a few important special cases of Noether's theorem. Consider spacetime translational symmetry. We know from theorem 3.1 that under such a symmetry, we can make the Lagrangian density have no explicit dependence on the coordinates. Therefore, such a symmetry implies we can take:

$$\partial_\mu \mathfrak{L} = 0. \quad (4.11.58)$$

Under a spacetime translation, the coordinates change by:

$$x'^\mu = x^\mu + \varepsilon a^\mu \quad (4.11.59)$$

where a^μ is the unit vector in the relevant direction of transformation. As well, the fields do not change at all as they are simply transported to their new locations:

$$\phi'^a(x') = \phi^a(x). \quad (4.11.60)$$

Therefore:

$$\mathcal{D}x^\mu = a^\mu, \quad \mathcal{D}\phi^a = 0. \quad (4.11.61)$$

Under such a transformation, (4.11.51) becomes:

$$a^\mu \partial_\mu \mathfrak{L} = \partial_\mu \mathcal{D}f^\mu \quad (4.11.62)$$

which vanishes by (4.11.58). So, $\partial_\mu \mathcal{D}f^\mu = 0$ and the general solution for $\mathcal{D}f^\mu$ becomes:

$$\mathcal{D}f^\mu = \partial_\nu \chi^{\mu\nu} \quad (4.11.63)$$

for some antisymmetric tensor field $\chi^{\mu\nu}$. For each of the 4 independent directions (meaning setting $a^\mu = \delta^\mu_{\nu_*}$ for ν_* a fixed number), we can define:

$$\Theta^{\rho\mu}_{\nu_*} = \chi^{\rho\mu}|_{a^\sigma = \delta^\sigma_{\nu_*}}. \quad (4.11.64)$$

Then, generically:

$$\chi^{\rho\mu} = \Theta^{\rho\mu}_{\nu} a^\nu \quad (4.11.65)$$

where $\Theta^{\rho\mu}_{\nu}$ is now a rank-3 tensor which is antisymmetric in its first two indices. Therefore, by theorem 4.7, the conserved Noether current for a system with translational symmetry in the a^μ direction is:

$$J^\mu = \left(\mathfrak{L} \delta^\mu_{\nu} - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a + \partial_\rho \Theta^{\rho\mu}_{\nu} \right) a^\nu. \quad (4.11.66)$$

The rank-2 tensor multiplying a^ν in this expression is known as the **Energy-Momentum Tensor** T^μ_{ν} :

$$T^\mu_{\nu} = \mathfrak{L} \delta^\mu_{\nu} - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a + \partial_\rho \Theta^{\rho\mu}_{\nu}. \quad (4.11.67)$$

Translational symmetry in the a^ν direction guarantees:

$$\partial_\mu (T^\mu_{\nu} a^\nu) = 0 \quad (4.11.68)$$

while full spacetime translational symmetry guarantees:

$$\partial_\mu T^\mu_{\nu} = 0. \quad (4.11.69)$$

Because the integral of $T^0_{\nu} a^\nu$ over all space gives the generator of translations in the a^ν direction, the total momentum 4-vector of the system is given by:

$$p_\mu = \int_{\mathbb{S}} T^0_{\mu} d\mathbb{S} \quad (4.11.70)$$

which is why T^μ_{ν} is associated with energy and momentum. This integral implies that $-T^0_0$ is the energy density of the system and T^0_a is the linear momentum density of the system. We introduced the energy-momentum tensor previously in problem 4.82 and we will see shortly how the two do in fact coincide. In a generic theory, if all that is known is that the theory is spacetime translationally invariant, there is no natural special choice for tensor field $\Theta^{\rho\mu}_{\nu}$.

Very often our theories of interest will have not just spacetime translational symmetry but also Lorentz symmetry, so that the theory together has symmetry under the full connected Poincare group. Let us now study the Noether current corresponding to Lorentz symmetry. By Theorem 4.8, we can take the Lagrangian density of the theory to be invariant under the connected Poincare group, and thus possess no explicit dependence on x and be a Lorentz scalar. Under a Lorentz transformation by transformation parameters $\varepsilon^{\alpha\beta}$, the coordinates change according to (4.9.1), (4.10.50), and (4.10.53):

$$x'^\mu = L^\mu_{\nu} x^\nu = \left(e^{\varepsilon^{\alpha\beta} J_{\alpha\beta}} \right)^\mu_{\nu} x^\nu = x^\mu + \varepsilon^{\alpha\beta} (x_\alpha \delta^\mu_\beta - x_\beta \delta^\mu_\alpha) + \mathcal{O}(\varepsilon^2) \quad (4.11.71)$$

$$\implies \mathcal{D} x^\mu = \theta^{\alpha\beta} (x_\alpha \delta^\mu_\beta - x_\beta \delta^\mu_\alpha). \quad (4.11.72)$$

The fields may transform however they happen to transform under a Lorentz transformation. In general, that transformation can be expanded in powers of $\theta^{\alpha\beta}$ so that we define $\mathcal{D}_{\alpha\beta} \phi^a$ to be antisymmetric in exchanging α and β and to satisfy:

$$\phi'^a(x') = \phi^a(x) + \varepsilon^{\alpha\beta} \mathcal{D}_{\alpha\beta} \phi^a + \mathcal{O}(\varepsilon^2) \quad (4.11.73)$$

$$\implies \mathcal{D} \phi^a = \theta^{\alpha\beta} \mathcal{D}_{\alpha\beta} \phi^a. \quad (4.11.74)$$

Because we assume the Lagrangian density is a Lorentz scalar and has spacetime translational symmetry, (4.11.51) becomes:

$$\partial_\mu \mathcal{D} f^\mu = 0 \quad (4.11.75)$$

which again is solved by:

$$\mathcal{D} f^\mu = \partial_\nu \chi^{\mu\nu} \quad (4.11.76)$$

for a generic antisymmetric tensor $\chi^{\mu\nu}$. For each of the 6 independent Lorentz transformation directions (meaning setting $\theta^{\alpha\beta} = \frac{1}{2}(\delta^\alpha_{\mu_*} \delta^\beta_{\nu_*} - \delta^\alpha_{\nu_*} \delta^\beta_{\mu_*})$ for μ_*, ν_* fixed numbers), we can define:

$$\Phi^{\rho\sigma}_{\mu_*\nu_*} = \chi^{\rho\sigma}|_{\theta^{\alpha\beta} = \frac{1}{2}(\delta^\alpha_{\mu_*} \delta^\beta_{\nu_*} - \delta^\alpha_{\nu_*} \delta^\beta_{\mu_*})}. \quad (4.11.77)$$

Then, generically:

$$\chi^{\rho\sigma} = -\Phi^{\rho\sigma}_{\alpha\beta}\theta^{\alpha\beta} \quad (4.11.78)$$

where $\Phi^{\rho\sigma}_{\alpha\beta}$ is now a rank-4 tensor which is antisymmetric in its first two indices and antisymmetric in its last two indices. By theorem 4.7, the conserved Noether current for a system with Lorentz symmetry in the $\theta^{\alpha\beta}$ direction is:

$$J^\mu = \left(\frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D}_{\alpha\beta} \phi^a + x_\alpha \left(\mathfrak{L} \delta^\mu_\beta - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\beta \phi^a \right) - x_\beta \left(\mathfrak{L} \delta^\mu_\alpha - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\alpha \phi^a \right) + \partial_\nu \Phi^{\mu\nu}_{\alpha\beta} \right) \theta^{\alpha\beta}. \quad (4.11.79)$$

The rank-3 tensor multiplying $\theta^{\alpha\beta}$ in this expression is known as the **Angular-Momentum Current Tensor** $\mathcal{J}^\mu_{\alpha\beta}$:

$$\mathcal{J}^\mu_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D}_{\alpha\beta} \phi^a + x_\alpha \left(\mathfrak{L} \delta^\mu_\beta - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\beta \phi^a \right) - x_\beta \left(\mathfrak{L} \delta^\mu_\alpha - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\alpha \phi^a \right) + \partial_\nu \Phi^{\mu\nu}_{\alpha\beta}. \quad (4.11.80)$$

Symmetry under Lorentz transformations in the $\theta^{\alpha\beta}$ direction guarantees:

$$\partial_\mu (\mathcal{J}^\mu_{\alpha\beta} \theta^{\alpha\beta}) = 0 \quad (4.11.81)$$

while full Lorentz invariance of the theory guarantees:

$$\partial_\mu \mathcal{J}^\mu_{\alpha\beta} = 0. \quad (4.11.82)$$

Because the integral of $\mathcal{J}^0_{\alpha\beta} \theta^{\alpha\beta}$ over all space gives the generator of Lorentz transformations in the $\theta^{\alpha\beta}$ direction, the total angular momentum tensor of the system is given by:

$$J_{\alpha\beta} = \int_{\mathbb{S}} \mathcal{J}^0_{\alpha\beta} d\mathbb{S}. \quad (4.11.83)$$

The angular momentum current tensor has three parts in its expression, the part due to $\mathcal{D}_{\alpha\beta} \phi^a$, the two terms proportional to x^μ which also almost contain a factor of the energy-momentum tensor, and the arbitrary piece $\partial_\nu \Phi^{\mu\nu}_{\alpha\beta}$.

The Poincare invariance of our Lagrangian density allows us to identify nice canonical choices for $\Theta^{\rho\mu}_\nu$ in the energy-momentum tensor and $\Phi^{\mu\nu}_{\alpha\beta}$ in the angular momentum current tensor, in the sense of making both tensors as simple as possible. Define the **spin current tensor** $S^\mu_{\alpha\beta}$ by:

$$S^\mu_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D}_{\alpha\beta} \phi^a. \quad (4.11.84)$$

This is named so because the part of the angular momentum current which is associated to only transforming the fields and not the coordinates. However, it is important to note that there is not a local gauge invariant distinction between spin angular momentum density and orbital angular momentum density because pieces in $\Phi^{\mu\nu}_{\alpha\beta}$ can shuffle terms between the two (one would tend to think of spin angular momentum as the coordinate origin independent piece of the angular momentum and orbital as the origin dependent piece; these distinction is not locally gauge invariant). There is a gauge invariant definition of total spin angular momentum (see problem 4.44 for the result in electromagnetism) however it is nonlocal in the sense that it cannot be written as the spatial integral of a function of the fields and a finite number of derivatives at a single point.

It is also useful to define the Noether stress tensor N^μ_ν by:

$$N^\mu_\nu = \mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a. \quad (4.11.85)$$

This way, the energy-momentum tensor and angular momentum current tensor can be written as:

$$T^\mu_\nu = N^\mu_\nu + \partial_\rho \Theta^{\rho\mu}_\nu \quad (4.11.86)$$

$$\mathcal{J}^\mu_{\alpha\beta} = S^\mu_{\alpha\beta} + x_\alpha N^\mu_\beta - x_\beta N^\mu_\alpha + \partial_\nu \Phi^{\mu\nu}_{\alpha\beta}. \quad (4.11.87)$$

In terms of the Noether stress tensor, the conservation law of the energy-momentum tensor becomes:

$$\partial_\nu N^\mu_\nu = 0. \quad (4.11.88)$$

In terms of the spin current tensor, the conservation law of the angular momentum current becomes:

$$\partial_\mu S^\mu_{\alpha\beta} = N_{\beta\alpha} - N_{\alpha\beta}. \quad (4.11.89)$$

This may also be written as:

$$\frac{N^{\mu\nu} + N^{\nu\mu}}{2} = N^{\mu\nu} + \frac{1}{2} \partial_\rho S^{\rho\mu\nu}. \quad (4.11.90)$$

The combination on the left-hand side is by constructing symmetric under interchanging μ and ν , and so the right-hand side is symmetric as well even though it is not manifest. This equation remains symmetric under adding symmetric terms and so:

$$\frac{N^{\mu\nu} + N^{\nu\mu}}{2} + \frac{1}{2}\partial_\rho S^{\mu\nu\rho} + \frac{1}{2}\partial_\rho S^{\nu\mu\rho} = N^{\mu\nu} + \frac{1}{2}\partial_\rho (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (4.11.91)$$

is also a symmetric tensor. The combination of spin current tensors inside the derivative on the right-hand side is antisymmetric under exchanging ρ and μ :

$$S^{\mu\rho\nu} + S^{\rho\nu\mu} + S^{\nu\rho\mu} = -S^{\mu\nu\rho} - S^{\rho\mu\nu} - S^{\nu\mu\rho} \quad (4.11.92)$$

and so we can take by definition:

$$\Theta^{\rho\mu\nu} = \frac{1}{2}(S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (4.11.93)$$

as it satisfies the necessary antisymmetry in ρ and μ . With this choice of Θ , the resulting energy-momentum tensor is:

$$T^{\mu\nu} = \mathfrak{L}\eta^{\mu\nu} - \frac{\partial\mathfrak{L}}{\partial\partial_\mu\phi^a}\partial^\nu\phi^a + \frac{1}{2}\partial_\rho(S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (4.11.94)$$

which by (4.11.91) is symmetric. This choice of definition of the energy-momentum tensor is called the Belinfante-Rosenfeld energy-momentum tensor and we will see in chapter 7 that in a Poincare invariant theory it really is the only natural choice of definition.

With this definition of $T^{\mu\nu}$, the angular momentum current tensor can be rewritten as:

$$\mathcal{J}^{\mu\alpha\beta} = x^\alpha T^{\mu\beta} - x^\beta T^{\mu\alpha} + S^{\mu\alpha\beta} - \frac{1}{2}x^\alpha\partial_\nu(S^{\nu\mu\beta} + S^{\mu\beta\nu} + S^{\beta\mu\nu}) + \frac{1}{2}x^\beta\partial_\nu(S^{\nu\mu\alpha} + S^{\mu\alpha\nu} + S^{\alpha\mu\nu}) + \partial_\nu\Phi^{\mu\nu\alpha\beta}. \quad (4.11.95)$$

With some algebra, the appearing factors of x^μ can all be pushed inside of the partial derivatives in exchange for some extra terms. Simplifying gives:

$$\mathcal{J}^{\mu\alpha\beta} = x^\alpha T^{\mu\beta} - x^\beta T^{\mu\alpha} + \partial_\nu \left(\Phi^{\mu\nu\alpha\beta} - \frac{1}{2}x^\alpha(S^{\nu\mu\beta} + S^{\mu\beta\nu} + S^{\beta\mu\nu}) + \frac{1}{2}x^\beta(S^{\nu\mu\alpha} + S^{\mu\alpha\nu} + S^{\alpha\mu\nu}) \right). \quad (4.11.96)$$

Then, choose $\Phi^{\mu\nu\alpha\beta}$ as:

$$\Phi^{\mu\nu\alpha\beta} = \frac{1}{2}x^\alpha(S^{\nu\mu\beta} + S^{\mu\beta\nu} + S^{\beta\mu\nu}) - \frac{1}{2}x^\beta(S^{\nu\mu\alpha} + S^{\mu\alpha\nu} + S^{\alpha\mu\nu}) \quad (4.11.97)$$

which does in fact have the required antisymmetry in μ and ν as well as in α and β , and so this is a legal choice of Φ . The resulting angular momentum current tensor is then simply:

$$\mathcal{J}^\mu_{\alpha\beta} = x_\alpha T^\mu_\beta - x_\beta T^\mu_\alpha \quad (4.11.98)$$

and angular momentum local conservation law simply gives:

$$T^{\mu\nu} = T^{\nu\mu}. \quad (4.11.99)$$

Thus, we have:

Theorem 4.9: Belinfante-Rosenfeld Theorem – Special Relativity

If the Lagrangian density of a local classical field theory has no explicit coordinate dependence, then the energy-momentum tensor:

$$T^\mu_\nu = \mathfrak{L}\delta^\mu_\nu - \frac{\partial\mathfrak{L}}{\partial\partial_\mu\phi^a}\partial_\nu\phi^a + \partial_\rho\Theta^{\rho\mu}_\nu \quad (4.11.100)$$

satisfies the local conservation law:

$$\partial_\mu T^\mu_\nu = 0. \quad (4.11.101)$$

$\Theta^{\rho\mu}_\nu$ is an arbitrary rank-3 tensor field which is antisymmetric in its first two indices.

If the Lagrangian density of that theory is additionally Lorentz invariant, then $\Theta^{\rho\mu}_\nu$ may be chosen

so that the energy-momentum tensor becomes:

$$T^\mu{}_\nu = \mathfrak{L}\delta^\mu{}_\nu - \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \partial_\nu \phi^a + \frac{1}{2} \partial_\rho (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (4.11.102)$$

where $S^\mu{}_{\alpha\beta}$ is the spin current tensor defined by:

$$S^\mu{}_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \partial_\mu \phi^a} \mathcal{D}_{\alpha\beta} \phi^a \quad (4.11.103)$$

and $\mathcal{D}_{\alpha\beta} \phi^a = -\mathcal{D}_{\beta\alpha} \phi^a$ is the rate of change of the fields near the identity under a Lorentz transformation with parameters $\theta^{\alpha\beta}$:

$$\phi'^a(x') = \phi^a(x) + \theta^{\alpha\beta} \mathcal{D}_{\alpha\beta} \phi(x) + \mathcal{O}(\theta^2). \quad (4.11.104)$$

Then, the angular momentum current tensor can be taken to be:

$$\mathcal{J}^\mu{}_{\alpha\beta} = x_\alpha T^\mu{}_\beta - x_\beta T^\mu{}_\alpha. \quad (4.11.105)$$

Lorentz symmetry guarantees that the angular momentum current tensor satisfies the local conservation law:

$$\partial_\mu \mathcal{J}^\mu{}_{\alpha\beta} = 0 \quad (4.11.106)$$

and equivalently that the energy-momentum tensor is symmetric:

$$T^{\mu\nu} = T^{\nu\mu}. \quad (4.11.107)$$

Let us now look at the energy-momentum tensor of electromagnetism. From the Lagrangian density for Maxwell's equations:

$$\mathfrak{L} = -\frac{1}{4} \mathcal{F}^{\mu\nu} \mathcal{F}_{\mu\nu} \quad (4.11.108)$$

using:

$$\frac{\partial \mathfrak{L}}{\partial \partial_\nu A_\mu} = \mathcal{F}^{\mu\nu} \quad (4.11.109)$$

the Noether stress tensor is:

$$N^\mu{}_\nu = \mathfrak{L}\delta^\mu{}_\nu - \frac{\partial \mathfrak{L}}{\partial \partial_\mu A_\rho} \partial_\nu A_\rho = -\mathcal{F}^{\rho\mu} \partial_\nu A_\rho - \frac{1}{4} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma} \delta^\mu{}_\nu \quad (4.11.110)$$

which is not gauge invariant. The Lagrangian density is manifestly a Lorentz scalar, because it is formed out of contractions of all indices of Lorentz tensors. Because the vector potential A_μ is a vector field, under a Lorentz transformation:

$$A'_\mu(x') = L_\mu{}^\nu A_\nu(x) = A_\mu(x) + \theta^{\alpha\beta} (A_\alpha \eta_{\beta\mu} - A_\beta \eta_{\alpha\mu}) + \mathcal{O}(\theta^2) \quad (4.11.111)$$

$$\implies \mathcal{D}_{\alpha\beta} A_\mu = A_\alpha \eta_{\beta\mu} - A_\beta \eta_{\alpha\mu}. \quad (4.11.112)$$

Therefore, the spin current tensor is:

$$S^\mu{}_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \partial_\mu A_\nu} \mathcal{D}_{\alpha\beta} A_\nu = \mathcal{F}^\mu{}_\alpha A_\beta - \mathcal{F}^\mu{}_\beta A_\alpha \quad (4.11.113)$$

which is also not gauge invariant. With these pieces together, we find the Belinfante-Rosenfeld energy-momentum tensor:

$$T^\mu{}_\nu = N^\mu{}_\nu + \frac{1}{2} \partial_\rho (S^{\rho\mu}{}_\nu + S^\mu{}_\nu{}^\rho + S_\nu{}^{\mu\rho}) \quad (4.11.114)$$

$$= \mathcal{F}^{\mu\rho} \partial_\nu A_\rho - \frac{1}{4} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma} \delta^\mu{}_\nu + \frac{1}{2} \partial_\rho (\mathcal{F}^{\rho\mu} A_\nu - \mathcal{F}^\rho{}_\nu A^\mu + \mathcal{F}^\mu{}_\nu A^\rho - \mathcal{F}^{\mu\rho} A_\nu + \mathcal{F}_\nu{}^\mu A^\rho - \mathcal{F}_\nu{}^\rho A^\mu) \quad (4.11.115)$$

$$= \mathcal{F}^{\mu\rho} \partial_\nu A_\rho - \frac{1}{4} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma} \delta^\mu{}_\nu - \partial_\rho (\mathcal{F}^{\mu\rho} A_\nu) \quad (4.11.116)$$

$$= -\mathcal{F}^{\mu\rho} \mathcal{F}_{\rho\nu} - \frac{1}{4} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma} \delta^\mu{}_\nu - A_\nu \partial_\rho \mathcal{F}^{\mu\rho}. \quad (4.11.117)$$

The equation of motion from the Lagrangian density is:

$$\partial_\nu \mathcal{F}^{\mu\nu} = 0 \quad (4.11.118)$$

and so the on-shell energy-momentum tensor for electromagnetism is:

$$T^{\mu\nu} = -\mathcal{F}^{\mu\rho}\mathcal{F}_\rho{}^\nu - \frac{1}{4}\mathcal{F}^{\rho\sigma}\mathcal{F}_{\rho\sigma}\eta^{\mu\nu} \quad (4.11.119)$$

which is both symmetric and gauge invariant. Also, it coincides perfectly with what we found perfectly in the homework!

The last special case of Noether's theorem we will consider at this time is when the symmetry transformation is the gauge transformation. Consider the Lagrangian density for Maxwell's equations with a current source:

$$\mathcal{L} = -\frac{1}{4}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu} + J^\mu A_\mu. \quad (4.11.120)$$

Under a gauge transformation, the transformed Lagrangian density becomes:

$$\mathcal{L}' = \mathcal{L} + \partial_\mu(J^\mu f) - f\partial_\mu J^\mu. \quad (4.11.121)$$

In order for the difference between $\mathcal{L}$ and $\mathcal{L}'$ to be a surface term for all f , we need $f\partial_\mu J^\mu$ to be a surface term for all f . However, because we can select f arbitrarily the only way to make this the case is if $\partial_\mu J^\mu = 0$, which is simply the continuity equation for the current density. In this sense, the requirement for gauge symmetry of the action implies the local conservation of charge or vice versa. As well, from the equation of motion of this Lagrangian density:

$$\partial_\nu \mathcal{F}^{\mu\nu} = J^\mu \quad (4.11.122)$$

we can see that the continuity equation is automatically implied by the antisymmetry of $\mathcal{F}^{\mu\nu}$:

$$\partial_{\mu\nu}^2 \mathcal{F}^{\mu\nu} = \partial_\mu J^\mu \implies \partial_\mu J^\mu = 0. \quad (4.11.123)$$

4.12 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 4.3: Calibrating relative motion** and
- **Problem 4.4: Clock Synchronization** establish how two observers can bring themselves into a state of no relative motion and synchronize clocks with light signals thus allowing them to agree on time measurements going forward.
- **Problem 4.10: Poincare Algebra** and
- **Problem 4.81: Covariantizing the Poincare algebra** compute the Poisson brackets of all of the conserved mechanical quantities in the relativistic theory and put those brackets into covariant form. These brackets will continue to appear going forward.
- **Problem 4.31: Electromagnetic Energy Conservation** and
- **Problem 4.32: Electromagnetic Linear Momentum Conservation** and
- **Problem 4.33: Electromagnetic Angular Momentum Conservation** and
- **Problem 4.34: Electromagnetic Dynamic Energy Momentum Conservation** establish the various conservation laws implied by Noether's theorem due to symmetry under the Poincare group.
- **Problem 4.36: Dispersion Relations and Fourier Amplitudes** and
- **Problem 4.44: Normal Mode Decomposition of the Electromagnetic Hamiltonian** and
- **Problem 4.45: Phase Velocity, Wave-Packet Velocity, Group Velocity** and
- **Problem 4.50: Wave-packet solutions** establish properties of wave solutions in Fourier space and their wave-packets solutions as well as their particle-like interpretation under appropriate circumstances.
- **Problem 4.71: 2-to-2 Scattering** introduces the Mandelstam variables and basic properties of two particle scattering which we will use often going forward.
- **Problem 4.73: Dimensional Analysis and restoring factors of ϵ_0 and c** establishes how to reintroduce the factors of ϵ_0 and c to convert from natural units to SI units.
- **Problem 4.74: Collapse of the Classical Atom** shows that the electromagnetic radiation given off by a classical atom would cause such an atom to collapse in less than a nanosecond, further demonstrating the inability of classical mechanics to explain the macroscopic stability of matter.
- **Problem 4.76: Tensor Product Practice** is important for getting comfortable with actually using the tensor product and also introduces the notion of entanglement which will become important in Part II.
- **Problem 4.79: Parity Transformations of common quantities** and
- **Problem 4.80: Time Reversal Transformations of common quantities** develop the transformation properties of common quantities under parity and time reversal.
- **Problem 4.82: Covariant Conservation Laws and the Energy-Momentum Tensor** introduces the energy-momentum tensor which will become extremely important later in our studies of both fluids and gravity.

In this chapter we developed the theory of relativistic particles interacting with the potentials thus arriving at the theory of **Lorentz Classical Mechanics** or (Special) Relativistic Classical Mechanics. To do so, we made the following experimentally motivated assumptions:

Assumptions generally made in Physics:

- PHSXI: Smoothness of Time and Time Evolution.**
- PHSXII: Smoothness of 3-dimensional Space.**
- PHSXIII: Time Translational Symmetry.**
- PHSXIV: Space Translational Symmetry.**
- PHSXV: Rotational Symmetry.**
- PHSXVI: Locality.**
- PHSXVII: Causality.**

Assumptions specific to Lorentz Classical Mechanics:

- LCMI: Matter consists of moving points.**
- LCMII: Lorentz Boost Symmetry.**
- LCMIII: Spacetime is static and Minkowskian.**

In doing so, we have added the assumption of causality, which is general to all physics, we have kept the assumption about the point nature of matter from the Galilean theory, and we have upgraded the Galilean

theory's notion of boost symmetry and the geometry of space and time to reflect that we must keep the speed of light the same for all observers rather than the passage of time. Interestingly, we did not have to assume parity symmetry in order to derive our results the way we did in the Galilean theory. Parity symmetry is automatic at the order to which we have gone in the relativistic Lagrangian. (It is possible to write down higher order terms in the electromagnetic Lagrangian which violate parity symmetry but have all other required symmetries, for example $(\vec{E} \cdot \vec{B})(|\vec{E}|^2 - c^2|\vec{B}|^2)$.)

In section 4.1, we developed the most general replacement for the failed Galilean boost and arrived at the Lorentz boost as the only alternative consistent with the existence of electromagnetic waves. In section 4.2, we codified these assumptions and used them to find the Lagrangian for a free relativistic particle. In section 4.3, we used our techniques around adding interaction terms to a free theory to write down the Hamiltonian and Lagrangian for a relativistic particle experiencing the potentials and then studied the resulting equations of motion for that particle. In section 4.4, we studied the Lorentz transformation properties of the potentials and fields so as to develop a Lagrangian density for them. In section 4.5, we used that Lagrangian density to derive the equations of motion for electromagnetism, known as Maxwell's equations. In section 4.6, we took the electromagnetic Lagrangian and found the corresponding electromagnetic Hamiltonian. In section 4.7, we discussed an issue with the relativistic theory: the most obvious theory of gravity to try is wrong. We also saw that the relativistic theory seems to be able to successfully describe the conservation laws necessary for when matter splits apart or combines to make new matter but this is seen as an effective theory only as the dynamical mechanism to cause these combinations and decays is not present within the theory. In section 4.8, we developed Lorentz Natural Units by understanding that c should not be understood as a fundamental constant which needs to be measured but more naturally as a fundamental conversion factor that relates lengths of distance and durations of time, thus eliminating the need to define those units separately. As well, we found that in contrast to the Galilean theory the effect of a charge distribution on itself in the relativistic theory cannot be smoothed away to 0 and does in fact inherently diverge for a point charge. This signals that the theory of point particles is incorrect. This is further confirmed by the inability of point particles to explain the experimental results of two-slit diffraction. The actual experimental result obtained even for a matter beam is the wave-like result. Thus, we will need to explore a wave description of matter (to be done in Part II). In section 4.9, we developed covariant index notation and the notion of a tensor so as to describe the relativistic theory in a way which most apparently displays its symmetries. In section 4.10 we proved that in fact all coordinate transformations which preserve the proper time are given by boosts, rotations, time reversal, and parity transformations and we classified the structure of the Lorentz group. In section 4.11 we generalized Noether's theorem to apply to local classical field theories and found that the existence of a symmetry in such a theory implies the existence of a local conservation law. In total we leave this chapter with an improved notion of boost which is finally consistent with electromagnetic waves but without an explanation for the occasional wave-like properties of matter or a relativistically compatible theory of gravity.

Now that we have defined Lorentz Natural Units, our only independent units are units of mass M and units of time T (as the previously independent unit of length L is now defined by the distance light travels in our unit of time and the speed of light is identically 1 length unit per time unit). Our derived units of length and charge are now expressed by:

$$L = T, \quad [q] = \sqrt{MT}. \quad (4.12.1)$$

The units of mass and time are chosen arbitrarily (for us, the kilogram and the second) and using all of our conventions established all other units can be determined and experimental quantities measured. The main experimental successes of the relativistic theory over the Galilean one are its ability to predict electromagnetic phenomena and the allowed decays and combinations of particles. Electromagnetism is by far the most precisely understood phenomenon in physics with precision experiments able to test it to better than one part in a trillion. So, while relativistic classical mechanics is necessarily flawed, within its domain of validity it is an incredibly powerful and predictive theory. Later on we will occasionally work with Galilean theories again because many real life scenarios occur at speeds much less than 1, but never again will we entertain that such theories may be fundamental. Special relativity permanently has supplanted them. When we do discuss Galilean theories (in particular in chapters 6 and 8) we will again explicitly write factors of ϵ_0 , μ_0 , and c , as is traditional in such a theory for the purpose of being easily compared to existing sources. At this point our view of physics is summarized by Figure 4.3.

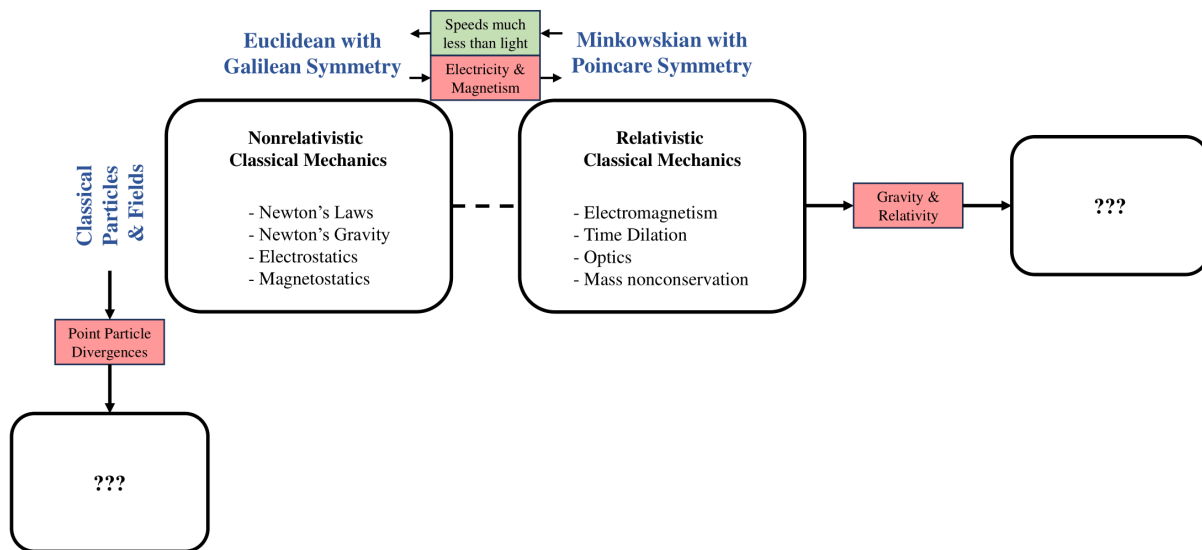


Figure 4.3: Our perspective on physics as of the end of this chapter. Lorentz boost symmetry was able to solve the problem of electromagnetic coexistence but did nothing to affect the problem of point particle divergences. As well, we found there is some more work to be done to make gravity consistent with this new boost symmetry.

This chapter is by no means a complete treatment of essential topics in Relativistic Classical Mechanics. For completeness sake, refer to any standard work on electromagnetism such as [121] (my favorite), [89], [128], [52] or classical mechanics such as [117], [37], [60], [2] for practice and applications.

Chapter 5

Classical Statistical Mechanics

They've done studies, you know. 60 percent of the time, it works every time.

– Anchorman: The Legend of Ron Burgundy [25]

It was an act of desperation. For six years I had struggled with the blackbody theory. I knew the problem was fundamental and I knew the answer. I had to find a theoretical explanation at any cost, except for the inviolability of the two laws of thermodynamics.

– Max Planck [44]

Tackling the issues of point particle divergences and absence of gravity in our previous theories will require us to modify our theories so far developed and study systems on very small distances (in the case of particles) and on very large distances (in the case of gravity). Before doing so, there are many interesting things to be studied at the intermediate and large scales where the theories we have already developed are valid. This brings us to the topic of statistical mechanics.

Statistical mechanics is the study of systems composed of an extremely large number of degrees of freedom. For example, our previous theories gave a description for each particle and thus in a system of N particles we have $6N$ variables to track (3 for each position $\vec{x}(t)$ in 3 dimensions and 3 for each conjugate momentum $\vec{p}(t)$). In an everyday sized box there are about 10^{25} molecules of air and so to exactly describe the behavior of the air in that box one would have to track around 6×10^{25} variables in time. The combined computing power of humanity isn't enough to stand a chance at doing this. Even if one could exactly track so many particles we would need the initial positions and momenta of all of those particles in order to begin tracking them. Clearly measuring instantaneously all of the positions and momenta of all of the molecules in a box of gas is quite a task to imagine! Many systems are chaotic (sensitive to initial conditions), especially large ones, and so approximately measuring the initial conditions isn't even helpful either as doing so is often insufficient to approximately compute the later conditions! So, is there any hope for studying large systems? This is why we need statistical mechanics.

Statistical mechanics seeks to find an approximate effective theory of just some macroscopically meaningful summary quantities which contain far less information than all of the variables of the microscopic system under consideration. The effective macroscopic theory we get out of statistical mechanics is called thermodynamics. Statistical mechanics provides the detailed relationship between those microscopic variables that define the full system and the macroscopic variables that are used in thermodynamics. That is, statistical mechanics derives the laws of the macroscopic theory of thermodynamics from microscopic considerations.

5.1 The Role and Meaning of Probability

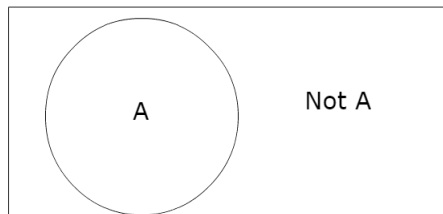
5.1.1 Defining Probability

In statistical mechanics we work with unbelievably unmanageably large systems (large in the sense of number of variables). Consequently, we will be unable to know the exact values of all variables in our

system. So, we need some way to mathematically cope with having incomplete information about our system. Fortunately, mathematicians have established how to do so in the theory of probability.

Probability is the mathematical formalism of how to systematically manage incomplete information. Because in probability one has incomplete information, any given system has a set of possible states it could be in. The space of all possible states a system may be in is called the sample space Ω . Every possible state in Ω is called an outcome (and so Ω may also be called the space of outcomes). For rolling a standard 6 sided die, the sample space is just the set $\Omega = \{1, 2, 3, 4, 5, 6\}$ for example. A set of some outcomes is called an event. For the case of the die, the set $\{2, 4, 6\}$ is an event and in words corresponds to the event that the die rolls an even number. The set of all possible events is called the event space $\mathfrak{F}$. Finally then, a probability measure Prob is a function which to each event assigns a real number between 0 and 1 (inclusive of both). That number it assigns is called the probability of the event and it is interpreted as our degree of belief that the event is true for the actual system at hand. If the probability is 1 then we believe as much as possible that the event is true and if the probability is 0 then we believe as much as possible that the event is false. If our die from before is “fair” then by definition each of the outcomes are equally probable and so it is exactly as probable to be even as odd and thus half of the time the die will roll an even number giving $\text{Prob}(\{2, 4, 6\}) = \frac{1}{2}$.

The triple $(\Omega, \mathfrak{F}, \text{Prob})$ together is called a probability space and the requirement that for all events the probability of that event be between 0 and 1 is called the **first Kolmogorov axiom** of probability. Whatever state the system we are describing is in it will be in some state (there will be some outcome) and so there is certainty that the state of the system lies in the sample space given that it is the set of all possible states. Consequently, $\text{Prob}(\Omega) = 1$. That is, the probability that there is an outcome is 1. This is the **second Kolmogorov axiom** of probability. In order to discuss the third and final Kolmogorov axiom, we should define some other concepts first. Any event A is by definition a subset of the sample space Ω , written $A \subseteq \Omega$. The set $\bar{A}$, called the complement of A or also “not A ”, is everything in the sample space Ω except the elements which are in A . Visually, if we draw the entire sample space Ω as a region then A will be some subset of that region and $\bar{A}$ will be everything outside of A but within Ω .



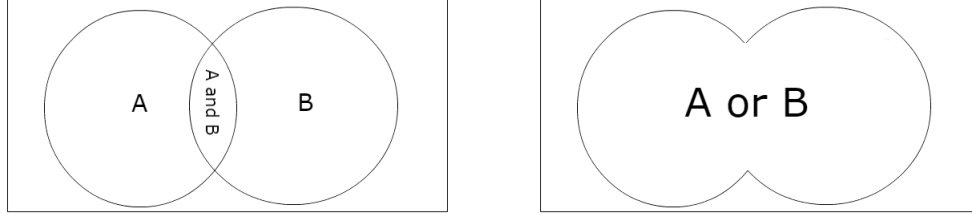
We can represent this also in a truth table. In a truth table, in columns on the left we consider an outcome which is either in each possible event or not in each possible event. If an outcome is not in an event, we enter 0 in that entry of the truth table and if the outcome is in an event, we enter 1 in that entry of the truth table. Then, in the columns on the right we compute, given the data on the left, whether that same outcome is in those events on the right. For example, the truth table for “not A ” is:

A	$\bar{A}$
0	1
1	0

In the first row, the outcome considered is taken not to be in A and so we enter a 0 under A ; consequently that outcome is in $\bar{A}$ and so we enter a 1 under $\bar{A}$. In the second row, the outcome considered is in A and so we enter a 1 under A ; consequently that outcome is not in $\bar{A}$ and so we enter a 0. For two events, we define $A \cup B$, read as “ A or B ” as the union of the two sets A, B . That is, $A \cup B$ is the set made from taking all of the elements of A and all of the elements of B and putting them together into one set. As well, we define $A \cap B$, read as “ A and B ” as the intersection of the two sets A, B . That is, $A \cap B$ is the set made from taking all of the elements of A which also are elements of B and putting them into one set. From these definitions, the truth tables for $A \cup B$ and $A \cap B$ are:

A	B	$A \cup B$	$A \cap B$
0	0	0	0
0	1	1	0
1	0	1	0
1	1	1	1

Visually, we can see these represented in the form of a Venn diagram:



Two events are said to be “disjoint” or “mutually exclusive” if their intersection is empty. That is, A and B are mutually exclusive if there are no outcomes which are both in A and in B . This means that the two regions A and B do not overlap at all in the Venn diagram. Then, the probability of $A \cup B$ is simply the probability of each of the two regions together and so is given by their sum:

$$\text{Prob}(A \cup B) = \text{Prob}(A) + \text{Prob}(B) \quad (A, B \text{ mutually exclusive.}) \quad (5.1.1)$$

This is the **third and final Kolmogorov** axiom. The three Kolmogorov axioms should seem quite intuitive but they are enough to completely establish all the rules of probability. For our first theorem let us prove how to generalize equation (5.1.1) for when A and B are not mutually exclusive. Notice that the sets $A \cap B$ and $A \cap \bar{B}$ are mutually exclusive (as one requires the outcome to be in B and the other requires the outcome to not be in B) and that their union is simply A . One can see both of these facts by looking at the truth table for these sets:

A	B	$A \cap B$	$A \cap \bar{B}$	$(A \cap B) \cup (A \cap \bar{B})$
0	0	0	0	0
0	1	0	0	0
1	0	0	1	1
1	1	1	0	1

The fact that there is no row in which both $A \cap B$ and $A \cap \bar{B}$ are 1 means that they are mutually exclusive. The fact that the column for $(A \cap B) \cup (A \cap \bar{B})$ is identical to the column for A means that they are equal. Then, using equation (5.1.1):

$$\text{Prob}(A) = \text{Prob}((A \cap B) \cup (A \cap \bar{B})) = \text{Prob}(A \cap B) + \text{Prob}(A \cap \bar{B}). \quad (5.1.2)$$

Also as can be seen from the truth table $A \cap \bar{B}$ and B are mutually exclusive and so:

$$\text{Prob}((A \cap \bar{B}) \cup B) = \text{Prob}(A \cap \bar{B}) + \text{Prob}(B). \quad (5.1.3)$$

As well, by truth table we can see that $(A \cap \bar{B}) \cup B = A \cup B$:

A	B	$A \cap \bar{B}$	$(A \cap \bar{B}) \cup B$
0	0	0	0
0	1	0	1
1	0	1	1
1	1	0	1

So, equation (5.1.3) becomes:

$$\text{Prob}(A \cup B) = \text{Prob}(A \cap \bar{B}) + \text{Prob}(B) \quad (5.1.4)$$

$$\implies \text{Prob}(A \cap \bar{B}) = \text{Prob}(A \cup B) - \text{Prob}(B). \quad (5.1.5)$$

Returning this result to equation (5.1.2) we have that for general events A and B without having to be mutually exclusive:

$$\boxed{\text{Prob}(A \cup B) = \text{Prob}(A) + \text{Prob}(B) - \text{Prob}(A \cap B).} \quad (5.1.6)$$

Visually, this is what you should expect from the Venn diagrams drawn. The measure of the region “ A or B ” is given by the total measure of region A together with the region B but one must subtract their overlap “ A and B ” in order to not double count.

We can use an event to define a reduced sample space. Instead of considering the full set of possible outcomes Ω , we can consider only the outcomes within some event A and define probabilities within that region. That is, we can consider the probability of B “given” A or B assuming A , written $B|A$ as the probability that an outcome lies within B assuming we already know that it lies within A . The probability that an outcome lies in B and in A is of course $\text{Prob}(A \cap B)$. The fraction of occurrences in which B is true given that A is true is then the fraction in which they are both true of the occurrences in which A is true. So, the probability $\text{Prob}(B|A)$ is defined as:

$$\boxed{\text{Prob}(B|A) \stackrel{\text{def}}{=} \frac{\text{Prob}(A \cap B)}{\text{Prob}(A)}}. \quad (5.1.7)$$

This formula, called the conditional probability, defines a new probability space with A as the sample space, the events $\{B \cap A : B \in \mathfrak{F}\}$ are the new event space, and this conditional probability formula gives the new probability measure.

We said probability is used to account for and manage incomplete information. This is directly manifested in conditional probability. Conditional probability gives us a mechanism for updating our calculations when we get new information. In our initial state of ignorance we have some sample space Ω and as we gain new information some outcomes are excluded giving a new sample space Ω' of the reduced possibilities; then our new probabilities are given by $\text{Prob}(A|\Omega')$ instead of the old probabilities $\text{Prob}(A)$. Consider both $A|B$ and $B|A$:

$$\text{Prob}(B|A) = \frac{\text{Prob}(A \cap B)}{\text{Prob}(A)}, \quad \text{Prob}(A|B) = \frac{\text{Prob}(A \cap B)}{\text{Prob}(B)} \quad (5.1.8)$$

$$\implies \text{Prob}(A \cap B) = \text{Prob}(B|A)\text{Prob}(A) = \text{Prob}(A|B)\text{Prob}(B) \quad (5.1.9)$$

$$\implies \boxed{\text{Prob}(B|A) = \frac{\text{Prob}(A|B)}{\text{Prob}(A)}\text{Prob}(B)}. \quad (5.1.10)$$

This last equation is known as **Bayes’ theorem**. On its own it may not seem that interesting, however it is extremely insightful. Suppose we have some scientific hypothesis which we are uncertain of the truth of. We have some degree of belief that our world satisfies that hypothesis which we call $\text{Prob}(\text{Hypothesis})$. Suppose further that we collect some data to test our hypothesis. Assuming our hypothesis is true we can use that hypothesis to predict what data should come about and thus we can compute $\text{Prob}(\text{Data}|\text{Hypothesis})$. Then, using Bayes’ theorem we can compute $\text{Prob}(\text{Hypothesis}|\text{Data})$, that is we can compute our updated degree of belief about our hypothesis given our new information collected in the data:

$$\text{Prob}(\text{Hypothesis}|\text{Data}) = \frac{\text{Prob}(\text{Data}|\text{Hypothesis})}{\text{Prob}(\text{Data})}\text{Prob}(\text{Hypothesis}). \quad (5.1.11)$$

So, Bayes’ theorem gives the formal mathematical way of updating your beliefs systematically from a prior degree of belief to a new degree of belief when you acquire new information. This is the core of the scientific method. The probabilities before updating are called priors and the probabilities after updating are called posteriors. It may seem that in order to use this one needs to somehow be able to compute $\text{Prob}(\text{Data})$, the probability of receiving the particular data regardless of whether the hypothesis is true. This can be accomplished using the third Kolmogorov axiom (let $H = \text{Hypothesis}$ and $D = \text{Data}$):

$$\text{Prob}(D) = \text{Prob}((D \cap H) \cup (D \cap \bar{H})) \quad (5.1.12)$$

$$= \text{Prob}(D \cap H) + \text{Prob}(D \cap \bar{H}) \quad (5.1.13)$$

$$= \text{Prob}(D|H)\text{Prob}(H) + \text{Prob}(D|\bar{H})\text{Prob}(\bar{H}). \quad (5.1.14)$$

To perform any calculations, it is necessary that using the hypothesis you are able to compute the probability the data is gotten assuming the hypothesis is true and using the converse of the hypothesis you are able to compute the probability the data is gotten assuming the hypothesis is false. Then, the probability $\text{Prob}(\bar{H})$ is given by:

$$1 = \text{Prob}(\Omega) = \text{Prob}(H \cup \bar{H}) = \text{Prob}(H) + \text{Prob}(\bar{H}) \implies \text{Prob}(\bar{H}) = 1 - \text{Prob}(H). \quad (5.1.15)$$

This then gives all of the necessary information to update our beliefs according to Bayes’ theorem. We will

make this more concrete in the homework.

Two events are said to be (statistically) independent if knowledge about one event tells you nothing about the other. That is, B is independent of A if $\text{Prob}(B|A)$ is the same as $\text{Prob}(B)$ as this means your degree of belief in B is unchanged by knowledge of A :

$$B \text{ independent of } A \implies \text{Prob}(B|A) = \text{Prob}(B) \quad (5.1.16)$$

$$\implies \frac{\text{Prob}(A \cap B)}{\text{Prob}(A)} = \text{Prob}(B) \quad (5.1.17)$$

$$\implies \text{Prob}(A \cap B) = \text{Prob}(A)\text{Prob}(B). \quad (5.1.18)$$

Hence, B is independent of A if and only if $\text{Prob}(A \cap B) = \text{Prob}(A)\text{Prob}(B)$ (as this algebra can be reversed). As well, it immediately follows that B is independent of A if and only if A is independent of B . In physics, we will assume that systems which are completely not interacting with each other (and which have never interacted) are statistically independent because due to their lack of interaction, there is nothing the state of one system can tell us about the state of the other.

We defined probability as a degree of belief; this is the Bayesian interpretation of probability. Another (likely familiar) notion of probability is the frequentist interpretation. The frequentist definition of the probability of an event is if one prepares the system of interest in the “same way” N different times and within those preparations the event in question occurs n times then the probability of the event is n/N in the limit that the number of preparations N is taken to infinity. These two definitions are not quite interchangeable but in many cases are compatible. When discussing cases in which it is possible to effectively repeat an experiment many times, frequentist thinking is often helpful. When discussing cases in which it is not or when making future predictions, Bayesian thinking is essential. I tend to insist on Bayesian thinking as more fundamental, but it is important to understand both.

The frequentist understanding has some problematic subtleties. The notion of “sameness” in preparation is peculiar for physics. In order to *exactly* redo an experiment we would have to recreate the entire universe and its whole history up to the moment of that experiment, which is clearly not possible. Instead, we can only approximately recreate experiments. So, this “sameness” really refers to an equivalence class of different preparations which for whatever system we are considering and whatever measurements we are performing we treat as the same without them microscopically actually being the same (the boundaries on what counts as the same and what doesn’t can be difficult to define, and is really only determined by experimental context). For statistical physics, we often have many constituents in a system which we are unable to distinguish between, so we consider measuring different constituents as if we are sampling from the “same” distribution many times. In order to compute an exact frequentist probability from data one needs to prepare and measure a system an infinite number of times, which is a bit impractical. Instead, frequentists estimate/approximate probabilities at a finite amount of data, which is perfectly valid. More problematically, the frequentist notion of probability requires it to be possible at least in imagination for a system to be prepared “the same way” (within the previously discussed equivalence class) so that it could theoretically be measured multiple times. But, maybe one would like to know the probability that there is a devastating earthquake tomorrow; there is only one tomorrow and only one earth to quake, so the frequentist can’t compute such a thing. The frequentist retort is to say that while there is only one tomorrow, it isn’t really different from any other day and so they could use available data to compute the probability that in a randomly selected 24 hour period there is a devastating earthquake and then define the probability that there is an earthquake tomorrow as that number. Subtly the last step of this logic is actually Bayesian. The frequentist is capable of estimating the probability that in an arbitrary 24 hour period there is a devastating earthquake from the large but finite amount of earthquake data that has been collected. But, by declaring that probability valid for the probability of an earthquake tomorrow, one is actually setting a degree of belief about tomorrow, not a frequentist probability because the singular tomorrow cannot be repeated. In essence, **the application of results from statistical samples to specific instances of systems is only valid when thinking in terms of degrees of belief, not in frequencies, because those specific instances cannot be recreated.** Because of this, you basically have to be Bayesian when making a prediction. We will see in the homework that in the case one can perform the frequentist infinitely many trials experiment the Bayesian results converge to the frequentist definition. In that way, the frequentist understanding of probability can be recovered when possible but is properly generalized by the Bayesian thinking. Both frequentist and Bayesian understandings of probability and the resultant statistical methods are popular and useful, though because of their different interpretations they do not typically answer the same questions.

5.1.2 Discrete Random Variables

A probability space allows us to consider the probabilities of various events but more often in physics we are interested in the values of quantities about our system, such as its energy or momentum, and so we would like to understand how to relate uncertain variables to events in probability space. This is accomplished through random variables. A random variable is a function from the sample space into some other set, usually a real or complex number or vector for us. For example, for a die roll the number that actually shows up on the die is a random variable. The sample space is each of the six sides and the function that is the random variable in this case just reads off the number printed on that side. For a more physical example, for a Galilean free particle with unknown momentum $\vec{p}$, its energy $E = \frac{|\vec{p}|^2}{2m}$ is a random variable that takes each possible $\vec{p}$ in the sample space and gives a corresponding real number to each one.

Let X be a random variable. Each outcome ω in the sample space Ω then gets mapped to some value by X . The set of all values X maps to is called the image of X , written $\text{Img}(X)$. So, $X(\omega)$ is a map from Ω into $\text{Img}(X)$. Suppose for now we are dealing with X discrete, so that its output is a natural number, or integer, or rational number, or some other countable set. Then, for each possible value x that X may take, we define the event that X takes that value and write that event as “ $X = x$ ”. Again, recall that an event is really a set and so when we say the event $X = x$ we really mean the set of all outcomes ω so that $X(\omega) = x$. The probability distribution function or probability mass function (pmf) for X , written $p_X(x)$ is defined by:

$$p_X(x) \stackrel{\text{def}}{=} \text{Prob}(X = x). \quad (5.1.19)$$

The pmf is automatically between 0 and 1 for all x (the possible values of X). Each event $X = x$ is mutually exclusive of other such events for different x . That is, there can be nowhere in sample space that $X = x_1$ and $X = x_2$ if $x_1 \neq x_2$. As well, the union $\cup_{x \in \text{Img}(X)} (X = x)$ goes over all values x that X may take and so covers the whole sample space. So, by the third Kolmogorov axiom:

$$1 = \text{Prob}(\Omega) = \text{Prob}(\cup_{x \in \text{Img}(X)} (X = x)) = \sum_{x \in \text{Img}(X)} \text{Prob}(X = x) \quad (5.1.20)$$

$$\implies \sum_{x \in \text{Img}(X)} p_X(x) = 1. \quad (5.1.21)$$

This is just the rather obvious statement that the probability that X takes some value of some kind is 1.

We can define functions of random variables, $f(X)$. By definition, a function of a random variable is a new random variable Y so that if X takes an outcome ω and spits out $x = X(\omega)$, then $Y = f(X)$ is defined so that $Y(\omega) = f(X(\omega)) = f(x)$. It just applies the function f to the output of X . This is quite natural as then for each outcome the random variable X is essentially replaced by its constant value x that it takes at that outcome and functions of X just become functions of x . The probability mass function for $f(X)$ then becomes by definition:

$$p_{f(X)}(y) = \text{Prob}(f(X) = y). \quad (5.1.22)$$

By definition, $f(X) = y$ if and only if $X = x$ for some x so that $f(x) = y$. The set of events $X = x$ for distinct such x are mutually exclusive and so:

$$\text{Prob}(f(X) = y) = \text{Prob}(\cup_{x|f(x)=y} (X = x)) = \sum_{x|f(x)=y} \text{Prob}(X = x) = \sum_{x|f(x)=y} p_X(x) \quad (5.1.23)$$

$$\implies p_{f(X)}(y) = \sum_{x|f(x)=y} p_X(x). \quad (5.1.24)$$

If $f(x)$ is an invertible function then there is only one term in this sum and the pmf's are equal just at the mapped forward arguments. If $f(x)$ is not invertible there is a contribution from each branch of the inverse.

We can turn an event into a random variable using the indicator function. The indicator function ϑ as we defined before in section 3.1 is defined so that it is 1 when its argument is true and 0 when its argument is false. So, the function $\vartheta(\omega \in A)$ is 1 for all outcomes ω which are in A and is 0 for all outcomes ω which are not in A . This is then a discrete random variable as it is a function from the sample space into just the set $\{0, 1\}$. As a short hand we denote this random variable as $\mathbb{1}_A = \vartheta(\omega \in A)$. The indicator function really is just the representation of the truth tables we have already discussed in an equation. The probability mass function for the indicator function is then:

$$p_{\mathbb{1}_A}(1) = \text{Prob}(\mathbb{1}_A = 1) = \text{Prob}(A), \quad p_{\mathbb{1}_A}(0) = \text{Prob}(\mathbb{1}_A = 0) = \text{Prob}(\bar{A}) = 1 - \text{Prob}(A). \quad (5.1.25)$$

Very nicely, every random variable can just be written as a sum of indicator functions. Let A_x be the event that $X = x$. Then, because each such event is mutually exclusive for different x their indicator functions don't overlap. For any outcome exactly one such indicator function is 1 and all of the others are zero. So:

$$\sum_{x \in \text{Img}(X)} \mathbb{1}_{A_x} = 1 \quad (5.1.26)$$

$$\implies X = X1 = \sum_{x \in \text{Img}(X)} X \mathbb{1}_{A_x}. \quad (5.1.27)$$

The product $X \mathbb{1}_{A_x}$ is 0 for all outcomes for which X is not x and it is x for all outcomes for which $X = x$. So:

$$X \mathbb{1}_{A_x} = x \mathbb{1}_{A_x} \quad (5.1.28)$$

$$\implies X = \sum_{x \in \text{Img}(X)} x \mathbb{1}_{A_x}. \quad (5.1.29)$$

Thus, every random variable can be written as a linear combination of indicator random variables.

Random variables can take many different values due to our incomplete information. So, it is useful to try to find a way of turning a random variable into a “best” single representative value. The typical way of defining “best” value is called the expectation of the random variable and for a random variable X it is written $\mathbb{E}(X)$. Generally we will be working with random variables which are numerical and so we will be able to add them and multiply them by constants. If $\mathbb{E}(X)$ is to be our best guess value for X then it must satisfy some basic properties. First, if X is guaranteed to take a particular value x then that value is clearly the best guess value for X and so $\mathbb{E}(X)$ must also take that value:

$$X = x \implies \mathbb{E}(X) = x. \quad (5.1.30)$$

Second, if we multiply our random variable by a constant a to get a new random variable aX the best guess value for aX should just be a times the best guess value for X :

$$\mathbb{E}(aX) = a\mathbb{E}(X). \quad (5.1.31)$$

This is absolutely necessary for our probability formalism to be independent of our choice of arbitrary physical units as changing units rescales our variables by constant multipliers. If we are changing vector bases then after changing bases the new components will be linear combinations of the old components. If we would like the best guess values to change bases in the same way as the random variables then we must have that the best guess of a linear combination is the linear combination of best guesses. That is, for random variables X and Y :

$$\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y). \quad (5.1.32)$$

Using these properties and the indicator decomposition of a random variable, we have:

$$\mathbb{E}(X) = \mathbb{E}\left(\sum_{x \in \text{Img}(X)} x \mathbb{1}_{A_x}\right) = \sum_{x \in \text{Img}(X)} x \mathbb{E}(\mathbb{1}_{A_x}). \quad (5.1.33)$$

Hence, we only need to know how to compute the expectation of indicator random variables in order to compute the expectation of any random variable. We know from equation (5.1.25) that the pmf for an indicator random variable is completely determined by a single number, the probability that the indicator takes the value 1. So, for an event A with probability $p_A = \text{Prob}(A)$ the expectation of the indicator of A must be *some* function of p_A :

$$\mathbb{E}(\mathbb{1}_A) = g(p_A). \quad (5.1.34)$$

Using our linearity property with another event B of probability p_B :

$$\mathbb{E}(\mathbb{1}_A + \mathbb{1}_B) = g(p_A) + g(p_B). \quad (5.1.35)$$

Now suppose B and A are mutually exclusive. Then, the indicator function of their union $\mathbb{1}_{A \cup B}$ is 1 if and only if exactly one of them is true and the same holds for the sum $\mathbb{1}_A + \mathbb{1}_B$. Thus:

$$A, B \text{ mutually exclusive} \implies \mathbb{1}_{A \cup B} = \mathbb{1}_A + \mathbb{1}_B \quad (5.1.36)$$

$$\implies \mathbb{E}(\mathbb{1}_{A \cup B}) = g(p_A) + g(p_B). \quad (5.1.37)$$

Using the definition of the function g and the third Kolmogorov axiom:

$$\mathbb{E}(\mathbb{1}_{A \cup B}) = g(\text{Prob}(A \cup B)) = g(\text{Prob}(A) + \text{Prob}(B)) = g(p_A + p_B). \quad (5.1.38)$$

So, for A and B mutually exclusive:

$$\mathbb{E}(\mathbb{1}_A + \mathbb{1}_B) = g(p_A + p_B) = g(p_A) + g(p_B). \quad (5.1.39)$$

This is now just an algebraic constraint on the function g that for two numbers x, y between 0 and 1 it must satisfy:

$$g(x + y) = g(x) + g(y). \quad (5.1.40)$$

Differentiating both sides with respect to y we have:

$$g'(x + y) = g'(y). \quad (5.1.41)$$

At $y = 0$ this gives:

$$g'(x) = g'(0) \quad (5.1.42)$$

$$\implies g(x) = g'(0)x + g(0). \quad (5.1.43)$$

Evaluating our original algebraic constraint at $x = y = 0$:

$$g(0) = 2g(0) \implies g(0) = 0. \quad (5.1.44)$$

So, we have:

$$g(x) = g'(0)x. \quad (5.1.45)$$

Now consider the indicator function of the whole sample space $\mathbb{1}_\Omega$. Because every outcome is in the sample space this indicator function is identically 1 and so by the constant property of the expectation (5.1.30):

$$\mathbb{E}(\mathbb{1}_\Omega) = \mathbb{E}(1) = 1. \quad (5.1.46)$$

As well, $\text{Prob}(\Omega) = 1$ and so:

$$\mathbb{E}(\mathbb{1}_\Omega) = g(\text{Prob}(\Omega)) = g(1). \quad (5.1.47)$$

Thus:

$$g(1) = g'(0)1 = 1 \implies g'(0) = 1 \quad (5.1.48)$$

$$\implies g(x) = x. \quad (5.1.49)$$

Altogether then we have that the expectation of $\mathbb{1}_A$ is simply the probability of A :

$$\mathbb{E}(\mathbb{1}_A) = \text{Prob}(A). \quad (5.1.50)$$

Returning this to our general formula for the expectation of a random variable we have:

$$\boxed{\mathbb{E}(X) = \sum_{x \in \text{Img}(X)} x \text{Prob}(X = x) = \sum_{x \in \text{Img}(X)} x p_X(x).} \quad (5.1.51)$$

This is the familiar formula for a weighted average where we are summing over all of the different possible values of X and weighting them by the probability that X actually takes that specific value. This expectation is also called the mean of the random variable X or the first moment of the random variable X . Commonly we will use the symbol μ_X as a shorthand for this expectation:

$$\mu_X \stackrel{\text{def}}{=} \mathbb{E}(X). \quad (5.1.52)$$

From here we can immediately compute the expectation of a function of a random variable using the definition of a function of a random variable:

$$\mathbb{E}(f(X)) = \sum_{y \in \text{Img}(f(X))} y \text{Prob}(f(X) = y). \quad (5.1.53)$$

Then, using our previous formula for the pmf of a function of a random variable:

$$\mathbb{E}(f(X)) = \sum_{y \in \text{Img}(f(X))} y \sum_{x | f(x)=y} \text{Prob}(X = x) \quad (5.1.54)$$

$$\implies \mathbb{E}(f(X)) = \sum_{y \in \text{Img}(f(X))} \sum_{x | f(x)=y} y \text{Prob}(X = x). \quad (5.1.55)$$

Because in the second sum we are considering only x so that $f(x) = y$, we can replace the factor of y

appearing there with $f(x)$:

$$\mathbb{E}(f(X)) = \sum_{y \in \text{Img}(f(X))} \sum_{x|f(x)=y} f(x) \text{Prob}(X = x). \quad (5.1.56)$$

Then, we are summing over all x so that $f(x) = y$ and then summing over all y . This is then equivalent to just summing over all x . Thus:

$$\mathbb{E}(f(X)) = \sum_{x \in \text{Img}(X)} f(x) \text{Prob}(X = x) = \sum_{x \in \text{Img}(X)} f(x) p_X(x). \quad (5.1.57)$$

So, to compute the expectation of a function of a random variable we don't even need to compute the pmf for that function, we can express the result cleanly in terms of the pmf of the underlying random variables. This last equation is known as the “law of the unconscious statistician” as someone who is not being careful might interpret this formula as a definition or assumption when in fact it is a theorem and wholly derived from our previous assumptions.

We've found that the expectation formula is the unique expression satisfying the desired properties we gave (equations (5.1.30)-(5.1.32)) but there is another sense in which it gives the “best guess” constant value for a random variable. It gives the lowest average error in approximating the the random variable by a constant under an appropriate definition of average error. Suppose we are working with a random variable X which is numerical. Then, for any guess value M , we can consider how far we are from the true value by considering the magnitude $|X - M|$. Our expected magnitude of error is then:

$$\varepsilon_1 = \mathbb{E}(|X - M|) = \sum_{x \in \text{Img}(X)} |x - M| p_X(x). \quad (5.1.58)$$

One idea of a “best guess” value for X would then minimize our expected error so that on average we are as close as possible. Then, we would select M so that:

$$\frac{\partial \varepsilon_1}{\partial M} \stackrel{!}{=} 0 \quad (5.1.59)$$

$$\frac{\partial \varepsilon_1}{\partial M} = \sum_{x \in \text{Img}(X)} \frac{M - x}{|M - x|} p_X(x). \quad (5.1.60)$$

The function $\frac{x}{|x|}$ is known as the sign function $\text{sgn}(x)$:

$$\text{sgn}(x) \stackrel{\text{def}}{=} \begin{cases} 1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \end{cases} = \frac{d|x|}{dx}. \quad (5.1.61)$$

Then:

$$\frac{\partial \varepsilon_1}{\partial M} = \sum_{\substack{x \in \text{Img}(X) \\ M > x}} p_X(x) - \sum_{\substack{x \in \text{Img}(X) \\ M < x}} p_X(x) \stackrel{!}{=} 0 \quad (5.1.62)$$

$$\implies \sum_{\substack{x \in \text{Img}(X) \\ M > x}} p_X(x) = \sum_{\substack{x \in \text{Img}(X) \\ M < x}} p_X(x) \quad (5.1.63)$$

$$\implies \text{Prob}(X < M) = \text{Prob}(X > M). \quad (5.1.64)$$

Such an M is called the **median** of a probability distribution. This is certainly not the same as the expectation of X in general. This error minimization we did we can see treats being above or below the median as equally bad regardless of how far above or below one is because it is simply the value with equal probability above and below.

Another reasonable error formula we could try to minimize is the expected squared distance:

$$\varepsilon_2 = \mathbb{E}((X - \mu)^2). \quad (5.1.65)$$

By virtue of the square having increasing derivative, this error penalizes large deviations more than small deviations. Then:

$$\frac{\partial \varepsilon_2}{\partial \mu} = \sum_{x \in \text{Img}(X)} 2(\mu - x) p_X(x) \stackrel{!}{=} 0 \quad (5.1.66)$$

$$\implies \mu \sum_{x \in \text{Img}(X)} p_X(x) - \sum_{x \in \text{Img}(X)} xp_X(x) = 0 \quad (5.1.67)$$

$$\implies \mu = \mathbb{E}(x). \quad (5.1.68)$$

Hence, the mean is the best guess value for minimizing the expected squared error. These two functions ε_1 and ε_2 are called “loss functions”. For practical applications many different “natural” loss functions may present themselves to be the quantity one would like to minimize. (For example, if one is estimating a parameter for engineering applications and errors lead to monetary damages of equipment one may want to minimize the expected cost of damage which may depend quite non-linearly on the error of the parameter.) As we see here, the expectation formula we have already found to be quite natural is the minimizer of a quadratic loss function. When we have minimized our expected squared error, that expected squared error takes some generally non-zero value. Its value is called the variance of X :

$$\boxed{\text{Var}(X) \stackrel{\text{def}}{=} \varepsilon_2|_{\mu=\mu_X} = \mathbb{E}(X - \mathbb{E}(X))^2.} \quad (5.1.69)$$

The variance is also called the second central moment of the random variable X . The standard deviation σ_X of a random variable is defined as the positive square root of its variance:

$$\sigma_X \stackrel{\text{def}}{=} \sqrt{\text{Var}(X)}. \quad (5.1.70)$$

So, σ_X^2 is the expected squared error of our best guess. The mean μ_X and standard deviation σ_X of a random variable then give two extremely important pieces of information. If one is to try to approximate a random variable as simply being given by a number then the “best” possible choice of such a candidate number is the mean μ_X . Then, the standard deviation σ_X characterizes the typical error in making such an approximation (in fact in the very same sense as the mean, σ_X^2 is the “best” possible choice for characterizing the squared error). In this way, μ_X is a measure of the “center” of a distribution (as in where the bulk of the probability is located) and σ_X is a measure of the “spread” of a distribution (as in how large of a region the bulk of the probability occupies). Because the standard deviation measures how spread out the probability mass function for a random variable is, physicists sometimes call σ_X the “fluctuation” of X as it gives the typical amount by which the true value of X differs (and thus “has fluctuated”) from the best guess value μ_X .

We have now defined the first and second moments of a random variable. In general, the n^{th} moment of a random variable M_n is defined by the expectation of X^n :

$$M_n = \mathbb{E}(X^n). \quad (5.1.71)$$

However, it is often more useful to consider the central moments $\bar{M}_n$ which are defined by the expectation of $(X - \mu_X)^n$:

$$\bar{M}_n = \mathbb{E}(X - \mu_X)^n. \quad (5.1.72)$$

Then, $M_1 = \mu_X$, $\bar{M}_1 = 0$, $\bar{M}_2 = \text{Var}(X)$. The central moments $\bar{M}_n$ of various random variables turn out to present themselves quite naturally as objects of study in a wide variety of problems, as we will see repeatedly. If the random variable X has units, then each $\bar{M}_n$ has units of X^n . So, it can be nice to define the (automatically unitless) normalized central moments m_n :

$$m_n = \mathbb{E} \left(\frac{X - \mu_X}{\sigma_X} \right)^n. \quad (5.1.73)$$

Then, $m_1 = 0$ and $m_2 = 1$. For $n > 2$, the various M_n , $\bar{M}_n$, m_n can all be computed from each other for given μ_X and σ_X and so they contain the same information; they are just not always equally clean ways of organizing that information.

Often of course we will deal with more than one random variable at a time. So, let X and Y be two different random variables. The joint probability mass function $p_{X,Y}(x,y)$ is defined by:

$$p_{X,Y}(x,y) \stackrel{\text{def}}{=} \text{Prob}(X = x \cap Y = y). \quad (5.1.74)$$

Then, if we sum this formula over all values of y we can recover the probability mass function for X using the third Kolmogorov axiom:

$$\sum_{y \in \text{Img}(Y)} p_{X,Y}(x,y) = \sum_{y \in \text{Img}(Y)} \text{Prob}(X = x \cap Y = y) \quad (5.1.75)$$

$$= \text{Prob}(\cup_{y \in \text{Img}(Y)} (X = x \cap Y = y)) = \text{Prob}(X = x) = p_X(x). \quad (5.1.76)$$

The identical calculation with the roles of X and Y reversed yields:

$$p_Y(y) = \sum_{x \in \text{Img}(X)} p_{X,Y}(x, y). \quad (5.1.77)$$

The individual distributions $p_X(x)$ and $p_Y(y)$ are called the marginal distributions for X and Y . The process of summing over one of the variables so that it does not appear in the final expression is called “integrating out” that variable. From here we can compute the expectations of X and Y in terms of the joint distribution:

$$\mathbb{E}(X) = \sum_{x \in \text{Img}(X)} xp_X(x) = \sum_{(x,y) \in \text{Img}((X,Y))} xp_{X,Y}(x, y), \quad (5.1.78)$$

$$\mathbb{E}(Y) = \sum_{(x,y) \in \text{Img}((X,Y))} yp_{X,Y}(x, y). \quad (5.1.79)$$

We can compute the expectation of any function of X and Y , $f(X, Y)$ quite easily. The proof of the law of the unconscious statistician never assumed that X was number valued. So, if we take the X appearing in the our already proven law of the unconscious statistician in equation (5.1.57) to be vector valued with components (X, Y) our two random variables then it immediately follows that:

$$\boxed{\mathbb{E}(f(X, Y)) = \sum_{(x,y) \in \text{Img}((X,Y))} f(x, y)p_{X,Y}(x, y).} \quad (5.1.80)$$

Thus, the joint distribution is necessary in general to compute expectations of functions of both X and Y .

Just as we can compute conditional probabilities of events and conditional probability really redefined a reduced sample space, we can define random variables on that reduced sample space and thus can define conditional probability mass functions. For example, we could compute the conditional probability mass function for Y given that X takes the value x . By the definition of conditional probability:

$$p_{Y|X}(y|x) = \text{Prob}(Y = y|X = x) = \frac{\text{Prob}(Y = y \cap X = x)}{\text{Prob}(X = x)} = \frac{p_{X,Y}(x, y)}{p_X(x)}. \quad (5.1.81)$$

Moreover, we say that two random variables are independent if knowledge of the value of one tells you nothing about the value of the other, just like with events. That is, two random variables X and Y are independent if the conditional distribution of Y given X is the same as the unconditional distribution of Y :

$$X, Y \text{ independent} \implies p_{Y|X}(y|x) = p_Y(y) \quad (5.1.82)$$

$$\implies \frac{p_{X,Y}(x, y)}{p_X(x)} = p_Y(y) \quad (5.1.83)$$

$$\implies p_{X,Y}(x, y) = p_X(x)p_Y(y). \quad (5.1.84)$$

So, X and Y are independent as random variables if and only if the events $X = x$ and $Y = y$ are independent as events for all values of x and y .

5.1.3 Continuous Random Variables

We can do essentially everything we did for discrete random variables for random variables which have continuous outputs, like the real numbers, though the situation is a bit more technically complicated. Let's suppose that we are dealing with a real valued random variable X . Then, define the cumulative distribution function (cdf) as the probability:

$$F_X(x) = \text{Prob}(X \leq x). \quad (5.1.85)$$

Let $b > a$ be two real numbers. Then, $X \leq b$ means that either $X \leq a$ or $a < X \leq b$. These two possibilities are mutually exclusive and so:

$$\text{Prob}(X \leq b) = \text{Prob}((X \leq a) \cup (a < X \leq b)) = \text{Prob}(X \leq a) + \text{Prob}(a < X \leq b). \quad (5.1.86)$$

So, we can identify the probability that X lie in the interval $(a, b]$ as:

$$\text{Prob}(a < X \leq b) = F_X(b) - F_X(a). \quad (5.1.87)$$

Automatically and unsurprisingly, this means that the cdf is a non-decreasing function. The cdf is necessarily between 0 and 1 for all x because it is a probability. As well, because X is necessarily some finite

real number:

$$\lim_{x \rightarrow -\infty} F_X(x) = \lim_{x \rightarrow -\infty} \text{Prob}(X \leq x) = 0 \quad (5.1.88)$$

$$\lim_{x \rightarrow \infty} F_X(x) = \lim_{x \rightarrow \infty} \text{Prob}(X \leq x) = 1. \quad (5.1.89)$$

The probability density function (pdf) $f_X(x)$ is defined as the derivative of the cdf:

$$f_X(x) \stackrel{\text{def}}{=} \frac{dF_X}{dx}. \quad (5.1.90)$$

Because the cdf is non-decreasing, the pdf is non-negative. However, the pdf is **NOT** a probability and so it is not required to be less than or equal to 1. By integrating both sides of the definition of the pdf we have:

$$\int_a^b f_X(x) dx = \int_a^b \frac{dF_X}{dx} dx = F_X(b) - F_X(a) \quad (5.1.91)$$

$$\implies \boxed{\text{Prob}(a < X \leq b) = \int_a^b f_X(x) dx.} \quad (5.1.92)$$

From this we can see the actual interpretation of the pdf. The probability density function is the probability per unit coordinate-length for the value of X . That is, just like the total mass in a region is gotten by integrating the mass density over that region the total probability of a variable being in a region is gotten by integrating the probability density over that region. An extremely common **WRONG** statement physicists will make is “ $f(x)dx$ is the probability to find X between x and $x + dx$ ”. If this is something you say, please, do better. The correct statement is that the probability X is between a and b is the integral of $f_X(x)$ with respect to x over that interval. If you are still treating the integral measure dx as “an infinitesimal number”, go read a math book.

We can define functions of continuous random variables as well. Consider some random variable $g(X)$ where g is a real valued function. Then:

$$F_{g(X)}(y) = \text{Prob}(g(X) \leq y). \quad (5.1.93)$$

Suppose we can divide the real line up into a list of disjoint intervals $M_1, \dots, M_n$ so that on each interval $g(x)$ is monotone. Then, as shown in problem 3.2 on each interval one can define a unique inverse function $g_k^{-1}(y)$ so that on that interval $g_k^{-1}(g(x)) = x$. Then, because these intervals are disjoint and so they make mutually exclusive events:

$$F_{g(X)}(y) = \text{Prob}(\cup_{k=1}^n (g(X) \leq y \cap X \in M_k)) = \sum_{k=1}^n \text{Prob}(g(X) \leq y \cap X \in M_k). \quad (5.1.94)$$

$$\implies f_{g(X)}(y) = \frac{dF_{g(X)}}{dy} = \sum_{k=1}^n \frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy}. \quad (5.1.95)$$

Let l_k be the lower limit of the interval M_k and r_k be the upper limit of M_k . Suppose we are considering an interval on which $g(x)$ is an increasing function. Then:

$$g(X) \leq y \implies g_k^{-1}(g(X)) \leq g_k^{-1}(y) \implies X \leq g_k^{-1}(y). \quad (5.1.96)$$

Consequently:

$$\text{Prob}(g(X) \leq y \cap X \in M_k) = \text{Prob}(X \leq g_k^{-1}(y) \cap l_k < X \leq r_k). \quad (5.1.97)$$

If $g_k^{-1}(y) > r_k$ then the first condition is redundant and we simply get $\text{Prob}(l_k < X < r_k)$, which is independent of y . Or, if $g_k^{-1}(y) \leq l_k$ then no value of X could satisfy both conditions and this probability becomes 0. So, this probability only varies with y for y so that $g_k^{-1}(y) \in M_k$. Thus:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{d\text{Prob}(X \leq g_k^{-1}(y) \cap l_k < X \leq r_k)}{dy}. \quad (5.1.98)$$

The indicator function here just enforces that the following expression is only non-zero for y so that $g_k^{-1}(y) \in M_k$. For y as specified this condition reduces to:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{d\text{Prob}(l_k < X \leq g_k^{-1}(y))}{dy} \quad (5.1.99)$$

$$= \vartheta(g_k^{-1}(y) \in M_k) \frac{d}{dy} \int_{l_k}^{g_k^{-1}(y)} f_X(x) dx \quad (5.1.100)$$

$$= \vartheta(g_k^{-1}(y) \in M_k) \frac{dg_k^{-1}(y)}{dy} f_X(g_k^{-1}(y)). \quad (5.1.101)$$

Let x_k be the value of $x \in M_k$ so that $y = g(x)$. The indicator function above is 1 when such an x_k exists and 0 when it does not. Then:

$$x_k = g_k^{-1}(y) \quad (5.1.102)$$

$$g_k^{-1}(g(x)) = x \implies \frac{d}{dx} (g_k^{-1}(g(x))) = 1 \quad (5.1.103)$$

$$\implies \left. \frac{dg_k^{-1}(y)}{dy} \right|_{y=g(x)} g'(x) = 1 \implies \frac{dg_k^{-1}}{dy} = \frac{1}{g'(x_k)}. \quad (5.1.104)$$

Because $g(x)$ is increasing on this interval its derivative is positive and so we have:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{1}{|g'(x_k)|} f_X(x_k). \quad (5.1.105)$$

Suppose instead we are dealing with an interval on which $g(x)$ is a decreasing function. Then:

$$g(X) \leq y \implies g_k^{-1}(g(X)) \geq g_k^{-1}(y) \implies X \geq g_k^{-1}(y). \quad (5.1.106)$$

Consequently:

$$\text{Prob}(g(X) \leq y \cap X \in M_k) = \text{Prob}(X \geq g_k^{-1}(y) \cap l_k < X \leq r_k). \quad (5.1.107)$$

If $g_k^{-1}(y) \leq l_k$ then the first condition is redundant and we simply get $\text{Prob}(l_k < X < r_k)$, which is independent of y . Or, if $g_k^{-1}(y) < r_k$ then no value of X could satisfy both conditions and this probability becomes 0. So, this probability only varies with y for y so that $g_k^{-1}(y) \in M_k$. So:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{d\text{Prob}(X \geq g_k^{-1}(y) \cap l_k < X \leq r_k)}{dy}. \quad (5.1.108)$$

For y as specified this condition reduces to:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{d\text{Prob}(g_k^{-1}(y) \leq X < r_k)}{dy} \quad (5.1.109)$$

$$= \vartheta(g_k^{-1}(y) \in M_k) \frac{d}{dy} \int_{g_k^{-1}(y)}^{r_k} f_X(x) dx \quad (5.1.110)$$

$$= \vartheta(g_k^{-1}(y) \in M_k) \left(-\frac{dg_k^{-1}(y)}{dy} \right) f_X(g_k^{-1}(y)). \quad (5.1.111)$$

Then, again using x_k and now that $g(x)$ is decreasing and so its derivative is negative:

$$\frac{d\text{Prob}(g(X) \leq y \cap X \in M_k)}{dy} = \vartheta(g_k^{-1}(y) \in M_k) \frac{1}{|g'(x_k)|} f_X(x_k). \quad (5.1.112)$$

This is precisely the same as (5.1.105) and so this equation holds whether $g(x)$ is increasing or decreasing. Then, equation (5.1.95) becomes:

$$f_{g(X)}(y) = \sum_{k=1}^n \vartheta(g_k^{-1}(y) \in M_k) \frac{f_X(x_k)}{|g'(x_k)|}. \quad (5.1.113)$$

The indicators then just select out all intervals which actually have x so that $g(x) = y$. Thus, the sum reduces to:

$$f_{g(X)}(y) = \sum_{x|y=g(x)} \frac{f_X(x)}{|g'(x)|}. \quad (5.1.114)$$

Notice that this is in fact the same change of variables formula as the Dirac delta as found in question 3.2. Any quantity with this change of variables property is called a “distribution”. This is why $f_X(x)$ is called a probability distribution or probability density and why the proper name for the Dirac delta is the Dirac delta distribution. In the case that $g(x)$ is a nice invertible function everywhere there is only one such branch and

we can write:

$$f_{g(X)}(y) = \frac{f_X(g^{-1}(y))}{|g'(g^{-1}(y))|}. \quad (5.1.115)$$

We can also define an expectation on continuous random variables. The most natural way to do anything continuous is to understand it as the limit of something discrete. Consider chopping up the real line into intervals of width ℓ for fixed ℓ so that interval n is given by $M_n = (n\ell, (n+1)\ell)$. Then if we take n across all integers this covers the whole real line. For a random variable X , define the random variable X_ℓ so that whenever $X \in M_n$, $X_\ell = n\ell$, the left endpoint of the interval. Plotting X_ℓ vs X shows that it is a staircase incrementing by ℓ at each integer multiple of ℓ . As we take $\ell \rightarrow 0$ the intervals will become smaller and smaller and so X_ℓ will be increasingly like X . As well, X_ℓ is a discrete random variable and so its expectation is:

$$\mathbb{E}(X_\ell) = \sum_{n \in \mathbb{Z}} n\ell \text{Prob}(X_\ell = n\ell). \quad (5.1.116)$$

We will define the expectation of X by the limit that our discretization goes to 0:

$$\mathbb{E}(X) = \lim_{\ell \rightarrow 0^+} \mathbb{E}(X_\ell). \quad (5.1.117)$$

Define $x_n = n\ell$. Then:

$$\mathbb{E}(X_\ell) = \sum_{n \in \mathbb{Z}} x_n \int_{x_n}^{x_n+\ell} f_X(x) dx = \sum_{n \in \mathbb{Z}} \int_{x_n}^{x_n+\ell} x_n f_X(x) dx. \quad (5.1.118)$$

For a real number x , the integer part or floor of x , $\lfloor x \rfloor$ is defined as the greatest integer less than or equal to x . Then, the decimal part of x , $\% (x)$ is defined as the amount by which x exceeds $\lfloor x \rfloor$:

$$\% (x) = x - \lfloor x \rfloor. \quad (5.1.119)$$

The decimal part of a real number is then necessarily greater than or equal to 0 and less than 1. Above we have that the integration variable x satisfies:

$$n \leq \frac{x}{\ell} \leq n+1. \quad (5.1.120)$$

Immediately then the integer part of $\frac{x}{\ell}$ is n . So:

$$\frac{x}{\ell} = \lfloor \frac{x}{\ell} \rfloor + \% \left(\frac{x}{\ell} \right) = n + \% \left(\frac{x}{\ell} \right) \quad (5.1.121)$$

$$\implies x_n = \ell n = x - \ell \% \left(\frac{x}{\ell} \right). \quad (5.1.122)$$

This allows us to rewrite our expectation as:

$$\mathbb{E}(X_\ell) = \sum_{n \in \mathbb{Z}} \int_{x_n}^{x_n+\ell} \left(x - \ell \% \left(\frac{x}{\ell} \right) \right) f_X(x) dx = \int_{-\infty}^{\infty} \left(x - \ell \% \left(\frac{x}{\ell} \right) \right) f_X(x) dx. \quad (5.1.123)$$

Because the fractional part is bounded above by 1:

$$0 \leq \ell \% \left(\frac{x}{\ell} \right) < \ell \quad (5.1.124)$$

$$\implies 0 \leq \lim_{\ell \rightarrow 0^+} \ell \% \left(\frac{x}{\ell} \right) \leq 0 \quad (5.1.125)$$

$$\implies \lim_{\ell \rightarrow 0^+} \ell \% \left(\frac{x}{\ell} \right) = 0. \quad (5.1.126)$$

So, in the $\ell \rightarrow 0^+$ limit:

$$\lim_{\ell \rightarrow 0^+} \mathbb{E}(X_\ell) = \lim_{\ell \rightarrow 0^+} \int_{-\infty}^{\infty} \left(x - \ell \% \left(\frac{x}{\ell} \right) \right) f_X(x) dx = \int_{-\infty}^{\infty} x f_X(x) dx. \quad (5.1.127)$$

Thus, for a continuous random variable the expectation is defined as:

$$\boxed{\mathbb{E}(X) = \int_{-\infty}^{\infty} x f_X(x) dx.} \quad (5.1.128)$$

The fact that the change of variables formula for pdf's matches the change of variables formula for the

Dirac delta gives a very convenient result. Consider the expectation:

$$\mathbb{E}(\delta(y - g(X))) = \int_{-\infty}^{\infty} \delta(y - g(x)) f_X(x) dx \quad (5.1.129)$$

and use the Dirac delta change of variables formula:

$$\delta(y - g(x)) = \sum_{x_k | g(x_k) = y} \frac{\delta(x - x_k)}{|g'(x_k)|}. \quad (5.1.130)$$

Then:

$$\mathbb{E}(\delta(y - g(X))) = \int_{-\infty}^{\infty} \sum_{x_k | g(x_k) = y} \frac{\delta(x - x_k)}{|g'(x_k)|} f_X(x) dx = \sum_{x | g(x) = y} \frac{f_X(x)}{|g'(x)|} = f_{g(X)}(y). \quad (5.1.131)$$

Hence, this expectation of the Dirac delta gives an easy way of expressing the distribution of a function of a random variable:

$$\boxed{f_{g(X)}(y) = \mathbb{E}(\delta(y - g(X)))}. \quad (5.1.132)$$

This makes it quite easy to prove the law of the unconscious statistician for continuous random variables as:

$$\mathbb{E}(g(X)) = \int_{-\infty}^{\infty} y f_{g(X)}(y) dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y \delta(y - g(x)) f_X(x) dy dx = \int_{-\infty}^{\infty} g(x) f_X(x) dx. \quad (5.1.133)$$

The last formula is exactly what we expected. The raw moments, central moments, and normalized central moments of a continuous random variable are all defined in the same way as the discrete case:

$$M_n = \mathbb{E}(X^n), \quad \bar{M}_n = \mathbb{E}(X - \mu_X)^n, \quad m_n = \mathbb{E}\left(\frac{X - \mu}{\sigma}\right)^n. \quad (5.1.134)$$

The mean still exactly has the interpretation as the best guess value which minimizes the expected squared error and the variance still exactly has the interpretation as that minimized value of the expected squared error. The median's definition and interpretation are unchanged as well.

So far we have only considered real valued continuous random variables. Now let us consider a random variable which takes a value in $\mathbb{R}^d$ so that $X(\omega) : \Omega \rightarrow \mathbb{R}^d$. Then, for M a region in $\mathbb{R}^d$, we can consider the probability that X lies within that region M . The probability density function for X is defined as the function so that the probability that X is in M is given by integrating that pdf over the region M :

$$\boxed{\text{Prob}(X \in M) = \int_M f_X(\vec{x}) d^d \vec{x}}. \quad (5.1.135)$$

Because the probability is necessarily non-negative for all M , $f_X(\vec{x})$ must be non-negative for all $\vec{x}$. However, because $f_X(\vec{x})$ is again not a probability it is not required to be less than 1. We can also develop a change of variables formula for this more general case. Consider a new random variable $Y = \vec{F}(X)$ where F is an invertible function from $\mathbb{R}^d$ into $\mathbb{R}^d$. Then, define the set $\vec{F}(M) = \{\vec{F}(\vec{x}) : \vec{x} \in M\}$. By definition of the probability density function:

$$\text{Prob}(Y \in \vec{F}(M)) = \int_{\vec{F}(M)} f_Y(\vec{y}) d^d \vec{y}. \quad (5.1.136)$$

We can compute the left hand side though using the pdf for X because, owing to the invertibility of $\vec{F}$, $X \in M$ if and only if $Y \in \vec{F}(M)$. Therefore:

$$\text{Prob}(Y \in \vec{F}(M)) = \text{Prob}(X \in M) = \int_M f_X(\vec{x}) d^d \vec{x} \quad (5.1.137)$$

$$\implies \int_{\vec{F}(M)} f_Y(\vec{y}) d^d \vec{y} = \int_M f_X(\vec{x}) d^d \vec{x}. \quad (5.1.138)$$

We can change variables in the integral on the left hand side to the integration variable $\vec{x}$ so that $\vec{y} = \vec{F}(\vec{x})$. Then using the standard Jacobian change of variables formula for integration:

$$\int_{\vec{F}(M)} f_Y(\vec{y}) d^d \vec{y} = \int_M f_Y(\vec{F}(\vec{x})) \left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} \right) \right| d^d \vec{x} \quad (5.1.139)$$

$$\implies \int_M f_Y(\vec{F}(\vec{x})) \left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} \right) \right| d^d \vec{x} = \int_M f_X(\vec{x}) d^d \vec{x}. \quad (5.1.140)$$

This is true for all integration regions M and so we have:

$$f_Y(\vec{F}(\vec{x})) \left| \det \left(\frac{\partial \vec{F}}{\partial \vec{x}} \right) \right| = f_X(\vec{x}) \quad (5.1.141)$$

$$\implies \boxed{f_Y(\vec{y}) = \frac{f_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|}} \quad (5.1.142)$$

where $\vec{y} = \vec{F}(\vec{x})$. Just as with the single variable case, this is precisely the change of variables formula satisfied by the multidimensional Dirac delta found in problem 3.3.

We can also generalize the expectation of the Dirac delta formula we found for changing variables in the single variable case to the multivariable case. Let $\vec{F}(\vec{x})$ be function from $\mathbb{R}^d$ into $\mathbb{R}^{d'}$ where $d' \leq d$. We will not expect this function to be invertible. Let $Y = \vec{F}(X)$ be a random variable. Then, the pdf for Y is by definition the function which satisfies:

$$\text{Prob}(Y \in N) = \int_N f_Y(\vec{y}) d^{d'} \vec{y}. \quad (5.1.143)$$

Let M be the set of values of X so that $\vec{F}(X) \in N$. Then, because $Y \in N$ if and only if $X \in M$, we immediately have:

$$\text{Prob}(Y \in N) = \text{Prob}(X \in M) = \int_M f_X(\vec{x}) d^d \vec{x} \quad (5.1.144)$$

$$\implies \int_N f_Y(\vec{y}) d^{d'} \vec{y} = \int_M f_X(\vec{x}) d^d \vec{x}. \quad (5.1.145)$$

We can rewrite the second integral by inserting a Dirac delta:

$$\int_{\mathbb{R}^{d'}} \delta(\vec{y} - \vec{F}(\vec{x})) d^{d'} \vec{y} = 1 \quad (5.1.146)$$

$$\implies \int_M f_X(\vec{x}) d^d \vec{x} = \int_{\mathbb{R}^{d'}} \int_M f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} d^{d'} \vec{y}. \quad (5.1.147)$$

The interior integrand is only non-zero for $\vec{y}$ which are in N due to the Dirac delta. So, we can reduce the integration region $\mathbb{R}^{d'}$ to N:

$$\int_M f_X(\vec{x}) d^d \vec{x} = \int_N \int_M f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} d^{d'} \vec{y}. \quad (5.1.148)$$

We can also replace the integration region M with $\mathbb{R}^d$ on the right hand side because the Dirac delta is 0 for all $\vec{x}$ outside of M whenever $\vec{y}$ is in N. Thus:

$$\int_M f_X(\vec{x}) d^d \vec{x} = \int_N \int_{\mathbb{R}^d} f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} d^{d'} \vec{y}. \quad (5.1.149)$$

Finally then, from equation (5.1.145) we have:

$$\int_N f_Y(\vec{y}) d^{d'} \vec{y} = \int_N \left(\int_{\mathbb{R}^d} f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} \right) d^{d'} \vec{y}. \quad (5.1.150)$$

for all integration regions N and thus:

$$f_Y(\vec{y}) = \int_{\mathbb{R}^d} f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x}. \quad (5.1.151)$$

This is the general change of variables formula regardless of whether $\vec{F}$ is invertible or even if $\vec{y}$ has the same dimension as $\vec{x}$.

Each component of X is just a real valued random variable. Let X^a be component a of X . Its expectation is then defined by the single variable formula (with no implicit summation intended anywhere in this calculation):

$$\mathbb{E}(X^a) = \int_{-\infty}^{\infty} x f_{X^a}(x) dx. \quad (5.1.152)$$

The pdf for a single component of X , called the marginal distribution for that component, can be computed easily from our change of variables formula:

$$f_{X^a}(x) = \int_{\mathbb{R}^d} f_X(\vec{x}') \delta(x - x'^a) d^d \vec{x}' = \int_{\mathbb{R}^{d-1}} f_X(x^1, \dots, x^{a-1}, x, x^{a+1}, \dots, x^d) dx^1 \dots dx^{a-1} dx^{a+1} \dots dx^d. \quad (5.1.153)$$

That is, the marginal distribution for a single component is gotten by just “integrating out” all of the other components. With this, the expectation for that single component becomes:

$$\mathbb{E}(X^a) = \int_{-\infty}^{\infty} x \int_{\mathbb{R}^{d-1}} f_X(x^1, \dots, x^{a-1}, x, x^{a+1}, \dots, x^d) dx^1 \dots dx^{a-1} dx^{a+1} \dots dx^d dx = \int_{\mathbb{R}^d} x^a f_X(\vec{x}) d^d \vec{x}. \quad (5.1.154)$$

So, because the expectation of each component of X is given by integrating that component against the pdf for X , the expectation of X is defined as:

$$\boxed{\mathbb{E}(X) = \int_{\mathbb{R}^d} \vec{x} f_X(\vec{x}) d^d \vec{x}.} \quad (5.1.155)$$

Plainly, component a of $\mathbb{E}(X)$ is simply $\mathbb{E}(X^a)$. From this we can prove the completely general law of the unconscious statistician:

$$\mathbb{E}(\vec{F}(X)) = \int_{\mathbb{R}^{d'}} \vec{y} f_Y(\vec{y}) d^{d'} \vec{y} = \int_{\mathbb{R}^{d'}} \vec{y} \int_{\mathbb{R}^d} f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} d^{d'} \vec{y} \quad (5.1.156)$$

$$= \int_{\mathbb{R}^{d'}} \int_{\mathbb{R}^d} \vec{F}(\vec{x}) f_X(\vec{x}) \delta(\vec{y} - \vec{F}(\vec{x})) d^d \vec{x} d^{d'} \vec{y} = \int_{\mathbb{R}^d} \vec{F}(\vec{x}) f_X(\vec{x}) \int_{\mathbb{R}^{d'}} \delta(\vec{y} - \vec{F}(\vec{x})) d^{d'} \vec{y} d^d \vec{x} \quad (5.1.157)$$

$$= \int_{\mathbb{R}^d} \vec{F}(\vec{x}) f_X(\vec{x}) d^d \vec{x}. \quad (5.1.158)$$

From this, we can immediately express the general change of variables formula as:

$$\boxed{f_Y(\vec{y}) = \mathbb{E}(\delta(\vec{y} - \vec{F}(X))).} \quad (5.1.159)$$

One potentially counterintuitive fact, at least initially, about continuous random variables is that for a continuous random variable with a bounded pdf, the probability that that variable takes any particular exact value is 0. By definition, the probability that a real valued random variable is in the interval $(a, b]$ is:

$$\text{Prob}(a < X \leq b) = \int_a^b f_X(x) dx. \quad (5.1.160)$$

As $b \rightarrow a$ this interval becomes the single point $X = a$. Therefore:

$$\text{Prob}(X = a) = \lim_{b \rightarrow a^+} \int_a^b f_X(x) dx. \quad (5.1.161)$$

If $f_X(x)$ is a bounded function then this integral goes to 0 as its integration region limits to null. Therefore, for the overwhelmingly typical case the probability that $X = a$ is 0 for all a . This does **NOT** mean X cannot equal a . That is not how probability works! All this says is that we overwhelmingly disbelieve that X will *exactly* equal a . For all practical purposes, one has finite error bars on measurements and should be concerned with the probability that X is between $a - \delta a$ and $a + \delta a$ where δa is your experimental resolution. Similarly, for continuous random variables the situation with conditional probability is much more subtle. In particular, because the probability that a random variable takes an exact value is generally 0, you cannot sensibly define a probability space conditioned on a random variable taking an exact value. That event has probability 0 and conditional probability would require then dividing by 0 according to equation (5.1.7). In order to meaningfully do conditional probability with continuous random variables, one must condition on that variable being in a range, not exactly at a point. Do not haphazardly try to condition on an event of probability 0, please!

Independence is often an important concept for continuous random variables. Naturally, two real valued random variables are independent if knowing that one variable lies in an interval tells you nothing about the distribution of the other. So, independence of X and Y are given by the condition:

$$\text{Prob}(c < Y \leq d | a < X \leq b) = \text{Prob}(c < Y \leq d) \quad (5.1.162)$$

$$\implies \frac{\text{Prob}(c < Y \leq d \cap a < X \leq b)}{\text{Prob}(a < X \leq b)} = \text{Prob}(c < Y \leq d) \quad (5.1.163)$$

$$\implies \int_c^d \int_a^b f_{(X,Y)}(x,y) dx dy = \int_c^d f_Y(y) dy \int_a^b f_X(x) dx. \quad (5.1.164)$$

For X and Y to be independent this must be true for all intervals and so we may differentiate both sides with respect to b and d to have:

$$f_{(X,Y)}(b,d) = f_X(b)f_Y(d). \quad (5.1.165)$$

Statistical independence for continuous random variables means that their probability densities multiply!

An important concept for multiple random variables is their correlation. For two numerically valued random variables X and Y the correlation or covariance is defined as:

$$\boxed{\text{Cov}(X,Y) = \mathbb{E}((X - \mathbb{E}(X))(Y - \mathbb{E}(Y)))}. \quad (5.1.166)$$

Automatically we can see that the variance of a random variable is its covariance with itself:

$$\text{Var}(X) = \mathbb{E}(X - \mathbb{E}(X))^2 = \text{Cov}(X, X). \quad (5.1.167)$$

By expanding out the products in the definition of the covariance formula and simplifying, we find the shorter formula:

$$\text{Cov}(X,Y) = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y). \quad (5.1.168)$$

If two random variables are independent then automatically a short calculation gives:

$$\text{Cov}(X,Y) = 0. \quad (5.1.169)$$

However, the converse is **NOT** true. Two variables may have vanishing correlation but that is absolutely not enough to conclude that they are independent. Independence implies the much stronger condition that if we consider the correlation of any two functions of the random variables individually and use the law of the unconscious statistician:

$$\text{Cov}(F(X), G(Y)) = 0. \quad (5.1.170)$$

That is, if two variables are independent the correlation of any functions each individually of those two random variables is 0. Now suppose two random variables X and Y satisfy the property that for any functions of each individually the correlation of those two functions as random variables is 0. Then, take:

$$F(x) = \delta(x - x_0), \quad G(y) = \delta(y - y_0) \quad (5.1.171)$$

for some constants x_0 and y_0 . The vanishing correlation condition then becomes:

$$\text{Cov}(F,G) = f_{(X,Y)}(x_0, y_0) - f_X(x_0)f_Y(y_0) \stackrel{!}{=} 0. \quad (5.1.172)$$

Hence, two random variables X, Y are independent if and only if the correlation $\text{Cov}(F(X), G(Y))$ vanishes for any functions F, G .

5.1.4 (2nd Pass) Overly Philosophical Rambling

I described probability as the mathematical formalism of how to systematically manage incomplete information. This understanding leads to thinking about the randomness that occurs in everyday life and experiments as being due to deterministic rules of time evolution but with some unknown exact values of some variables. Some may argue that while this is a version of probability, there is another version I have not discussed. More specifically, one may consider the idea of a fundamentally probabilistic or fundamentally random system meaning a system whose rules of time evolution themselves are nondeterministic so that no amount of additional information could determine the outcome of them. When applied to physics, I do not believe this to be a meaningful or valid scientific concept (for quite trivial reasons).

At each time t the universe is in some state $\Phi(t)$. The full function $\Phi(t)$ for all t is then a set of information $\mathcal{I}$. If at time t_1 you were given the additional information $\mathcal{I}$ you would then know the state of the universe at time $t_2 > t_1$ simply by reading off $\Phi(t_2)$ within that information and thus there always exists some information such that if you are allowed to know that information the system is deterministic. The fact that the universe exists and it does not seem possible (or even seem to make sense as an idea) to “repeat” an exact moment in time means that each event in the universe simply happens. It is not possible to do “repeat trials” of exact moments in the universe and so it is not possible to check if in literally the exact same scenario a different result would or would not be achieved. The time evolution of the universe is trivially deterministic because it is simply determined by what actually happens. Even if one did have an exact repeated state of the universe so that $\Phi(t_1) = \Phi(t_2)$ for $t_1 \neq t_2$ and then had that $\Phi(t_1 + \delta t) \neq \Phi(t_2 + \delta t)$ so

that apparently deterministic time evolution was broken, this could alternatively be explained by a violation of time translation symmetry. It is always possible to make the t dependence of the U function in (1.1.1) be such that whatever $\Phi(t)$ you want is found with deterministic time evolution but perhaps without time translation symmetry. Thus, in an experiment it is never possible to distinguish a violation of determinism from a violation of time translational symmetry.

The deterministic rule I gave above for the time evolution of the universe is very stupid. It can simply be said as “at each time everything is the way it is”, which is true but not useful. (I only waste time making that vacuous statement to illustrate how equivalently vacuous of an idea fundamental probabilism is.) The goal in physics is to find as simple of a description of as much of the time evolution of the universe as possible. We want our description to have predictive power (meaning using math it should be able to turn information about the present into information about other times). However, any description we ever have will necessarily have limited predictive power because we will always only have limited information about the present (due to the finite precision of measurements, the fact that seemingly much of the universe is outside of our past lightcone, and so on). Because of this lack of information probability will always be an essential part of actually doing physics. But, this gives precisely zero evidence for the idea of fundamental randomness. While some systems may be most readily and helpfully described probabilistically it does not mean that the actual world being described is probabilistic. When we do physics we only ever find a description of the world around us; do not confuse our status quo best description with the actual universe itself. **You cannot drink a theory of hydrodynamics.** Some readers might believe this discussion will later be modified or made more complicated when we begin doing quantum mechanics; it will not. None of the experimental or theoretical structure of classical, statistical, or quantum physics contradicts or conflicts with determinism. Some aspects of quantum mechanics we will discuss in Part II conflict with certain naive assumptions about which parts of a system may be meaningfully treated as statistically independent but say nothing about determinism. If in your head you are shouting “But what about Bell’s theorem!”, I encourage you to read [79] and to wait until Part II. Bell’s theorem does not imply what you probably think it implies.

Exercises

Problem 5.1: ★ Characteristic function of a probability distribution. For making calculations with probability distributions one of the most useful tools is the characteristic function of that distribution. For a single real valued random variable X , define the characteristic function $\varphi_X(t)$ by:

$$\varphi_X(t) = \mathbb{E}e^{itX}.$$

- Let the pdf of X be $f_X(x)$. Show that $\varphi_X(t)$ (up to a normalization convention) is the Fourier transform of $f_X(x)$.
- Show that $f_X(x)$ can be recovered from $\varphi_X(t)$ using the inverse Fourier transform.
- Show that $\varphi_X(t)$ exists/converges for all random variables X .
- Suppose $\varphi_X(t)$ has a Taylor series about 0. Show then that the Taylor series for $\varphi_X(t)$ gives:

$$\mathbb{E}(X^n) = \frac{1}{i^n} \left(\frac{\partial}{\partial t} \right)^n \varphi_X(t) \Big|_{t=0}.$$

Problem 5.2: Addition of Independent Random Variables. Let X and Y be independent real valued random variables with pdfs $f_X(x)$ and $f_Y(y)$ and let $Z = X + Y$.

- Show that the pdf for Z is given by:

$$f_Z(z) = \int_{-\infty}^{\infty} f_X(x)f_Y(z-x)dx.$$

- Show that characteristic functions of the three variables are related by:

$$\varphi_Z(t) = \varphi_X(t)\varphi_Y(t).$$

Problem 5.3: Bernoulli Distribution. The most simple non-trivial probability distribution is the Bernoulli Distribution, which is just a (possibly unfair) coin flip. A Bernoulli random variable X takes the value 1 with probability φ and the value 0 with probability $1 - \varphi$ where φ is called the success probability and thus is a real number in the interval $[0, 1]$.

- Show that the pmf for the Bernoulli Distribution is:

$$p(x) = \varphi^x(1 - \varphi)^{1-x}$$

where x may take the values of 0 or 1.

- (b) Show that the characteristic function for the Bernoulli distribution is:

$$\varphi(t) = 1 - \wp + \wp e^{it}.$$

- (c) Show that the moments of the Bernoulli distribution are given by:

$$\mathbb{E}(X^n) = \wp$$

for all integer $n > 0$.

Problem 5.4: Binomial Distribution. The Bernoulli distribution represents a trial in which there is a single success or failure. If one takes many identically independently distributed (iid) such trials and considers the distribution of the total number of successes and total number of failures, the result is the binomial distribution. Let $X_1, \dots, X_N$ be iid Bernoulli trials (meaning independent and with the same $\wp$) and let $Y = X_1 + \dots + X_N$. Then, Y has the binomial distribution.

- (a) Show using the result of problem 5.2 that the characteristic function of the binomial distribution is:

$$\varphi(t) = (1 - \wp + \wp e^{it})^N.$$

- (b) Use the binomial theorem and the inverse Fourier transform to show that the binomial distribution has pmf:

$$p(n) = \frac{N!}{n!(N-n)!} \wp^n (1-\wp)^{N-n}$$

where n is the total number of successes and thus is an integer between 0 and N .

- (c) Show that the mean and variance of the binomial distribution are:

$$\mu = \wp N, \quad \sigma^2 = N\wp(1-\wp)$$

and that these are simply N times the corresponding values for a Bernoulli distribution. Show that this pattern does not hold for the higher order central moments.

Problem 5.5: Multinoulli and Multinomial Distributions. Just like the Bernoulli distribution is the distribution of a general coin flip, the multinoulli distribution is the distribution of a general dice roll. Let $\wp_1, \dots, \wp_d$ be probabilities which add up to 1 and d a positive integer. Then, a random variable X is multinoulli distributed if it equals the value k with probability $\wp_k$. If $d = 6$ and $\wp_k = 1/6$ then we have a standard fair six sided die. Otherwise, this is a generalization which allows an unfair die of any number of sides. For $d = 2$, this is a Bernoulli distribution (up to an overall shift of the random variable by 1).

- (a) Show that the characteristic function of the multinoulli distribution is given by:

$$\varphi(t) = \wp_1 e^{it} + \dots + \wp_d e^{idt}.$$

- (b) When adding multinoulli distributions there are two interesting ways to do it. One could add the results of the different dice rolls directly or count the occurrences of each roll outcome. For $d = 2$ these are essentially the same as the sum of roll results tells you the number of the successes and the number of rolls minus successes equals the number of failures. For $d > 2$ these are different. The first of these where we just add the dice rolls directly will not be so useful for us. Instead, we will care about counting the occurrences of each result. We can still formulate this as a sum by introducing the “bucket” multinoulli distribution. Let the list $(n_1, \dots, n_d)$ be the number of occurrences of the multinoulli giving outcome 1, 2, ..., d . Then, a single multinoulli trial gives $(1, 0, \dots, 0)$ with probability $\wp_1$, ..., $(0, \dots, 0, 1)$ with probability $\wp_d$. Let the multivariable characteristic function be defined by:

$$\varphi(t_1, \dots, t_d) = \mathbb{E} e^{it_1 n_1 + \dots + it_d n_d}.$$

Show that for the bucket multinoulli distribution this gives:

$$\varphi(t_1, \dots, t_d) = \wp_1 e^{it_1} + \dots + \wp_d e^{it_d}.$$

- (c) Now let us actually consider N iid multinoulli trials. The sum of the bucket multinoulli variables (adding the lists component by component) gives a list $(n_1, \dots, n_d)$ with the total number of occurrences of each possible value of the multinoulli trial. Show that the pmf for this list is:

$$p(n_1, \dots, n_d) = \frac{N!}{n_1! \dots n_d!} \wp_1^{n_1} \dots \wp_d^{n_d}$$

where $0 \leq n_k \leq N$ and $n_1 + \dots + n_d = N$. This distribution is known as the multinomial distribution and we see that it represents the distribution of results of counting the occurrences of different outcomes

of independent trials of a given random variable.

Problem 5.6: ★ The Gamma function and Sterling's Theorem.

- (a) Define the Gamma function $\Gamma(x)$ by:

$$\Gamma(x) \stackrel{\text{def}}{=} \int_0^{\infty} e^{-t} t^{x-1} dt.$$

Show using integration by parts that the Gamma function satisfies the identity:

$$\Gamma(x+1) = x\Gamma(x).$$

As well, show that $\Gamma(1) = 1$ and that for non-negative integer n :

$$n! = \Gamma(n+1) = \int_0^{\infty} e^{-t} t^n dt.$$

Thus, the Gamma function (up to a shift in the argument by 1) acts as a generalization of the factorial to continuous argument.

- (b) It will be useful for us to understand how $N!$ behaves for large N . Using the expression derived for $N!$ make the change of integration variable to $z = \frac{t-N}{\sqrt{N}}$. Show that:

$$N! = N^{N+\frac{1}{2}} e^{-N} \int_{-\sqrt{N}}^{\infty} e^{-\sqrt{N}z} \left(1 + \frac{z}{\sqrt{N}}\right)^N dz.$$

- (c) Define Sterling's function $\text{St}(N)$ by:

$$\text{St}(N) \stackrel{\text{def}}{=} \frac{N!}{\sqrt{2\pi N} e^{-N} N^N}.$$

Show that exactly:

$$\text{St}(N) = \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{N}}^{\infty} e^{-\sqrt{N}z} \left(1 + \frac{z}{\sqrt{N}}\right)^N dz$$

and that in the limit $N \rightarrow \infty$ the above integral becomes a Gaussian integral so that:

$$\lim_{N \rightarrow \infty} \text{St}(N) = 1.$$

Thus, we can always express the factorial as:

$$N! = \sqrt{2\pi N} e^{-N} N^N \text{St}(N)$$

and for large N the Sterling's function appearing here simply approaches 1 (and it does so quite quickly). This result is known as Sterling's theorem.

Problem 5.7: Poisson Distribution. Consider a type of event which occurs discretely (such as lightning striking) but which may happen at any moment in time. In any given sub-interval of time, the event either happens or it does not and so it can be viewed as a Bernoulli trial. The total number of occurrences is then given by summing over each such Bernoulli trial (assuming that in these sub-intervals the event does not happen more than once) and so can be viewed as a binomial distribution. In order for the event to not occur more than once in each sub-interval we need to take the time of the sub-intervals to limit toward 0. This means we need to consider a large number of Bernoulli trials and thus have a binomial distribution with large N . In order to keep the average number of events finite, we need that average $\mu = \varphi N$ (using the binomial distribution mean) to remain fixed as $N \rightarrow \infty$. This defines the Poisson distribution: the distribution of the number of counts of independently occurring discrete events over a continuous interval. It is equivalently given by a binomial distribution with $N \rightarrow \infty$ and $\varphi = \frac{\mu}{N}$ where μ is fixed.

- (a) Show using the formula for the binomial distribution and Sterling's theorem that the Poisson distribution has pmf:

$$p(n) = \frac{e^{-\mu}}{n!} \mu^n.$$

- (b) Show that the characteristic function of the Poisson distribution is:

$$\varphi(t) = e^{\mu(e^{it}-1)}$$

and that the mean and variance of the Poisson distribution are both equal to μ .

Problem 5.8: Gaussian Distribution. Suppose that N iid Bernoulli trials with success probability $\wp$ are performed and an object is moved to the left by ℓ each time 0 is obtained and right by r each time 1 is obtained.

- (a) If X_k is Bernoulli trial k and Y_k is how much the object is moved due to that trial, show that:

$$Y_k = -\ell + (r + \ell)X_k$$

and that the mean and variance of Y_k are given by:

$$\mathbb{E}Y_k = (r + \ell)\wp - \ell, \quad \text{Var}(Y_k) = (r + \ell)^2\wp(1 - \wp).$$

- (b) Let Z be the total displacement of the object after the N trials. Show that it is given by:

$$Z = \sum_{k=1}^N Y_k = -N\ell + (r + \ell) \sum_{k=1}^N X_k$$

with mean, variance, and characteristic function:

$$\mathbb{E}Z = -N\ell + N(r + \ell)\wp, \quad \text{Var}(Z) = N(r + \ell)^2\wp(1 - \wp), \quad \varphi(t) = e^{-iN\ell t} \left(1 - \wp + \wp e^{i(r+\ell)t}\right)^N.$$

- (c) Assume that we take $N \rightarrow \infty$ while keeping the mean μ and variance σ^2 of Z fixed. Show that in this limit the characteristic function of Z becomes:

$$\varphi(t) = e^{i\mu t - \frac{\sigma^2 t^2}{2}}$$

and that consequently the pdf of Z becomes (using the Gaussian integral):

$$f(z) = \frac{e^{-\frac{(z-\mu)^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}}.$$

This is known as the Gaussian (or Normal) distribution with mean μ and variance σ^2 . As we see it is the distribution of the total of a sum of many independent small up or down fluctuations.

- (d) Show that the sum of independent Gaussians is Gaussian with mean and variance both given by the sums of the means and variances of the individual Gaussians.

Problem 5.9: Cauchy Distribution. Let X and Y be independent Gaussian random variables with mean 0 and variances σ_1^2 and σ_2^2 . Let $Z = z_0 + \frac{Y}{X}$ where z_0 is a constant and let $\Gamma = 2\frac{\sigma_2^2}{\sigma_1^2}$. This Z follows the Cauchy distribution (also called the Lorentz distribution by physicists, or the Breit-Wigner distribution by high-energy physicists).

- (a) Show that the pdf for Z is given by:

$$f(z) = \frac{\Gamma}{2\pi} \frac{1}{\frac{\Gamma^2}{4} + (z - z_0)^2}.$$

- (b) Show that the mode and median of Z are z_0 (and so z_0 is called the center or maximum of the distribution). As well, show that at $z = z_0 \pm \frac{\Gamma}{2}$ the pdf is half of its maximum value and so the interval over which the pdf is at least half its maximum value has width Γ . This Γ is correspondingly called the full-width at half-maximum (FWHM) of the distribution.
- (c) Show that the characteristic function of the Cauchy distribution is:

$$\varphi(t) = e^{iz_0 t - \frac{\Gamma}{2}|t|}.$$

Consequently, show that neither the mean, the variance, nor any other higher moments of the Cauchy distribution exist (they do not converge).

Problem 5.10: Geometric Distribution. Suppose we have a (potentially unfair) coin with success (heads) probability $\wp$ and that we flip the coin over and over until we get heads, then we stop. The distribution on the number of flips we must perform is called the geometric distribution.

- (a) Show that the probability we have not yet received heads after n flips is $(1 - \wp)^n$. Using this, show that the pmf for the geometric distribution (the probability we stop after precisely n flips) is:

$$p(n) = \wp(1 - \wp)^{n-1}$$

- (b) Show that the characteristic function for the geometric distribution is:

$$\varphi(t) = \frac{\wp}{e^{-it} - 1 + \wp}$$

and that its mean is $\frac{1}{\wp}$ and variance is $\frac{1-\wp}{\wp^2}$.

Problem 5.11: Exponential Distribution. Suppose we have a geometric distribution where we flip the coin with a frequency f (meaning ft flips occur in a time t) which we take to limit toward infinity while keeping the average time it takes for a success to happen to be fixed. The resulting random variable is said to be exponentially distributed. Such a distribution then describes the time it takes for an event which may happen independently at any moment in time to happen for the first time. This is the common distribution for decay processes where one material transitions into another at some rate which is predictable on average. Similarly, if a tool is used for a task continuously but may break independently at any time, the exponential distribution is appropriate for modeling how long the tool will last.

- (a) For our geometric distribution and finite f , let T be the random variable giving the time at which we stop flipping. Show that the coin is flipped for the n^{th} time at time $\frac{n}{f}$ and that T has the characteristic function:

$$\varphi(s) = \mathbb{E}e^{isT} = \frac{\wp}{e^{-i\frac{s}{f}} - 1 + \wp}$$

where $\wp$ is defined as in the geometric distribution question.

- (b) Now suppose we take $f \rightarrow \infty$ as described and let $\tau = \mathbb{E}T$ called the lifetime of the event be fixed. Show that $\wp = \frac{1}{f\tau}$ and that in the $f \rightarrow \infty$ limit:

$$\varphi(s) = \frac{1}{1 - is\tau}.$$

Consequently, show that the pdf of the exponential distribution is:

$$f(t) = \frac{1}{\tau} e^{-\frac{t}{\tau}} \vartheta(t)$$

and that its mean is τ and variance is τ^2 .

Problem 5.12: Gamma Distribution. Suppose we have N continuously flipped coins as described in the previous question (and so all with the same lifetime τ). We flip the first coin until we get a success, then we immediately start to flip the second coin until we get a success, and so on until we finish flipping the last coin. The total time T it takes for us to finish flipping all of the coins is distributed according to the Gamma distribution. In the tool analogy, if we had a batch of N such tools where we use one at a time until it breaks and then switch to the next tool, the Gamma distribution would be appropriate for modeling how long it takes us to run out of tools.

- (a) Show that T is the sum of N identically independently distributed exponential distributions.
 (b) Show that the characteristic function of the Gamma distribution can be written as:

$$\varphi(s) = \frac{1}{(1 - is\tau)^N} = \frac{1}{(N-1)!(i\tau)^{N-1}} \left(\frac{\partial}{\partial s} \right)^{N-1} \frac{1}{1 - is\tau}.$$

- (c) Show that the pdf of the Gamma distribution is:

$$f(t) = \frac{t^{N-1}}{\Gamma(N)\tau^N} e^{-\frac{t}{\tau}} \vartheta(t)$$

and that its mean is $N\tau$ and variance is $N\tau^2$.

- (d) Let $Z = \frac{T - N\tau}{\sqrt{N\tau}}$. Show that in the $N \rightarrow \infty$ limit Z is distributed according to the normal distribution with mean 0 and variance 1. So, explain that in the large N limit a Gamma distribution behaves like a normal distribution with mean $N\tau$ and variance $N\tau^2$.

Problem 5.13: Beta Distribution. Suppose we have $N_1 + N_2$ tools as in the previous question. Suppose we use the first N_1 of them one at a time until they all break. Let T_1 be the time it takes for those N_1 tools to break and let T_2 be the time it takes for the remaining N_2 tools to break after that. Let $R = \frac{T_1}{T_1 + T_2}$ be the fraction of the total use time we got out of the full set of $N_1 + N_2$ which was spent solely on the first N_1 tools. That is, R represents the fraction of the total use time the N_1 tools contribute. This R is distributed according to the Beta distribution.

- (a) Show that the pdf of the Beta distribution must satisfy:

$$f_R(r) = \int_{-\infty}^{\infty} \delta\left(\frac{t_1}{t_1 + t_2} - r\right) f_1(t_1) f_2(t_2) dt_1 dt_2$$

where $f_1(t_1)$ and $f_2(t_2)$ are the pdf's of the N_1 and N_2 tool sets:

$$f_1(t_1) = \frac{t_1^{N_1-1}}{\Gamma(N_1)\tau^{N_1}} e^{-\frac{t_1}{\tau}} \vartheta(t_1), \quad f_2(t_2) = \frac{t_2^{N_2-1}}{\Gamma(N_2)\tau^{N_2}} e^{-\frac{t_2}{\tau}} \vartheta(t_2).$$

- (b) Complete the integration in the previous part to show that the Beta distribution is explicitly given by:

$$f_R(r) = \frac{\Gamma(N_1 + N_2)}{\Gamma(N_1)\Gamma(N_2)} r^{N_1-1} (1-r)^{N_2-1}$$

for $r \in [0, 1]$ and 0 otherwise.

- (c) Show that the normalization of the Beta distribution immediately implies the (non-obvious) identity:

$$\int_0^1 r^{N_1-1} (1-r)^{N_2-1} dr = \frac{\Gamma(N_1)\Gamma(N_2)}{\Gamma(N_1 + N_2)} = B(N_1, N_2)$$

where here we have defined the Beta function $B(N_1, N_2)$.

- (d) Show that the mean and variance of the Beta distribution are:

$$\mathbb{E}(R) = \frac{N_1}{N_1 + N_2}, \quad \text{Var}(R) = \frac{N_1 N_2}{(N_1 + N_2)^2 (N_1 + N_2 + 1)}.$$

Problem 5.14: Checking Coin Fairness. Suppose we have a coin with an unknown probability φ of flipping heads. We flip the coin N times and among those attempts we receive heads n times. Here we will develop an answer to the question: what is the best estimate for φ ?

- (a) Let D (short for data) be the event that we get n heads from N coin flips at fixed φ . Show that:

$$\text{Prob}(D|\varphi) = \frac{N!}{n!(N-n)!} \varphi^n (1-\varphi)^{N-n}.$$

- (b) Suppose you have a prior distribution $f(\varphi)$ which is the probability distribution giving your degree of belief in the possible values of φ before taking any data. Show using Bayes theorem that after collecting the data you should have posterior probability distribution $f(\varphi|D)$ for φ :

$$f(\varphi|D) = C(N, n) \varphi^n (1-\varphi)^{N-n} f(\varphi)$$

where $C(N, n)$ depends on N and n but does not depend on φ . Show that $C(N, n)$ is determined by the requirement that $f(\varphi|D)$ be a correctly normalized pdf.

- (c) A common choice of prior distribution for $f(\varphi)$ is:

$$f(\varphi) = \frac{1}{\pi} \frac{1}{\sqrt{\varphi(1-\varphi)}}$$

which is known as Jeffrey's prior for this problem. Because the prior distribution is intended to give your degrees of belief about the unknown parameters before collecting any data, there is no correct or incorrect prior to pick, it is literally subjective. However, there are correct or incorrect rationales given for why some priors are preferable or tend to give posterior distributions with more desirable properties. Because the posterior is proportional to the prior, any region on which the prior is identically 0 will always remain that way no matter what data is received. For this reason it is typically best to avoid choosing priors which have regions on which they are exactly 0, as they resist being corrected by data. This is a good reason. Another common line of reasoning is to choose a prior which is a uniform distribution because "if we know nothing about the problem, we should assume all values are equally probable". People who say this will call the uniform distribution an "uninformative prior". This is an incorrect reason. A uniform distribution does not stay uniform under a change of variables (if the distribution for φ is uniform then the distribution for φ^2 isn't) and so if uniform is intended to represent "uninformative" it only could possibly do so in a preferred system of variables. In fact, for a given $f(\varphi)$ there is a change of variables to a new variable $q = q(\varphi)$ so that q is uniformly distributed making the choice of a uniform prior nothing but selecting out which variable you say is preferred. A uniform prior is in this way extremely informative as it implicitly selects a favorite coordinate system. There is significant statistics literature debunking the idea of the existence of "uninformative" priors [19]. Jeffrey's prior is a formal system of creating priors which does not select out any special system of variables, however it isn't perfect either for reasons we will discuss later. Show that if you use Jeffrey's prior your posterior distribution is:

$$f(\varphi|D) = \frac{\Gamma(n + \frac{1}{2}) \Gamma(N - n + \frac{1}{2})}{\Gamma(N + 1)} \varphi^{n-\frac{1}{2}} (1-\varphi)^{N-n-\frac{1}{2}}.$$

Show that this is a Beta distribution with $N_1 = n + \frac{1}{2}$ and $N_2 = N - n + \frac{1}{2}$.

- (d) Show using the above posterior distribution that the best guess value of φ and the variance of φ are:

$$\mathbb{E}_{\varphi} = \frac{n + \frac{1}{2}}{N + 1}, \quad \text{Var}(\varphi) = \frac{(n + \frac{1}{2})(N - n + \frac{1}{2})}{(N + 1)^2(N + 2)}.$$

- (e) Let $q = \frac{n}{N}$ be the fraction of flips which are heads. By the frequentist understanding of probability as $N \rightarrow \infty$, q becomes the probability of flipping heads. Show using the results of the previous part that in the large N limit:

$$\mathbb{E}_{\varphi} = q, \quad \text{Var}(\varphi) = 0$$

and thus explain that in the limit of large data the Bayesian understanding of probability exactly matches the frequentist one.

Problem 5.15: Generating random variables with an arbitrary distribution. Suppose one has the ability to generate random numbers independently from each other each with the uniform distribution from 0 to 1. Let U be a random variable with this distribution. Let $F(x)$ be the cdf for a real valued random variable X . Show that the random variable $F^{-1}(U)$ is distributed exactly like X and so by “inverting the cdf” we can generate any random variable we like from a uniformly random variable. Essentially every computer has a “random number generator” which generates numbers “uniformly” from 0 to 1 and so this can be used to generate random variables with an arbitrary distribution on a computer¹.

Problem 5.16: The Law of Large Numbers. Suppose we have N random variables $X_1, \dots, X_N$ which are all identically independently distributed with finite mean μ . Let $\varphi_1(t)$ be the characteristic function of any of these random variables and let $\bar{X}$ be the sample mean of these variables:

$$\bar{X} = \frac{\sum_{k=1}^N X_k}{N}.$$

- (a) Show that the characteristic function $\varphi_N(t)$ for the sample mean is:

$$\varphi_N(t) = \varphi_1^N\left(\frac{t}{N}\right).$$

- (b) Show that for $\varphi_1(t)$:

$$\varphi_1(t) = 1 + i\mu t + o(t)$$

where the little o notation $o(t)$ means terms which go to 0 faster than t .

- (c) Using the results of the previous two parts show that in the large N limit:

$$\lim_{N \rightarrow \infty} \varphi_N(t) = \lim_{N \rightarrow \infty} \left(1 + \frac{i\mu t}{N} + o\left(\frac{t}{N}\right)\right)^N = e^{i\mu t}.$$

Thus show that in the large N limit the sample mean converges² to a constant random variable

¹There are many subtleties to computer randomness and number generation. Computers only generate decimal numbers to finite precision, not full real numbers and so they are only capable of exactly producing discrete random variables. Any “continuous” variables made by a computer are approximations. Because probability is the theory of how to manage incomplete information, data is said to be random if it is determined by information which is not known. What counts as random is consequently dependent on what information you have. The random number generators in computers compute those random numbers in a completely deterministic way but from obscure initial data. In some cases the computer simply performs a sophisticated calculation from some “seed” number already stored in the computer which produces a result that would be very difficult to predict unless one knew both the algorithm used and the seed. Such a computation is called “pseudorandom”. Other times, the computer uses a seed given by the results of physical measurements such as the very rapidly fluctuating temperatures within the computer or some other parameter which would be essentially impossible to predict from outside of the computer, which people call “truly random”. However, theoretically, if the universe was prepared exactly the same way (if such a thing were possible) the same result would be achieved or if one knew the exact initial conditions of the physical properties of the computer and had arbitrary computing power that seed could be computed and so “true randomness” and “pseudorandomness” are only different at the level of what information is known and available. The distinction between true randomness and pseudorandomness is a practical distinction of what initial conditions could ever reasonably be known and what computations could be performed; it is not a fundamental physical distinction. “Fundamental randomness”, meaning randomness that no amount of physical information and initial conditions could ever predict even in principle would be basically scientifically meaningless as argued in 5.1.4.

²In probability theory there are many distinct senses of convergence of different strength. The proof given here is enough to prove the so-called weak law of large numbers, that the sample mean converges in probability to the actual mean (the probability the sample mean is within ε of μ goes to 1 for all positive ε). In fact a stronger sense of convergence is also true, the so-called

identically equal to the mean for any underlying distribution with finite mean. This is known as the Law of Large Numbers.

Problem 5.17: Central Limit Theorem. Suppose we have exactly the same setup as in the previous problem except now in addition to finite mean the underlying variables X_k also have finite variance σ^2 . Define the sample deviation:

$$Z = \sqrt{N} \frac{\bar{X} - \mu}{\sigma}.$$

- (a) Show that the characteristic function φ_Z for Z is:

$$\varphi_Z(t) = e^{-i\frac{\sqrt{N}}{\sigma}\mu t} \varphi_1^N\left(\frac{t}{\sigma\sqrt{N}}\right).$$

- (b) Show that for $\varphi_1(t)$:

$$\varphi_1(t) = 1 + i\mu t - \frac{t^2}{2}(\sigma^2 + \mu^2) + o(t^2) = e^{it\mu - \frac{\sigma^2}{2}t^2} + o(t^2).$$

- (c) Using the results of the previous two parts show that in the large N limit:

$$\lim_{N \rightarrow \infty} \varphi_Z(t) = e^{-\frac{t^2}{2}}.$$

Compute the pdf for Z to show that in the large N limit Z has a normal distribution with mean 0 and variance 1. Thus show that in the large N limit the sample mean asymptotically has a normal distribution with mean μ and variance $\frac{\sigma^2}{N}$ for any underlying distribution with finite mean and variance. This is known as the Central Limit Theorem and it is one of the fundamental reasons the normal distribution appears so often. Even in systems which have completely different distributions, sample means of large samples of those systems still have a normal distribution.

Problem 5.18: Chebyshev's Inequality and Markov's Inequality.

- (a) Let X be a non-negative random variable ($\text{Prob}(X < 0) = 0$) with finite expectation and pdf $f(x)$ and let a be a non-negative constant. Show that:

$$\mathbb{E}(X) = \int_0^a xf(x)dx + \int_a^\infty xf(x)dx \geq a\text{Prob}(X > a).$$

Thus, show that:

$$\text{Prob}(X > a) \leq \frac{\mathbb{E}(X)}{a}.$$

This is known as Markov's inequality.

- (b) Let X be a real valued random variable with finite mean μ and variance σ^2 . For $k > 0$, using that $|X - \mu| > k\sigma$ if and only if $(X - \mu)^2 > k^2\sigma^2$ and Markov's inequality show that:

$$\text{Prob}(|X - \mu| > k\sigma) \leq \frac{1}{k^2}.$$

This is known as Chebyshev's Inequality. This inequality places a fundamental limit on how probable it can be for a random variable to differ from its mean by at least a given amount. Thus, this concretely establishes at least how tightly a random variable is bound to be centered about its mean with width characterized by its standard deviation.

Problem 5.19: Propagation of small errors. Let $X^1, \dots, X^d$ be d random variables, not necessarily distributed the same way or independent or related in any way. However, suppose that each of these X^k have finite mean (let $\mu^k = \mathbb{E}(X^k)$) and that the covariances $\text{Cov}(X^k, X^n)$ exist and are finite for each k and n . If each X^k has pdf which decays sufficiently quickly to 0 away from μ^k so that within the precision relevant to experiment we only need the lowest order corrections to $X^k - \mu^k$, show that in this approximation for any smooth function G :

$$\mathbb{E}G(X^1, \dots, X^d) \approx G(\mu^1, \dots, \mu^d) + \frac{1}{2} \frac{\partial^2 G(\mu^1, \dots, \mu^d)}{\partial \mu^k \partial \mu^n} \text{Cov}(X^k, X^n) + \text{Higher Order Terms}$$

strong law of large numbers, that the probability the sample mean converges to μ is 1.

$$\text{Var}(G) \approx \frac{\partial G(\mu^1, \dots, \mu^d)}{\partial \mu^k} \frac{\partial G(\mu^1, \dots, \mu^d)}{\partial \mu^n} \text{Cov}(X^k, X^n) + \text{Higher Order Terms}.$$

Thus in the limit of small errors the means and matrix of covariances of our random variables are enough to compute the mean and variance of any smooth functions of our random variables. This is a reasonable introductory method for approximating error bars in quantities which are calculated (the G) from experimental data (the X^k) and so is sometimes called “freshman error propagation”.

Problem 5.20: Physical Coin Flipping. We have been so far discussing coin flips as events with unpredictable results. However, we know from the laws of mechanics how to exactly predict the result of a coin flip if we know its initial conditions. All of the unpredictability of a coin flip then comes from the fact that when a human person flips a coin they typically do so with very little precise control over those initial conditions.

- (a) Suppose a person flips a coin with upward component of its velocity v and angular velocity ω causing the coin to flip heads to tails to heads in the air. Assume the coin is initially heads up and that the person catches the coin at the same height from which it started. A coin of finite radius will hit the person’s hand with its center of mass at different heights and thus different times depending on how much it has rotated. Assume the coin’s velocity is small enough to neglect this effect. Show that the coin rotates by a total angle:

$$\theta = \frac{2v\omega}{g}$$

and that the coin will land heads if the nearest integer to $\frac{2v\omega}{\pi g}$ is even and will land tails if it is odd.

- (b) Show that for large ω small variations in v are capable of switching the result of the flip from heads to tails. Thus, the larger the angular velocity the coin is flipped with the more sensitive the result becomes to the initial conditions of the flip, leading to a coin which is effectively unpredictable.

Problem 5.21: Optimal Dice Design. As long as people have been playing games involving chance, some people have been practicing how to cheat the odds. If you could flip a coin consistently with the same initial conditions, you would take all of the randomness out of coin flipping. The same is true for rolling dice. In order to combat this, the numbers are laid out on dice so as to maximize their sensitivity to initial conditions, making controlling the results precisely as hard as possible. Show that in general this means that the numbers on a die with an arbitrary number of sides should be distributed so that if one selects a direction going out of the center of the die distributed uniformly on the sphere then the variance in which number that direction points to is as large as possible. In particular show that this means for a six sided die the opposite sides should sum to 7.

Problem 5.22: Least Squares Linear Fitting. Loss functions have many diverse applications but one of the most classic is for finding the best fit values for parameters to data. Suppose we have two sequences of data $X^1, \dots, X^N$, and $Y^1, \dots, Y^N$ which according to some theory we expect to be linearly related to each other for some parameters m and b with unknown values by:

$$Y^k \approx mX^k + b.$$

This is called our “model”. Let ε^2 be the quadratic error in this approximation summed over each data point:

$$\varepsilon^2(m, b) = \sum_{k=1}^N (Y^k - mX^k - b)^2$$

and take this ε^2 as our loss function. That is, the best fit values of m and b are taken to be those which minimize this error.

- (a) By minimizing ε^2 show that the best fit values of m and b are:

$$m_{\text{best}} = \frac{\overline{XY} - \overline{X}\overline{Y}}{\overline{X^2} - \overline{X}^2}, \quad b_{\text{best}} = \overline{Y} - m_{\text{best}}\overline{X}$$

where the bar over a quantity is defined by:

$$\overline{F} = \frac{1}{N} \sum_{k=1}^N F^k.$$

Please be careful and note that $\overline{X^2}$ and $\overline{X}^2$ are not the same.

- (b) Show then that the minimum value for ε^2 is:

$$\varepsilon_{\min}^2 = N \frac{(\overline{X^2} - \overline{X}^2)(\overline{Y^2} - \overline{Y}^2) - (\overline{XY} - \overline{X}\overline{Y})^2}{\overline{X^2} - \overline{X}^2}.$$

The smaller this is the better we would say the fit is. The precise details of the theory of goodness of fit are quite complicated, I suggest reading [4], [20], [53] for an introduction.

- (c) For simplicity, assume that in data collection each X^k and Y^k are normally distributed and independent and that the variances of all of the X^k are the same value σ_X^2 and the variances of all the Y^k are the same value σ_Y^2 . As well, assume the errors are small enough to reasonably use the freshman error propagation formula. Show then that this gives as an estimate for the variances of m and b :

$$\sigma_m^2 = \frac{1}{N} \frac{\overline{Y^2} - \overline{Y}^2}{(\overline{X^2} - \overline{X}^2)^2} \sigma_X^2 + \frac{1}{N} \frac{\sigma_Y^2}{\overline{X^2} - \overline{X}^2}$$

$$\sigma_b^2 = \frac{1}{N} \frac{(\overline{XY} - \overline{X}\overline{Y})^2 + \overline{X^2}(\overline{Y^2} - \overline{Y}^2)}{(\overline{X^2} - \overline{X}^2)^2} \sigma_X^2 + \frac{1}{N} \frac{\overline{X^2}}{\overline{X^2} - \overline{X}^2} \sigma_Y^2.$$

Problem 5.23: Chi-Squared Distribution. When using a quadratic loss function such as in the previous question with variables that are normally distributed, one inevitably encounters the χ^2 (pronounced chi-squared) Distribution.

- (a) Let $X_1, \dots, X_N$ be N iid random variables with normal distribution of mean μ and variance σ^2 . Let:

$$\varepsilon^2 = \sum_{k=1}^N \frac{(X_k - \mu)^2}{\sigma^2}.$$

Show that the pdf for ε^2 is:

$$f_{\varepsilon^2}(y) = \frac{y^{\frac{N}{2}-1} e^{-\frac{y}{2}}}{2^{\frac{N}{2}} \Gamma(\frac{N}{2})} \vartheta(y)$$

This is known as a χ^2 distribution with N “degrees of freedom”, which is just a name for the parameter appearing in the distribution. Show that this is a gamma distribution with $\tau = 2$ and the N appearing in the Gamma distribution replaced by $\frac{N}{2}$.

- (b) Let $X_1, \dots, X_N$ be N iid random variables with normal distribution exactly like before. Let:

$$\varepsilon^2 = \sum_{k=1}^N \frac{(X_k - \bar{X})^2}{\sigma^2}$$

where $\bar{X}$ is the sample mean of the X_k . Show that this ε^2 also has a χ^2 distribution except with $N - 1$ “degrees of freedom”.

Problem 5.24: ★ Borel-Kolmogorov Paradox or how I learned to start living and stop dividing by 0.

- (a) It is tempting to extend our conditional probability definition to continuous random variables and attempt to define the pdf for a random variable Y given that another random variable X takes a definite known value x . That is, we may like to define $f_{Y|X}(y|X=x)$. Show that if X is a discrete random variable the correct definition of such for continuous Y is:

$$f_{Y|X}(y|X=x) = \frac{f_{YX}(y \cap X=x)}{\text{Prob}(X=x)}$$

where $f_{YX}(y \cap X=x)$ is defined so that:

$$\int_a^b f_{YX}(y \cap X=x) dy = \text{Prob}(a < Y \leq b \cap X=x)$$

for all $a \leq b$.

- (b) Show that if X is a discretization of a continuous random variable Z with the discretization controlled by a parameter ε then in the limit that the discretization becomes continuous the result derived in the

previous section involves dividing by 0. The numerator also goes to 0 for a continuous random variable. Show that by l'Hopital's theorem one would get in the $\varepsilon \rightarrow 0$ continuous limit:

$$f_{Y|Z}(y|Z=z) = \lim_{\varepsilon \rightarrow 0} f_{Y|X}(y|X=x) = \frac{f_{YZ}(y,z)}{f_Z(z)}.$$

Thus, one may believe this is the correct definition for conditional probability of continuous random variables. However, this definition unfortunately depends on the way the discretization is taken and is not actually meaningful.

- (c) Consider a unit vector $\vec{n}$ of uniformly distributed random direction in 3 dimensions. That is, $\vec{n} = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$ and θ and φ are random variables distributed so that the probability $\vec{n}$ lands in any region on the unit sphere is proportional to the surface area of that region. Show that the joint pdf for θ and φ (with the usual ranges for spherical coordinates) is:

$$f(\theta, \varphi) = \frac{\sin \theta}{4\pi}.$$

- (d) Suppose we want to find the conditional distribution of where this vector $\vec{n}$ points to given that we know it points to some direction on a particular great circle (a great circle is a circle on a sphere with the same radius as that sphere). Suppose this great circle is the great circle defined by the condition $\theta = \frac{\pi}{2}$ (the equatorial great circle). Show that under our naive expression for continuous conditional probability we would have:

$$f\left(\varphi|\theta = \frac{\pi}{2}\right) = \frac{1}{2\pi}$$

and thus the azimuthal angle φ is uniformly distributed on the great circle, as you would expect from the spherical symmetry of the initial distribution.

- (e) Suppose now we take the great circle to be defined by the condition $\varphi = 0$ (the prime meridian great circle). Show that under our naive expression for continuous conditional probability we would have:

$$f(\theta|\varphi = 0) = \frac{1}{2} \sin \theta$$

and thus the zenith angle θ is not uniformly distributed on the great circle, even though the initial distribution was spherically symmetric. Even worse, we could have labeled our spherical coordinates differently so that this great circle was the equatorial great circle and the previous was the prime meridian and gotten this distributions to be completely swapped. The result of the naive conditional probability formula for continuous probability distributions is not consistent with changing your coordinates. This is the Borel-Kolmogorov paradox. The origin of the Borel-Kolmogorov paradox is that in different coordinates different discretization procedures lead to different results here which do not disappear even in the continuous limit. Essentially discretizing in θ as must be done in the first case involves considering the limit of a ring of vanishing thickness around the equator while discretizing in φ as must be done in this second case involves considering the limit of a wedge (like an orange slice) of vanishing thickness cut between the poles. These different limiting procedures give different results. So far in this book we have gone along with life assuming no such thing would happen, that in the continuous limit any artifacts of how we took that limit would disappear. This is true for many things under reasonable conditions but it is absolutely **NOT** true when applied generically to conditional probability. To define continuous conditional probability you need a preferred limiting procedure to take as representative (typically such a procedure is inspired by symmetries). This can be formalized with a result from measure theory known as the disintegration theorem. Fortunately, these difficulties are not really an issue for practical considerations of real data as no measurements are ever made with infinite precision. Any real life conditioning should be done by conditioning on the variable of interest being between the (finitely separated) lower and upper limits that have been set on it by measurement.

5.2 The Liouville Equation

Now let us actually begin doing statistical mechanics. Suppose we have some dynamical system defined by D variables, $\phi^1, \dots, \phi^D$. Then, by theorem 1.1 there is a velocity field function so that:

$$\frac{d\phi^a}{dt} = V^a(t, \phi). \quad (5.2.1)$$

The space of all possible values of ϕ is the phase space $\mathbb{P}$. Of course we will typically deal with a phase space where the ϕ^a are just canonical coordinates Q and conjugate momenta P and the velocity field will be given by Hamilton's equations:

$$\phi = \begin{pmatrix} Q \\ P \end{pmatrix}, \quad \frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a}. \quad (5.2.2)$$

While this will be the case we typically apply later on, there is some benefit of simplicity of notation to not explicitly putting in Hamilton's equations for now. When we are using a canonical phase space we let $D = 2d$ where d is the number of coordinates Q^a .

When we do statistical mechanics, we will often have D extremely large; large to the point that it is completely impractical to know what the initial conditions of our system are. Because we will not know the initial conditions of our dynamical system, there will be some probability distribution on the space of initial conditions. That is, there will be some function $f_0(\phi)$ so that the probability that the state of our system at time $t = 0$ is in some region M_0 of the phase space is given by:

$$\text{Prob}(\Phi(0) \in M_0) = \int_{M_0} f_0(\phi) d\mathbb{P} \quad (5.2.3)$$

where $\Phi(0)$ is a random variable representing the unknown initial state of our system and $d\mathbb{P}$ is the volume measure on phase space defined by:

$$d\mathbb{P} = \frac{d\phi^1 \dots d\phi^D}{(2\pi\hbar)^{\frac{D}{2}}}. \quad (5.2.4)$$

The factors of $2\pi\hbar$ are conventional (and thus make $f_0(\phi)$ not quite exactly the pdf for the initial conditions, just proportional to it). Here $\hbar$ is an arbitrary positive constant which is required to have the units necessary to make $f_0(\phi)$ is unitless. The motivation behind the factors of $2\pi\hbar$ is just to make a particular calculation in chapter 9 nicer and of course one could exclude them and just have slight adjustments to be made to a very small number of later formulas. For everything in this chapter, these $2\pi\hbar$'s cancel out anyway in all experimental results and do not matter. Those familiar with quantum mechanics will notice that $\hbar$ is the same symbol used for a particular constant in quantum mechanics and that they even have the same units (when the phase space is the phase space of a Hamiltonian system) and it is convenient later in chapter 9 to choose this $\hbar$ to be the same one as in quantum mechanics. However, in classical statistical mechanics the value of this $\hbar$ *never* matters. Because $f_0(\phi)$ differs from the proper probability density function on phase space by some factors of 2π , it has a slightly different name. This $f_0(\phi)$ is called the initial **phase space density (psd)**.

Our initial random variable $\Phi(0)$ in phase space will evolve according to the equations of motion over time to a new random variable $\Phi(t)$. What is the distribution of that random variable? Well, any set of initial conditions M_0 in phase space will evolve to some new set of later conditions $M(t)$ under the equations of motion. Further, because we assume as always that the dynamics are invertible, the only way a point in phase space evolves to end up in $M(t)$ is if it began in M_0 . So, the probability that $\Phi(0)$ is in M_0 is exactly the same as the probability that $\Phi(t)$ is in $M(t)$:

$$\text{Prob}(\Phi(0) \in M_0) = \text{Prob}(\Phi(t) \in M(t)). \quad (5.2.5)$$

We define the phase space density $f(t, \phi)$ as the pdf for $\Phi(t)$ adjusted in the same way by factors of $2\pi\hbar$:

$$\text{Prob}(\Phi(t) \in M) = \int_M f(t, \phi) d\mathbb{P}. \quad (5.2.6)$$

Then:

$$\int_{M_0} f_0(\phi) d\mathbb{P}_0 = \int_{M(t)} f(t, \phi) d\mathbb{P}. \quad (5.2.7)$$

where the subscript 0 on $d\mathbb{P}_0$ is just used to indicate that the variables integrated over represent the initial

conditions. We can also write the right hand side in terms of initial conditions by using the time evolution function introduced in section 1.1:

$$\phi^a(t) = U^a(t, \phi_0). \quad (5.2.8)$$

Then, $M(t) = U(t, M_0)$ as sets and so changing variables to the initial conditions in the integration:

$$\int_{M_0} f_0(\phi_0) d\mathbb{P}_0 = \int_{M_0} f(t, U(t, \phi_0)) \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) d\mathbb{P}_0. \quad (5.2.9)$$

These integrals match for all integration regions and so:

$$f_0(\phi_0) = f(t, U(t, \phi_0)) \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right). \quad (5.2.10)$$

Thus, in principle in order to find the phase space density at later times from the phase space density at an initial time we first need to solve the equations of motion and define $\phi(t)$ as the solution to that equation of motion. This gives the solution for the psd by:

$$\boxed{f(t, \phi) = \frac{f_0(\phi_0)}{\det \left(\frac{\partial \phi}{\partial \phi_0} \right)}}. \quad (5.2.11)$$

While this is the explicit solution it is typically not very practically useful. Instead, it is useful to find an equation of motion for the phase space density by differentiating equation (5.2.10) with respect to t :

$$\frac{d}{dt} f_0(\phi_0) = \frac{d}{dt} \left(f(t, U(t, \phi_0)) \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) \right). \quad (5.2.12)$$

The left hand side does not depend on time and so gives 0. The right hand side is more interesting:

$$\frac{d}{dt} \left(f(t, U(t, \phi_0)) \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) \right) = \frac{d}{dt} (f(t, U(t, \phi_0))) \det \frac{\partial U(t, \phi_0)}{\partial \phi_0} + f(t, U(t, \phi_0)) \frac{d}{dt} \det \frac{\partial U(t, \phi_0)}{\partial \phi_0} \quad (5.2.13)$$

$$\frac{d}{dt} f(t, U(t, \phi_0)) = \left. \frac{\partial f}{\partial t}(t, \phi) \right|_{\phi=U(t, \phi_0)} + \left. \frac{\partial f}{\partial \phi^a}(t, \phi) \right|_{\phi=U(t, \phi_0)} \frac{dU^a}{dt}(t, \phi_0). \quad (5.2.14)$$

Because $\phi(t) = U(t, \phi_0)$ is the solution to the underlying equation of motion:

$$\frac{dU^a}{dt}(t, \phi_0) = \frac{d\phi^a}{dt} = V^a(t, \phi) \quad (5.2.15)$$

$$\implies \frac{d}{dt} f(t, U(t, \phi_0)) = \frac{\partial f}{\partial t}(t, \phi(t)) + \frac{\partial f}{\partial \phi^a}(t, \phi(t)) V^a(t, \phi(t)). \quad (5.2.16)$$

Differentiating the determinant is quite a bit trickier. For a general $N \times N$ matrix M the determinant is defined by:

$$\det M = \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} M^{a_1}_{b_1} \dots M^{a_N}_{b_N} \quad (5.2.17)$$

where $\epsilon^{a_1 \dots a_N}$ is the N dimensional Levi-Civita symbol (here we are raising and lowering indices with the identity matrix, not the Minkowski metric, so the lowered and raised versions of ϵ are the same). It is defined so that $\epsilon_{123 \dots N} = 1$ and so that it is anti-symmetric under interchanging any pair of indices. The linear order variation of the determinant is then:

$$\delta \det M = \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} (\delta M^{a_1}_{b_1} M^{a_2}_{b_2} \dots M^{a_N}_{b_N} + \dots + M^{a_1}_{b_1} \dots M^{a_{N-1}}_{b_{N-1}} \delta M^{a_N}_{b_N}). \quad (5.2.18)$$

The N terms in the variation are actually all equal. One can see this by renaming indices so that the last factor of M is always the one which is varied. This will always require an even number of index interchanges because however many interchanges of a indices are required, the same number are required for interchanges of b indices and so over all the sign of the expression does not change. So:

$$\delta \det M = \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} N M^{a_1}_{b_1} M^{a_2}_{b_2} \dots M^{a_{N-1}}_{b_{N-1}} \delta M^{a_N}_{b_N} \quad (5.2.19)$$

$$= \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} N M^{a_1}_{b_1} M^{a_2}_{b_2} \dots M^{a_{N-1}}_{b_{N-1}} \delta_c^{a_N} \delta M^c_{b_N} \quad (5.2.20)$$

$$= \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} N M^{a_1}_{b_1} M^{a_2}_{b_2} \dots M^{a_{N-1}}_{b_{N-1}} M^{a_N}_d (M^{-1})^d_c \delta M^c_{b_N}. \quad (5.2.21)$$

The combination $\epsilon_{a_1 \dots a_N} M^{a_1}_{b_1} M^{a_2}_{b_2} \dots M^{a_N}_{b_N}$ is automatically antisymmetric in all of the b indices. Because there are only N possible values for each b index and it is antisymmetric in all N of them, this combination is determined by its value when the indices simply run from 1 to N and all other values are given by either 0 or appropriate index interchanges. Thus, it is in fact proportional to $\epsilon_{b_1 \dots b_N}$ for some constant C :

$$\epsilon_{a_1 \dots a_N} M^{a_1}_{b_1} \dots M^{a_N}_{b_N} = C \epsilon_{b_1 \dots b_N} \quad (5.2.22)$$

$$\implies \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} M^{a_1}_{b_1} \dots M^{a_N}_{b_N} = C \epsilon^{b_1 \dots b_N} \epsilon_{b_1 \dots b_N}. \quad (5.2.23)$$

The combination $\epsilon^{b_1 \dots b_N} \epsilon_{b_1 \dots b_N}$ sums over all ways to order the N distinct values of the b indices, giving $N!$. Then:

$$\epsilon^{b_1 \dots b_N} \epsilon_{b_1 \dots b_N} = N! \quad (5.2.24)$$

$$\implies C = \frac{1}{N!} \epsilon_{a_1 \dots a_N} \epsilon^{b_1 \dots b_N} M^{a_1}_{b_1} \dots M^{a_N}_{b_N} = \det M \quad (5.2.25)$$

$$\implies \epsilon_{a_1 \dots a_N} M^{a_1}_{b_1} \dots M^{a_N}_{b_N} = \det M \epsilon_{b_1 \dots b_N}. \quad (5.2.26)$$

Returning this result to our variation of the determinant:

$$\delta \det M = \frac{1}{N!} \epsilon^{b_1 \dots b_N} N \det M \epsilon_{b_1 \dots b_{N-1} d} (M^{-1})^d_c \delta M^c_{b_N}. \quad (5.2.27)$$

The combination $\epsilon^{b_1 \dots b_N} \epsilon_{b_1 \dots b_{N-1} d}$ is 0 if $b_N \neq d$ because there are N possibilities for each and neither can be any of the $N - 1$ values of b_1 through b_{N-1} without making the individual Levi-Civita symbols vanish. This leaves the same single non-trivial possibility for each and so this combination is proportional to $\delta_d^{b_N}$. As well, this combination sums over all ways to order the $N - 1$ distinct values of the b indices other than b_N and thus is $(N - 1)!$ whenever $b_N = d$. So:

$$\epsilon^{b_1 \dots b_N} \epsilon_{b_1 \dots b_{N-1} d} = (N - 1)! \delta_d^{b_N} \quad (5.2.28)$$

and with this:

$$\delta \det M = (M^{-1})^d_c \delta M^c_d \det M \quad (5.2.29)$$

$$\implies \boxed{\delta \det M = \text{Tr}(M^{-1} \delta M) \det M.} \quad (5.2.30)$$

Equation (5.2.30) then is the general formula for differentiating a determinant.

Returning to equation (5.2.13) then:

$$\frac{d}{dt} \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) = \text{Tr} \left(\left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right)^{-1} \frac{d}{dt} \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) \right) \det \left(\frac{\partial U(t, \phi_0)}{\partial \phi_0} \right) \quad (5.2.31)$$

$$= \text{Tr} \left(\left(\frac{\partial \phi}{\partial \phi_0} \right)^{-1} \frac{d}{dt} \left(\frac{\partial \phi}{\partial \phi_0} \right) \right) \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \quad (5.2.32)$$

$$= \text{Tr} \left(\frac{\partial \phi_0}{\partial \phi} \cdot \frac{\partial \dot{\phi}}{\partial \phi_0} \right) \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \quad (5.2.33)$$

$$= \text{Tr} \left(\frac{\partial \phi_0}{\partial \phi} \cdot \frac{\partial V}{\partial \phi_0} \right) \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \quad (5.2.34)$$

$$= \text{Tr} \left(\frac{\partial V}{\partial \phi} \right) \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \quad (5.2.35)$$

$$= \frac{\partial V^a}{\partial \phi^a} \det \left(\frac{\partial \phi}{\partial \phi_0} \right). \quad (5.2.36)$$

Now returning all of our results to equation (5.2.12):

$$0 = \left(\frac{\partial f}{\partial t}(t, \phi) + \frac{\partial f}{\partial \phi^a}(t, \phi) V^a(t, \phi) \right) \det \left(\frac{\partial \phi}{\partial \phi_0} \right) + f(t, \phi) \frac{\partial V^a}{\partial \phi^a} \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \quad (5.2.37)$$

$$\implies \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \phi^a} V^a + f(t, \phi) \frac{\partial V^a}{\partial \phi^a} = 0 \quad (5.2.38)$$

$$\implies \boxed{\frac{\partial f}{\partial t}(t, \phi) + \frac{\partial}{\partial \phi^a} (f(t, \phi) V^a(t, \phi)) = 0.} \quad (5.2.39)$$

This last equation is known as Liouville's equation. It gives the equation of motion for the phase space density

as derived from the underlying equations of motion of the random variable $\Phi(t)$. This equation is actually in the form of a continuity equation where we view the phase space density like a mass density in the phase space and we view the combination fV^a as the current density on phase space. Thus, Liouville's equation is really the statement of local probability conservation in phase space.

Liouville's equation leads to a very nice result for the evolution of expectations in time. Consider some function $G(t, \phi)$ defined on the phase space and allowed to explicitly depend on time. Then, the expectation of this quantity is given by the law of the unconscious statistician as:

$$\mathbb{E}G = \int_{\mathbb{P}} G(t, \phi) f(t, \phi) d\mathbb{P}. \quad (5.2.40)$$

Using Liouville's equation:

$$\frac{d}{dt} \mathbb{E}G = \int_{\mathbb{P}} \left(\frac{\partial G}{\partial t} f + G \frac{\partial f}{\partial t} \right) d\mathbb{P} = \int_{\mathbb{P}} \frac{\partial G}{\partial t} f d\mathbb{P} + \int_{\mathbb{P}} G \left(-\frac{\partial}{\partial \phi^a} (fV^a) \right) d\mathbb{P} \quad (5.2.41)$$

$$= \mathbb{E} \left(\frac{\partial G}{\partial t} \right) - \int_{\mathbb{P}} \left(\frac{\partial}{\partial \phi^a} (GfV^a) - \frac{\partial G}{\partial \phi^a} V^a f \right) d\mathbb{P}. \quad (5.2.42)$$

By the divergence theorem, the total derivative term becomes a surface integral. Because f must integrate over the phase space to 1 (by the second Kolmogorov axiom), f must decay far out into the phase space and so the surface term vanishes. With this:

$$\frac{d}{dt} \mathbb{E}G = \mathbb{E} \left(\frac{\partial G}{\partial t} + V^a \frac{\partial G}{\partial \phi^a} \right). \quad (5.2.43)$$

If we were to consider time dependent ϕ satisfying the underlying equations of motion:

$$\frac{dG(t, \phi(t))}{dt} = \frac{\partial G}{\partial t} + \frac{\partial G}{\partial \phi^a} \dot{\phi}^a = \frac{\partial G}{\partial t} + \frac{\partial G}{\partial \phi^a} V^a(t, \phi). \quad (5.2.44)$$

So, we can identify the quantity appearing in the expectation as what the time derivative of G would be under the underlying equations of motion. That is:

$$\boxed{\frac{d}{dt} \mathbb{E}G = \mathbb{E} \left(\frac{dG}{dt} \right)} \quad (5.2.45)$$

where the time derivative inside the expectation is taken as a time derivative under the flow of the underlying equations of motion.

Consider the case that our phase space variables are canonical coordinate and momenta so that $\phi = (Q, P)$ and the equations of motion are given by Hamilton's equations. Then, Liouville's equation becomes:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial Q^a} \left(f \frac{\partial \mathcal{H}}{\partial P_a} \right) + \frac{\partial}{\partial P_a} \left(f \left(-\frac{\partial \mathcal{H}}{\partial Q^a} \right) \right) = 0 \quad (5.2.46)$$

$$\implies \frac{\partial f}{\partial t} + \frac{\partial f}{\partial Q^a} \frac{\partial \mathcal{H}}{\partial P_a} + f \frac{\partial^2 \mathcal{H}}{\partial Q^a \partial P_a} - \frac{\partial f}{\partial P_a} \frac{\partial \mathcal{H}}{\partial Q^a} - f \frac{\partial^2 \mathcal{H}}{\partial Q^a \partial P_a} = 0 \quad (5.2.47)$$

$$\implies \boxed{\frac{\partial f}{\partial t} + \{f, \mathcal{H}\} = 0}. \quad (5.2.48)$$

Hence, Liouville's equation is very nicely stated in terms of the Poisson bracket. As well, the time derivative of the expectation formula then immediately becomes:

$$\frac{d}{dt} \mathbb{E}G = \mathbb{E} \left(\frac{\partial G}{\partial t} + \{G, \mathcal{H}\} \right). \quad (5.2.49)$$

The determinant in equation (5.2.36) can be explicitly solved for quite nicely:

$$\frac{d}{dt} \left(\ln \det \left(\frac{\partial \phi}{\partial \phi_0} \right) \right) = \frac{\partial V^a}{\partial \phi^a} \quad (5.2.50)$$

$$\implies \det \left(\frac{\partial \phi}{\partial \phi_0} \right) = e^{\int_0^t \frac{\partial V^a}{\partial \phi^a} dt}. \quad (5.2.51)$$

By equation (5.2.11) the solution to the Liouville equation is in principle exactly known before one even starts computing. However, that solution requires solving the underlying equations of motion and so using it is

often just as hard as just solving the underlying system exactly anyway. However, for a Hamiltonian system:

$$\frac{\partial V^a}{\partial \phi^a} = \frac{\partial}{\partial Q^a} \dot{Q}^a + \frac{\partial}{\partial P_a} \dot{P}_a = \frac{\partial^2 \mathcal{H}}{\partial Q^a \partial P_a} - \frac{\partial^2 \mathcal{H}}{\partial Q^a \partial P_a} = 0. \quad (5.2.52)$$

That is, a Hamiltonian system has a divergence free velocity field (also called incompressible). So, for a Hamiltonian system the coordinate transformation from the initial point in phase space to a later point in phase space along that trajectory always has:

$$\det \left(\frac{\partial \phi}{\partial \phi_0} \right) = \det \left(\frac{\partial(Q, P)}{\partial(Q_0, P_0)} \right) = 1. \quad (5.2.53)$$

This is not surprising as the Hamiltonian generates time evolution as a canonical transformation, the derivative matrix of which is always symplectic, and all symplectic matrices have determinant 1. So, the phase space density of a Hamiltonian system evolves according to equation (5.2.11) as:

$$f(t, Q, P) = f(0, Q_0, P_0) \quad (5.2.54)$$

where Q_0 and P_0 are the initial conditions which would lead to (Q, P) after a time t has elapsed.

It also follows that the change of variables formula for the phase space density simplifies for canonical transformations of a Hamiltonian system. Consider new coordinates and momenta (Q', P') which are defined from our old coordinates and momenta (Q, P) . Then, by equation (5.1.142):

$$f'(t, Q', P') = \frac{f(t, Q, P)}{|\det \left(\frac{\partial(Q', P')}{\partial(Q, P)} \right)|}. \quad (5.2.55)$$

However, the determinant appearing in the denominator we have just found to be 1. So:

$$f'(t, Q', P') = f(t, Q, P). \quad (5.2.56)$$

That is, under a symplectic change of variables the phase space density for the new variables is just the phase space density of the old variables with the old variables rewritten in terms of the new variables. In this way, the phase space density is invariant under canonical transformations.

There is an interesting and important duality in the Liouville equation which will appear for us in many different contexts going forward. For any function $G(t, \phi)$ on the phase space, we can use our phase space density at time t exactly as in equation (5.2.40). There we are integrating over the phase space at time t and ϕ does not explicitly depend on time. Instead, we could also consider just $f(0, \phi_0)$, the phase space density of the initial conditions and use the solution to the Liouville equation in equation (5.2.11) and the change of variables formula for an integral to express this as integral over the initial conditions:

$$\mathbb{E}G = \int_{\mathbb{P}_0} G(t, U(t, \phi_0)) \frac{f(0, \phi_0)}{\det \left(\frac{\partial \phi}{\partial \phi_0} \right)} \det \left(\frac{\partial \phi}{\partial \phi_0} \right) d\mathbb{P}_0 = \int_{\mathbb{P}_0} G(t, U(t, \phi_0)) f(0, \phi_0) d\mathbb{P}_0. \quad (5.2.57)$$

This last formula is of the form of an expectation value only with the initial phase space density as the distribution and where we have evolved the ϕ^a variables according to the underlying equations of motion. Thus, we can either write any expectation value of the theory as an integral over the phase space at the present time with a time evolving phase space density or we can write it as an integral over the initial phase space with a static phase space density but evolving the underlying coordinates in time. In this way, all of the time dependence can be shuffled between the phase space density and the coordinates on phase space. When we use $f(t, \phi)$ it is called the **Passive Picture** as the coordinates do not move. Then, the phase space density is just like a fluid moving around on phase space. When we use $f(0, \phi_0)$ and evolve the coordinates in time it is called the **Active Picture**. Then, the phase space density is just an initial distribution and all of the coordinates move around exactly according to their underlying equations of motion. These two pictures are exactly mathematically identical and simply different ways of organizing the same information.

The units of the constant $\hbar$ introduced in equation (5.2.4) are quite important to study. The requirements that the total probability on phase space be 1 and the phase space density be unitless give:

$$\int_{\mathbb{P}} f(t, Q, P) \frac{d^d Q d^d P}{(2\pi\hbar)^d} = 1 \implies [f] \frac{[Q]^d [P]^d}{[\hbar]^d} = 1 \quad (5.2.58)$$

$$[f] = 1 \implies [\hbar] = [Q][P]. \quad (5.2.59)$$

By equation the Hamilton-Jacobi with S being the action:

$$P = \frac{\partial S_c}{\partial Q} \implies [Q][P] = [S] \implies [\hbar] = [S]. \quad (5.2.60)$$

Hence $\hbar$ has units of the action. However, notice that our entire analytical mechanical formalism is independent of our choice of units of action (as described in problem 1.28). That is, if we consider a theory which is described by the action $S[Q]$ with equations of motion given by:

$$\frac{\delta S}{\delta Q^a} \stackrel{!}{=} 0 \implies \text{Equations of motion.} \quad (5.2.61)$$

Then, for any real constant $\alpha \neq 0$, the action defined by:

$$S'[Q] = \alpha S[Q] \quad (5.2.62)$$

gives equations of motion which hold if and only if the unscaled equations hold:

$$\frac{\delta S'}{\delta Q^a} = \alpha \frac{\delta S}{\delta Q^a} = 0 \iff \frac{\delta S}{\delta Q^a} = 0. \quad (5.2.63)$$

Therefore, if we rescale the action of the entire theory by the same constant uniformly the predictions are unchanged. This is not a symmetry/gauge transformation because this constant cannot depend on any parameters (without affecting the equation of motion) and we can only use this trick once (once you set the scale, you can't set it again without messing up the one you already set because interaction terms you add on after also have to be scaled in the same way). We can also calculate how this extends down to the Lagrangian and Hamiltonian:

$$\mathcal{L}' = \frac{dS'}{dt} = \alpha \frac{dS}{dt} = \alpha \mathcal{L} \quad (5.2.64)$$

$$P'_a = \frac{\partial \mathcal{L}'}{\partial \dot{Q}^a} = \alpha \frac{\partial \mathcal{L}}{\partial \dot{Q}^a} = \alpha P_a \quad (5.2.65)$$

$$\mathcal{H}' = P'_a \dot{Q}^a - \mathcal{L}' = \alpha (P_a \dot{Q}^a - \mathcal{L}) = \alpha \mathcal{H}. \quad (5.2.66)$$

Consequently, requiring the phase space density to remain invariant under changing the units of the action (which is natural because the phase space density is unitless) gives that the phase space measure must also be invariant under this change so that the probabilities are unaffected:

$$d\mathbb{P}' = d\mathbb{P} \implies \frac{d^d Q' d^d P'}{(2\pi\hbar')^d} = \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (5.2.67)$$

$$\implies \alpha^d \frac{d^d Q d^d P}{\hbar'^d} = \frac{d^d Q d^d P}{\hbar^d} \implies \hbar' = \alpha \hbar. \quad (5.2.68)$$

This scaling should not be surprising as $\hbar$ just has the same units as the action and so it inherits the same scaling. Because $\hbar$ has the same units as the action, the value of $\hbar$ is fixed whenever we fix the units of the action. That is, $\hbar$ is **NOT** a fundamental constant, just an artifact of our choice of units of action. We keep explicit factors of $\hbar$ for now but in later chapters we will see how to remove them in the same way as we did for c and ϵ_0 . So, how do we fix the units of the action? If we recall our actions from classical mechanics, for example equation (2.5.2), we can see that the units of the action are given by:

$$\mathcal{L} = \frac{1}{2} m |\dot{x}|^2 \implies [\mathcal{L}] = \frac{[S]}{T} = M \frac{L^2}{T^2} \implies [S] = \frac{ML^2}{T}. \quad (5.2.69)$$

Thus, we can see that the units of the action were fixed whenever we fixed our units of mass. In classical mechanics, we developed units of mass by selecting an arbitrary mass as a reference point. We can see that under this same α scaling:

$$\mathcal{L}' = \frac{1}{2} m' |\dot{x}|^2 = \alpha \mathcal{L} = \alpha \left(\frac{1}{2} m |\dot{x}|^2 \right) \implies m' = \alpha m. \quad (5.2.70)$$

The use of $\hbar$ in the phase space measure then is introduced for the purpose of providing a factor to absorb this scaling so that the phase space density is independent of the units of the action or equivalently independent of the reference mass used to define units of mass. For now it is not clear why we should care for this, but it will become clear in Part II. Regardless, introducing this factor is entirely harmless and arbitrary. One could never use the $2\pi\hbar$'s in the phase space measure in this chapter and no experimental results would be affected.

All of these results give us:

Theorem 5.1: Liouville's Theorem

If a dynamical system $\Phi = (\phi^1, \dots, \phi^d)$ evolves with velocity field $V^a(t, \phi)$ according to the equations of motion:

$$\frac{d\phi^a}{dt} = V^a(t, \phi) \quad (5.2.71)$$

and the initial conditions of this dynamical system have phase space density $f_0(\phi)$ then the phase space density $f(t, \phi)$ of this system at any other time is given by:

$$f(t, \phi(t)) = \frac{f_0(\phi(0))}{\det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right)} \quad (5.2.72)$$

or equivalently satisfies the Liouville equation:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \phi^a} (f V^a) = 0. \quad (5.2.73)$$

If that dynamical system is on a canonical phase space (Q, P) with equations of motion given by Hamilton's equations from a Hamiltonian $\mathcal{H}$ then the Liouville equation becomes:

$$\frac{\partial f}{\partial t} + \{f, \mathcal{H}\} = 0 \quad (5.2.74)$$

and the solution becomes:

$$f(t, Q(t), P(t)) = f_0(Q(0), P(0)). \quad (5.2.75)$$

Regardless of whether the system is Hamiltonian, expectations of functions on the dynamical system $G(t, \phi)$ satisfy:

$$\mathbb{E}G = \int_{\mathbb{P}} G(t, \phi) f(t, \phi) d\mathbb{P} = \int_{\mathbb{P}_0} G(t, \phi(t)) f(0, \phi_0) d\mathbb{P}_0 \quad (5.2.76)$$

$$\frac{d}{dt} \mathbb{E}(G) = \mathbb{E} \left(\frac{dG}{dt} \right). \quad (5.2.77)$$

When one is doing statistical mechanics the fundamental dynamical quantity is the phase space density $f(t, Q, P)$. Thus, you may wonder if it is possible to derive the equation of motion for f (the Liouville equation) from a variational principle or Hamiltonian where f is the variable to be varied. In fact, this is possible [50]. To be clear about notation, we write $\{\cdot, \cdot\}_{QP}$ for the usual Poisson bracket of the Q, P phase space variables:

$$\{A, B\}_{QP} = \frac{\partial A}{\partial Q^a} \frac{\partial B}{\partial P_a} - \frac{\partial B}{\partial Q^a} \frac{\partial A}{\partial P_a}. \quad (5.2.78)$$

We would like to find a Poisson bracket $\{\cdot, \cdot\}_f$ where the psd f is treated as the variable (and so derivatives will be taken with respect to f). We will call the Hamiltonian from which f get its equation of motion $\mathcal{H}_f$. We would like that equation of motion to be the Liouville equation. Thus, we want to find $\mathcal{H}_f$ and $\{\cdot, \cdot\}_f$ so that:

$$\frac{\partial f}{\partial t} = \{f, \mathcal{H}_f\}_f = -\{f, \mathcal{H}\}_{QP} \quad (5.2.79)$$

by (5.2.48). Certainly $\mathcal{H}_f$ will have to be related to the Hamiltonian $\mathcal{H}(Q, P)$ for the underlying variables. In fact, one can naturally take:

$$\mathcal{H}_f = \mathbb{E}(\mathcal{H}) = \int_{\mathbb{P}} f(t, Q, P) \mathcal{H}(t, Q, P) d\mathbb{P} \quad (5.2.80)$$

Returning this to equation (5.2.79) gives:

$$\int \mathcal{H}(t, Q', P') \{f(t, Q, P), f(t, Q', P')\}_f d\mathbb{P}' = -\frac{\partial f}{\partial Q^a} \frac{\partial \mathcal{H}}{\partial P_a} + \frac{\partial f}{\partial P_a} \frac{\partial \mathcal{H}}{\partial Q^a}. \quad (5.2.81)$$

To make this true for all $\mathcal{H}$, replace the function $\mathcal{H}$ with some function $B(t, Q, P)$ and integrate both sides against another arbitrary function $A(t, Q, P)$. Then, after a slight integration by parts, the $\{\cdot, \cdot\}_f$ bracket

must satisfy:

$$\int_{\mathbb{P}\mathbb{P}'} \{f(t, Q, P), f(t, Q', P')\}_f A(t, Q, P) B(t, Q', P') d\mathbb{P} d\mathbb{P}' = \int f \{A, B\}_{QP} d\mathbb{P} \quad (5.2.82)$$

$$\implies \boxed{\{\mathbb{E}(A), \mathbb{E}(B)\}_f = \mathbb{E}(\{A, B\}_{QP})}. \quad (5.2.83)$$

Taking the functional derivative of both sides with respect to A and B gives that the bracket is precisely:

$$\boxed{\{f(t, Q, P), f(t, Q', P')\}_f = \{(2\pi\hbar)^d \delta(Q - Q') \delta(P - P'), f(t, Q, P)\}_{QP}}. \quad (5.2.84)$$

The factor of $(2\pi\hbar)^d$ enters because the phase space measure $d\mathbb{P}$ used (consistently with (5.2.4)) includes the inverse of such a factor. If that $(2\pi\hbar)^d$ was not used in defining $d\mathbb{P}$, no factor would enter here. With a bit of labor one can show that this bracket satisfies the necessary properties of bilinearity, antisymmetry, the Jacobi identity, and the Leibniz property and thus is a genuine Poisson bracket. Therefore, classical statistical mechanics on a Hamiltonian system can be understood as actually a classical field theory where the phase space density $f(t, Q, P)$ is the classical field (and it is a field on the underlying phase space) equipped with the Poisson bracket (5.2.84) and with its Hamiltonian given by the expectation of the underlying classical Hamiltonian $\mathcal{H}(t, Q, P)$.

Exercises

Problem 5.25: Practice with the generic Liouville equation. Consider a dynamical system of two variables $x(t)$ and $y(t)$ satisfying:

$$\dot{x} = y, \quad \dot{y} = -x - 2\gamma y$$

for a positive constant $\gamma < 1$. Suppose that the system begins with phase space density:

$$f_0(x, y) = \frac{\hbar}{\sigma^2} e^{-\frac{x^2 + y^2}{2\sigma^2}}$$

where σ is a positive constant. Show that with the conventions established this phase space density is properly normalized:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_0(x, y) \frac{dx dy}{2\pi\hbar} = 1$$

and solve Liouville's equation to find the phase space density $f(t, x, y)$ as a function of time.

5.3 The First Law of Thermodynamics

For the total expected energy of a system we write E :

$$E = \mathbb{E}(\mathcal{H}). \quad (5.3.1)$$

Suppose we consider a system with phase space (Q, P) and free Hamiltonian $\mathcal{H}(Q, P)$ which experiences some external forces so that its equations of motion are:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a} + F_a^{\text{ext}}. \quad (5.3.2)$$

Then, by equation (5.2.45) and the work-energy theorem:

$$\frac{dE}{dt} = \frac{d}{dt} \mathbb{E}(\mathcal{H}) = \mathbb{E} \left(F_a^{\text{ext}} \frac{dQ^a}{dt} \right). \quad (5.3.3)$$

As we are describing extremely large systems and cannot possibly track all of the individual variables of those systems, it is useful to split the variables into two classes. **Macroscopic variables** are the variables in a system which are experimentally accessible, meaning we have the ability to measure and influence them specifically. **Microscopic variables** are all of the variables in a system which are not within our direct control. So, let $Q = (Q_m, Q_M)$ and $P = (P_m, P_M)$ where the Q_m^a and P_{ma} are the microscopic coordinates and their canonical momenta and the Q_M^a and P_{Ma} are the macroscopic coordinates and their canonical momenta. Immediately we have that:

$$\frac{dE}{dt} = \mathbb{E} \left(F_{ma}^{\text{ext}} \frac{dQ_m^a}{dt} \right) + \mathbb{E} \left(F_{Ma}^{\text{ext}} \frac{dQ_M^a}{dt} \right). \quad (5.3.4)$$

So, the change in energy of our system decomposes into changes due to forces on the microscopic variables and changes due to forces on the macroscopic forces. In statistical mechanics, W , the work done on a system is defined by the change in the expected energy of that system due to external forces on its macroscopic variables. That is:

$$W = \int_{t_0}^{t_f} \mathbb{E} \left(F_{Ma}^{\text{ext}} \frac{dQ_M^a}{dt} \right) dt. \quad (5.3.5)$$

More particularly, we write the instantaneous work done on the system by this integrand:

$$dW = \mathbb{E} \left(F_{Ma}^{\text{ext}} \frac{dQ_M^a}{dt} \right) dt. \quad (5.3.6)$$

Just as with equation (2.7.59), the bar is struck through the differential to indicate that the integral will generally depend on a specific path of integration (and so dW is an inexact differential). Similarly, $\mathcal{Q}$, the heat added to a system, is defined by the change in the expected energy of that system due to external forces on its microscopic variables. That is:

$$\mathcal{Q} = \int_{t_0}^{t_f} \mathbb{E} \left(F_{ma}^{\text{ext}} \frac{dQ_m^a}{dt} \right) dt. \quad (5.3.7)$$

Then, we also write:

$$d\mathcal{Q} = \mathbb{E} \left(F_{ma}^{\text{ext}} \frac{dQ_m^a}{dt} \right) dt. \quad (5.3.8)$$

This way the total change in energy is exactly given by:

$$\Delta E = \int_{t_0}^{t_f} \frac{dE}{dt} dt = W + \mathcal{Q} \quad (5.3.9)$$

$$\implies dE = dW + d\mathcal{Q}. \quad (5.3.10)$$

Because the expected energy is a function of the state of the system (it is determined by $f(t, Q, P)$), its derivative is a total differential and so no bar is necessary. Equation (5.3.10) is known as the **first law of thermodynamics**.

Because by definition the macroscopic variables are variables we can access and control meaningfully in experiment and work is change in energy due to forces on macroscopic variables, the work done on a system by external forces can be experimentally manipulated, controlled, and used. Alternatively, because by definition the microscopic variables are variables we cannot access and control meaningfully, the heat that is added to a system during a process is not directly manipulable on a variable by variable level. Previously when we

did mechanics we treated every variable as being directly accessible and so our work in previous chapters essentially treated all variables as macroscopic. Just as before in section 2.7, the external forces appearing above fundamentally originate from our system being a subsystem of an even larger system with those forces being due to the interaction terms in the total Hamiltonian for the full system. If one is lucky enough to have such a detailed full theory, one could use it to compute the external forces on the subsystem precisely.

Often (but not necessarily always) the systems we consider will be comprised of many (potentially interacting) copies of a smaller system, like a box of interacting molecules or gas. Then, the microscopic variables are generally taken to be the specific variables which describe a single copy of the small system and the macroscopic variables are taken to be either the total or average values of mechanical variables over all of the copies. For example, the position of a single molecule of gas is microscopic. But, the total energy, total linear momentum, or center of mass position of the entire gas are all macroscopic.

Together, we have:

Theorem 5.2: First Law of Thermodynamics

For a system under external macroscopic forces F_{Ma} on its macroscopic variables Q_M^a and microscopic forces F_{ma} on its microscopic variables Q_m^a , the change in its expected energy E between times t_0 and t_f is given by:

$$\Delta E = W + Q \quad (5.3.11)$$

where the work W and heat Q are defined by:

$$W \stackrel{\text{def}}{=} \int_{t_0}^{t_f} \mathbb{E} \left(F_{Ma} \frac{dQ_M^a}{dt} \right) dt, \quad Q \stackrel{\text{def}}{=} \int_{t_0}^{t_f} \mathbb{E} \left(F_{ma} \frac{dQ_m^a}{dt} \right) dt. \quad (5.3.12)$$

Exercises

Problem 5.26: Work done by changes in volume. Consider a thermodynamic system which is in a container of volume $\mathbb{V}$. Suppose that a wall of that container is subject to an external pressure p_{ext} (recall that pressure is defined as the force into a surface per unit surface area). Recall the expression for the work done on an object displaced by $d\vec{x}$ by an external force $\vec{F}_{\text{ext}}$:

$$dW = \vec{F}_{\text{ext}} \cdot d\vec{x}$$

and use it to show that the work done on the thermodynamic system when its volume is compressed by an external pressure is:

$$dW = -p_{\text{ext}} d\mathbb{V}.$$

5.4 Microcanonical Ensemble

Suppose we have some Hamiltonian system obeying the Liouville equation:

$$\frac{\partial f}{\partial t} + \{f, \mathcal{H}\} = 0 \quad (5.4.1)$$

with a time independent Hamiltonian $\mathcal{H}(Q, P)$. One useful criterion for distinguishing microscopic and macroscopic variables is the typical rate at which they evolve. Variables which change values more quickly than an experimenter can measure are essentially automatically microscopic. For a variable to be macroscopic its value needs to be stable on experimentally relevant timescales so that it can be measured and intentionally adjusted. For this reason, the adiabatic invariants of a system are generally macroscopic quantities. Because we are generally interested in the stable quantities of a system, we will often allow that system to evolve for so long that we can essentially only concern ourselves with the long term value of its phase space density. For calculation purposes it is more useful to work directly with the time averaged distribution $\bar{f}$ defined by:

$$\bar{f}(Q, P) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau f(t, Q, P) dt. \quad (5.4.2)$$

Using l'Hopital's rule we can see that $\bar{f}(Q, P)$ is the long term value of the distribution f :

$$\bar{f}(Q, P) = \lim_{\tau \rightarrow \infty} \frac{\frac{\partial}{\partial \tau} \int_0^\tau f(t, Q, P) dt}{\frac{\partial}{\partial \tau} \tau} = \lim_{\tau \rightarrow \infty} f(\tau, Q, P). \quad (5.4.3)$$

The above is true if such a limit exists. Many systems oscillate indefinitely, but they do so around well-defined time averages, which explains why the time average is generally the more useful quantity. Then:

$$\{\bar{f}, \mathcal{H}\} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \{f, \mathcal{H}\} dt = - \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \frac{\partial f}{\partial t} dt = \lim_{\tau \rightarrow \infty} \frac{f(0, Q, P) - f(\tau, Q, P)}{\tau}. \quad (5.4.4)$$

Using equation (5.2.55):

$$\{\bar{f}, \mathcal{H}\} = \lim_{\tau \rightarrow \infty} \frac{f(0, Q, P) - f(0, Q_0, P_0)}{\tau}. \quad (5.4.5)$$

We will generally have phase space densities which are initially bounded functions, meaning that at $t = 0$ the probability density of any value of (Q, P) is finite. Then, the numerator here is finite and the denominator limits to ∞ , giving:

$$\{\bar{f}, \mathcal{H}\} = 0. \quad (5.4.6)$$

Hence, the steady state distribution $\bar{f}$ automatically Poisson commutes with the Hamiltonian.

Suppose our system has K independent conserved quantities. That is, there are functions $G_1(Q, P)$, ..., $G_K(Q, P)$ which cannot be written in terms of each other so that each is conserved by the underlying equations of motion:

$$\frac{dG_k}{dt} = 0 \implies \{G_k, \mathcal{H}\} = 0. \quad (5.4.7)$$

If we have been careful so that this is a complete set of conserved quantities (meaning the system has no other conserved quantities which cannot be written in terms of these), then necessarily it automatically follows that $\bar{f}$ can be written as some function of these conserved quantities:

$$\bar{f}(Q, P) = F(G_1(Q, P), \dots, G_K(Q, P)). \quad (5.4.8)$$

Of course, one of these conserved quantities is automatically the energy. This function F can be determined from the initial distribution f_0 . The initial phase space probability density, being a probability distribution, is intended to represent our density of degree of belief that the initial conditions take particular values. As such, the correct initial distribution to take in general depends on the experimental setup. If the way the system is prepared tends to bias the variables in a particular way, that bias must be accurately reflected in our selection of the initial conditions in our calculations involving that distribution to make accurate predictions. This is no different than how in mechanics in order for one's calculation to give the correct prediction one must use the correct initial conditions for the equations of motion.

Often (but not necessarily always), we will model our system as not biasing toward any values of the conserved quantities other than the energy. That is, we often model our system by assuming that the experimenter prepares the system in a way in which they control the energy of the system but at fixed energy do not bias the distribution of initial conditions in any other way. Mathematically, this means we are

assuming the initial conditions are of the form:

$$f_0(Q, P) = F_0(\mathcal{H}(Q, P)) \quad (5.4.9)$$

We automatically have that:

$$f(t, Q, P) = f(0, Q_0, P_0) = F_0(\mathcal{H}(Q_0, P_0)) = F_0(\mathcal{H}(Q, P)) \implies \bar{f} = F_0(\mathcal{H}(Q, P)). \quad (5.4.10)$$

Moreover, suppose the experimenter has the ability to control their preparation of the system so that in fact the system has definite energy E . Then, the phase space density will have a Dirac delta to enforce that particular value of the energy:

$$\bar{f} = N\delta(E - \mathcal{H}). \quad (5.4.11)$$

Here N is some normalization factor. This factor is present because by the definition of probability the integral of the phase space density over the entire phase space is 1:

$$\int_{\mathbb{P}} \bar{f} d\mathbb{P} = N \int_{\mathbb{P}} \delta(E - \mathcal{H}) d\mathbb{P} = 1. \quad (5.4.12)$$

This condition then determines the value of N . Together we have:

Theorem 5.3: Microcanonical Ensemble

The time-averaged or long term behavior of a system's phase space density, defined by:

$$\bar{f}(Q, P) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau f(t, Q, P) dt \quad (5.4.13)$$

will satisfy:

$$\{\bar{f}, \mathcal{H}\} = 0 \quad (5.4.14)$$

and consequently will be a function solely of the conserved quantities of the system. If the experimental setup of the system is so that the initial conditions are not biased with regard to any of these initial conditions except the energy, then $\bar{f}$ will be a function of the energy only. If in addition the experimenter is able to precisely control the initial energy of the system, then the time averaged behavior of the system will tend to the microcanonical ensemble phase space density:

$$f_{\text{micro}}(Q, P|E) = \frac{1}{g(E)} \delta(E - \mathcal{H}(Q, P)). \quad (5.4.15)$$

where the density of states $g(E)$ is a normalization factor defined as the area of the surface in phase space with energy E :

$$g(E) \stackrel{\text{def}}{=} \int_{\mathbb{P}} \delta(E - \mathcal{H}) d\mathbb{P}. \quad (5.4.16)$$

There is another way to understand the microcanonical ensemble as the “least presumptive” distribution for a fixed given energy in a sense we will discuss in a section 5.6.

Exercises

Problem 5.27: Practice with the density of states.

- (a) Consider a single free nonrelativistic particle of mass m in a volume $\mathbb{V}$. Show that its density of states is:

$$g(E) = \frac{\mathbb{V}}{\pi^2 \hbar^3} \sqrt{\frac{m^3 E}{2}} \vartheta(E).$$

- (b) Consider two noninteracting subsystems, with Hamiltonians $\mathcal{H}_1$ and $\mathcal{H}_2$ so that their total Hamiltonian is $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$. Let $g_1(E)$ be the density of states of system 1 and $g_2(E)$ be the density of states of system 2. Show that the density of states of the combined system is:

$$g(E) = \int_{-\infty}^{\infty} g_1(E_1) g_2(E - E_1) dE_1.$$

- (c) Using dimensional analysis, show that the density of states for N free nonrelativistic particles of mass

m in a volume $\mathbb{V}$ is:

$$g_N(E) = \frac{C_N}{E} \left(\frac{\mathbb{V} m^{\frac{3}{2}} E^{\frac{3}{2}}}{h^3} \right)^N \vartheta(E)$$

for some dimensionless coefficient C_N which depends on N .

(d) Define the coefficient D_N :

$$D_N = \Gamma\left(\frac{3N}{2}\right) C_N.$$

Show using the result of part (b) that D_N satisfies the recursion relation:

$$D_{N+1} = D_1 D_N.$$

To do so it will be useful to remember the definition of the Gamma and Beta functions, and to reference the results of question 5.13. Use this to show that:

$$g_N(E) = \frac{\mathbb{V}^N}{\Gamma\left(\frac{3N}{2}\right)} \left(\frac{mE}{2\pi h^2} \right)^{\frac{3N}{2}} \frac{\vartheta(E)}{E}$$

5.5 Canonical Ensemble

In our previous analysis we never used that the system under consideration was “large” in any way. Let us do so now. That is, suppose our total system is described by a phase space (Q, q, P, p) with Hamiltonian:

$$\mathcal{H}_{\text{total}}(Q, q, P, p) = \mathcal{H}(Q, P) + \mathcal{H}_{2|1}(q, p|Q, P). \quad (5.5.1)$$

The coordinates and momenta written with capital letters as (Q, P) will be the coordinates and momenta of our system of interest whereas the coordinates and momenta written with lowercase letters as (q, p) will be the coordinates and momenta of some other variables which interact with our system of interest. Let the (Q, P) space have dimension $2d$ and the (q, p) space have dimension $2N$. The large N limit then corresponds to the limit that our system of interest is interacting with an environment of a large number of degrees of freedom. This would be relevant for describing say the motion of a specific object with position and momentum (Q, P) being bombarded by a large number of other objects, such as due to moving through a gas or fluid.

We will consider the environmental variables (q, p) to be near stable equilibrium (the value of that equilibrium may in principle depend on (Q, P)). That is, we will assume that the system interacts only at the lowest order of approximation with the environmental variables so that their Hamiltonian can be expanded as a Taylor series to lowest non-trivial order. So, in general we would take $\mathcal{H}_{2|1}$ to be an arbitrary quadratic function of q, p . From theorem 1.14, any stable quadratic Hamiltonian can be transformed by symplectic transformation into being a sum of harmonic oscillators. That is, it is guaranteed that under these assumptions the Hamiltonian for the (q, p) coordinates can be put into the form:

$$\mathcal{H}_{2|1}(q, p|Q, P) = \sum_{n=1}^N \left(\frac{p_n^2}{2} + \frac{\omega_n^2}{2} (q_n - F_n(Q, P))^2 \right). \quad (5.5.2)$$

The functions $F_n(Q, P)$ simply serve to reflect that the value of q_n at which the stable equilibrium occurs in principle may depend on the underlying values of (Q, P) due to the interactions between them.

Now suppose the the total system is prepared as we assumed in the previous section so that in the long run its statistics are described by the micro-canonical ensemble phase space density:

$$f_{\text{micro}}(Q, q, P, p|E) = \frac{1}{g(E)} \delta(E - \mathcal{H}_{\text{total}}(Q, q, P, p)) \quad (5.5.3)$$

Any quantity of the (Q, P) subsystem would only need their distribution to compute expectations and so viewing the (q, p) as microscopic variables from the environment, it is natural to integrate them out. So, we are interested in the marginal phase space density:

$$f_{\text{sys}}(Q, P|E) = \int_{\mathbb{R}^{2N}} f_{\text{micro}}(Q, q, P, p|E) \frac{d^N q d^N p}{(2\pi\hbar)^N}. \quad (5.5.4)$$

The factors of $2\pi\hbar$ are due to the definition of the phase space measure in equation (5.2.4). Explicitly using our approximation for $\mathcal{H}_{2|1}$:

$$f_{\text{sys}}(Q, P|E) = \int_{\mathbb{R}^{2N}} \frac{1}{g(E)} \delta \left(E - \mathcal{H}(Q, P) - \sum_{n=1}^N \left(\frac{p_n^2}{2} + \frac{\omega_n^2}{2} (q_n - F_n(Q, P))^2 \right) \right) \frac{d^N q d^N p}{(2\pi\hbar)^N}. \quad (5.5.5)$$

Define the integration variables (for $1 \leq n \leq N$):

$$x_n = \frac{\omega_n}{\sqrt{2\hbar}} (q_n - F_n), \quad x_{N+n} = \frac{p_n}{\sqrt{2\hbar}}. \quad (5.5.6)$$

Then:

$$f_{\text{sys}}(Q, P|E) = \frac{1}{g(E)} \frac{1}{\pi^N \prod_{n=1}^N \omega_n} \int_{\mathbb{R}^{2N}} \delta \left(E - \mathcal{H}(Q, P) - \sum_{n=1}^{2N} x_n^2 \right) d^{2N} x. \quad (5.5.7)$$

Define as well the vector $\vec{x}$ in $\mathbb{R}^{2N}$ with components given by the x_n . The Dirac delta appearing in the integral can be simplified using the result of problem 3.2:

$$\delta(E - \mathcal{H} - |\vec{x}|^2) = \frac{\delta(\sqrt{E - \mathcal{H}} - |\vec{x}|)}{2\sqrt{E - \mathcal{H}}}. \quad (5.5.8)$$

Finally, put the above integral into $2N$ dimensional spherical coordinates and let S_n be the surface area of the unit sphere of dimension n . Then, the volume measure is:

$$d^{2N} \vec{x} = r^{2N-1} dr dS_{2N-1}. \quad (5.5.9)$$

Thus, the integral becomes:

$$f_{\text{sys}}(Q, P|E) = \frac{1}{g(E)} \frac{1}{\pi^N \prod_{n=1}^N \omega_n} \int_0^\infty \int_{S_{2N_1}} \frac{\delta(\sqrt{E - \mathcal{H}} - r)}{2\sqrt{E - \mathcal{H}}} r^{2N-1} dS_{2N-1} dr \quad (5.5.10)$$

$$= \frac{S_{2N-1}}{2g(E)\pi^N \prod_{n=1}^N \omega_n} (E - \mathcal{H})^{N-1} \quad (5.5.11)$$

$$= \frac{S_{2N-1}E^{N-1}}{2g(E)\pi^N \prod_{n=1}^N \omega_n} \left(1 - \frac{\mathcal{H}}{E}\right)^{N-1}. \quad (5.5.12)$$

The entire prefactor here does not depend on (Q, P) and so is just a normalization. It can be determined just by the requirement that integrating f_{sys} over the entire (Q, P) phase space should give 1. We see that the only (Q, P) dependence is through the factor $\left(1 - \frac{\mathcal{H}}{E}\right)^{N-1}$. Because we are intending to take there to be a large number of environmental variables, we would like to take $N \rightarrow \infty$. However, doing so for any value of $\mathcal{H} > 0$ at fixed E causes the mentioned factor to go to 0. This is not surprising as if we take the number of available variables to be large but fix the total available energy, the energy available per variable limits toward 0. So, if we want to consider a subsystem with non-zero energy interacting with an environment we need to also scale the total energy E with N . We could have also predicted this by using that we already know that when two systems do not interact their total energy is sum of their individual energies and so energy scales with the size of the system. This line of reasoning is especially appealing given that we have expanded in the limit of weak interactions. So, for the large N limit to be valid we need the total energy E to scale linearly with the number of environmental variables:

$$E = E_0 + NT \quad (5.5.13)$$

where E_0 and T are some parameters independent of N that characterize the scaling. In the large N limit the distribution we have computed is called the canonical ensemble:

$$f_{\text{canon}}(Q, P|T) = \lim_{N \rightarrow \infty} \frac{S_{2N-1}N^{N_1}T^{N-1}}{2g(E)\pi^N \prod_{n=1}^N \omega_n} \left(1 + \frac{E_0 - \mathcal{H}}{NT}\right)^{N-1}. \quad (5.5.14)$$

This last limit can be computed using the compound interest definition of the exponential function:

$$e^x = \lim_{N \rightarrow \infty} \left(1 + \frac{x}{N}\right)^N. \quad (5.5.15)$$

Then:

$$f_{\text{canon}}(Q, P|T) = C(E_0, T) e^{\frac{E_0 - \mathcal{H}}{T}} = \frac{e^{-\frac{\mathcal{H}}{T}}}{Z(T)}. \quad (5.5.16)$$

The factor $Z(T)$ is called the partition function and it is determined by the requirement that the phase space density integrates to 1 over the (Q, P) phase space:

$$\int_{\mathbb{P}} f_{\text{canon}}(Q, P|T) d\mathbb{P} = \frac{1}{Z(T)} \int_{\mathbb{P}} e^{-\frac{\mathcal{H}(Q, P)}{T}} d\mathbb{P} = 1 \quad (5.5.17)$$

$$\implies Z = \int_{\mathbb{P}} e^{-\frac{\mathcal{H}}{T}} d\mathbb{P}. \quad (5.5.18)$$

Notice that f_{canon} is actually independent of E_0 .

So, if a system with phase space (Q, P) and free Hamiltonian $\mathcal{H}$ is placed in a very large background of weakly interacting variables, the steady state or equilibrium distribution of that system is given by the Boltzmann distribution or canonical ensemble:

$$\boxed{f_{\text{canon}}(Q, P|T) = \frac{e^{-\frac{\mathcal{H}(Q, P)}{T}}}{Z}}. \quad (5.5.19)$$

This distribution depends on the parameter T , called the temperature, which we have not yet specified. In the large N limiting procedure the total system energy was given by $E = E_0 + NT$ and so the temperature T has the interpretation as the average energy contribution per harmonic oscillator degree of freedom to the system. Our model of an environment consisting of a large number of stable degrees of freedom is called a thermal reservoir or thermal bath. The temperature then is the characteristic typical energy of each oscillator

in that bath. It is also common to define the variable β by:

$$\beta \stackrel{\text{def}}{=} \frac{1}{T}. \quad (5.5.20)$$

This β is called the “inverse temperature” or simply the “thermodynamic beta”. Expressed in terms of β the canonical ensemble becomes:

$$f_{\text{canon}}(Q, P|\beta) = \frac{e^{-\beta\mathcal{H}}}{Z(\beta)}. \quad (5.5.21)$$

The energy of the system which is placed in the bath can be efficiently computed in terms of the partition function and this beta:

$$E = \mathbb{E}(\mathcal{H}) = \int_{\mathbb{P}} f_{\text{canon}} \mathcal{H} d\mathbb{P} = \frac{1}{Z} \int_{\mathbb{P}} \mathcal{H} e^{-\beta\mathcal{H}} d\mathbb{P} = -\frac{1}{Z} \frac{\partial}{\partial \beta} \int_{\mathbb{P}} e^{-\beta\mathcal{H}} d\mathbb{P} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \quad (5.5.22)$$

$$\implies \boxed{E = -\frac{\partial}{\partial \beta} \ln Z.} \quad (5.5.23)$$

We can formally establish the meaning of temperature in terms of the bath in another way. If we were to take our (Q, P) degrees of freedom to themselves be a single harmonic oscillator we would have (using our results on the Gaussian integral):

$$\mathcal{H} = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 Q^2 \quad (5.5.24)$$

$$\implies Z = \int_{\mathbb{P}} e^{-\beta\mathcal{H}} d\mathbb{P} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{\beta}{2m}P^2 - \frac{m\omega^2\beta}{2}Q^2} \frac{dQdP}{2\pi\hbar} = \frac{1}{2\pi\hbar} \sqrt{\frac{2\pi m}{\beta}} \sqrt{\frac{2\pi}{m\omega^2\beta}} = \frac{1}{\hbar\omega\beta} \quad (5.5.25)$$

$$\implies E = -\frac{\partial}{\partial \beta} \ln \left(\frac{1}{\hbar\omega\beta} \right) = \frac{1}{\beta} = T. \quad (5.5.26)$$

Hence, for a harmonic oscillator placed in a thermal bath of temperature T , the expected energy of that harmonic oscillator is exactly T . However, our thermal bath consists of weakly interacting harmonic oscillators and so any specific oscillator in that bath could be considered as our system with the rest of the bath acting as the bath to that system. This reveals that for each harmonic oscillator in the bath, the expected energy of that oscillator is precisely T . This solidifies the interpretation of temperature T as the energy per harmonic oscillator degree of freedom of the bath.

To this point we have taken the thermal bath to consist of many weakly coupled harmonic oscillators. However, because any linearly stable theory near equilibrium becomes harmonic oscillators by the theorem of normal modes, we can in general take a large number of any weakly coupled stable systems to act as the bath. In that case, the temperature T would not be the energy per such stable system exactly. Instead, using the Hamiltonian for a single such system one would compute the expected energy as a function of T by equation (5.5.23) to establish the relationship between temperature and energy for that system. In fact, this thinking reveals an extremely important insight. Many macroscopic systems consist of an extremely large number of weakly interacting copies of essentially the same subsystem (the molecules in an every day material, for example). So, each subsystem can be treated as the (Q, P) phase space with all of the other subsystems acting as the bath. This should be valid in the large N limit. In other words, we can treat any very large system as acting as its own bath.

When two systems do not interact, we found that their Hamiltonians (and thus energies) add. Any quantity which is additive for non-interacting systems is called **extensive**. That is for systems 1 and 2 non-interacting the quantity X is extensive if:

$$X_{\text{total}} = X_1 + X_2 \quad (\text{Extensive}). \quad (5.5.27)$$

When interactions are present few if any quantities remain additive, though they may approximately be so for weak interactions. Energy, total linear momentum, total angular momentum, total volume, total number of particles in a system of any given species, and total electric charge are all extensive. Alternatively, for two systems 1 and 2 which are not interacting a quantity X is called intensive if whenever the values of that quantity coincides for the individual systems then the value also coincides for the total system:

$$X_1 = X_2 \implies X_{\text{total}} = X_1 = X_2 \quad (\text{Intensive}). \quad (5.5.28)$$

For example, the center of mass of a system is intensive. It immediately follows that the ratio of any

two extensive quantities X and Y is intensive:

$$Z = \frac{Y}{X}, \quad Z_1 = Z_2, \quad Y_{\text{total}} = Y_1 + Y_2, \quad X_{\text{total}} = X_1 + X_2 \quad (5.5.29)$$

$$\Rightarrow Z_{\text{total}} = \frac{Y_{\text{total}}}{X_{\text{total}}} = \frac{Y_1 + Y_2}{X_1 + X_2} = \frac{Z_1 + Z_2 \frac{X_2}{X_1}}{1 + \frac{X_2}{X_1}} = Z_1 = Z_2. \quad (5.5.30)$$

As well, the ratio of an extensive quantity to an intensive quantity is extensive. The ratio of an intensive quantity to an intensive quantity is intensive. The derivative of an extensive quantity with respect to an extensive quantity is intensive. The derivative of an extensive quantity with respect to an intensive quantity is extensive. The derivative of an intensive quantity with respect to an intensive quantity is intensive.

An immediate special case of the definitions of extensive and intensive is that if we consider N copies of a system and let X_1 be the value of some quantity in a single copy of that system an extensive quantity has $X = NX_1$ whereas an intensive quantity has $X = X_1$. In this way, we can understand extensive quantities as quantities which scale proportionally to the size of the system and intensive quantities as quantities which are independent of the scale of the system. Because temperature is the energy of the bath per harmonic oscillator degree of freedom, it is the derivative of the total energy (extensive) with respect to the number of degrees of freedom (extensive) and thus is intensive.

Generically, conserved quantities can be expressed extensively. Suppose we have two non-interacting systems which share a continuous symmetry so that the respective generators from Noether's theorem are:

$$G_1 = P_{1a} \mathcal{D}Q_1^a - \mathcal{H}_1 \mathcal{D}t - \mathcal{D}f_1, \quad G_2 = P_{2a} \mathcal{D}Q_2^a - \mathcal{H}_2 \mathcal{D}t - \mathcal{D}f_2. \quad (5.5.31)$$

Then, by Noether's theorem the generator of the symmetry for the combined system is:

$$G = P_a \mathcal{D}Q^a - \mathcal{H} \mathcal{D}t - \mathcal{D}f = P_{1a} \mathcal{D}Q_1^a + P_{2a} \mathcal{D}Q_2^a - (\mathcal{H}_1 + \mathcal{H}_2) \mathcal{D}t - \mathcal{D}f_1 - \mathcal{D}f_2 = G_1 + G_2. \quad (5.5.32)$$

Hence, the conserved quantities produced by Noether's theorem are automatically extensive.

We found that any large system can be treated as acting as its own bath. What we mean is that if a system is composed of N weakly interacting subsystems and it is prepared in the microcanonical ensemble then in the limit that N is taken to infinity keeping all intensive quantities fixed (and thus scaling all extensive quantities proportionally to N) that system's phase space equilibrium phase space distribution will be given by the canonical ensemble. This limiting procedure is known as the thermodynamic limit.

There is naively a contradiction in the previous line of reasoning. If a system is prepared in the microcanonical ensemble then f_{micro} is the correct distribution to use for computing its properties. If a system acts as its own bath then we instead say that the system is in the canonical ensemble and then f_{canon} is the correct distribution to use for computing its properties. How can these simultaneously be true? They are only simultaneously true in the thermodynamic limit (which makes the treatment of a system as its own bath valid). Let us show this properly.

Both f_{micro} and f_{canon} are functions of (Q, P) only through the energy $\mathcal{H}(Q, P)$. The microcanonical ensemble has definite energy E whereas the canonical ensemble decays exponentially with increasing energy with β as the rate of exponential decay. Directly from the partition function, the variance of the energy is given by:

$$\delta E^2 = \mathbb{E}(\mathcal{H}^2) - E^2 = \frac{1}{Z} \int_{\mathbb{P}} \mathcal{H}^2 e^{-\beta \mathcal{H}} d\mathbb{P} - E^2 \quad (5.5.33)$$

$$= \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2} \left(\frac{\partial Z}{\partial \beta} \right)^2 = \frac{\partial}{\partial \beta} \left(\frac{1}{Z} \frac{\partial Z}{\partial \beta} \right) = -\frac{\partial E}{\partial \beta}. \quad (5.5.34)$$

This is a quite nice general formula for computing the variance of the energy. Then, the squared relative fluctuation (ratio of the variance to the mean squared) of the energy is:

$$\boxed{\left(\frac{\delta E}{E} \right)^2 = -\frac{1}{E^2} \frac{\partial E}{\partial \beta}.} \quad (5.5.35)$$

The energy is extensive but the temperature (and so the thermodynamic beta) is intensive. Consequently, the derivative of E with respect to β is extensive and so the numerator here scales proportionally to the size of the system while the denominator scales proportionally to the square of the size of the system. For N copies of a subsystem with energy E_1 and energy variance δE_1^2 then:

$$\frac{\delta E}{E} = \frac{1}{\sqrt{N}} \frac{\delta E_1}{E_1}. \quad (5.5.36)$$

In the thermodynamic limit $N \rightarrow \infty$ and so the relative fluctuation of the energy goes to 0. Thus, in the thermodynamic limit the energy of the canonical ensemble can be taken to be exactly given by the expectation of the Hamiltonian. Because the energy becomes an exact definite value and the canonical ensemble is only a function of the energy, in the thermodynamic limit the canonical ensemble exactly matches the microcanonical ensemble. This is the formal meaning behind “any large system acts as its own bath”.

Of course, not every quantity is either intensive or extensive. The product of two extensive quantities scales like the square of the system size and so is neither. As well, when we consider two non-interacting systems the partition function is multiplicative:

$$Z = \int_{\mathbb{P}} e^{-\beta \mathcal{H}} d\mathbb{P} = \int_{\mathbb{P}_1} \int_{\mathbb{P}_2} e^{-\beta \mathcal{H}_1 - \beta \mathcal{H}_2} d\mathbb{P}_1 d\mathbb{P}_2 = \left(\int_{\mathbb{P}_1} e^{-\beta \mathcal{H}_1} d\mathbb{P}_1 \right) \left(\int_{\mathbb{P}_2} e^{-\beta \mathcal{H}_2} d\mathbb{P}_2 \right) = Z_1 Z_2. \quad (5.5.37)$$

The phase space density in the canonical ensemble is multiplicative as well for non-interacting systems:

$$f(Q_1, Q_2, P_1, P_2) = \frac{e^{-\beta \mathcal{H}}}{Z} = \frac{e^{-\beta(\mathcal{H}_1 + \mathcal{H}_2)}}{Z_1 Z_2} = \frac{e^{-\beta \mathcal{H}_1}}{Z_1} \frac{e^{-\beta \mathcal{H}_2}}{Z_2} = f_1(Q_1, P_1) f_2(Q_2, P_2). \quad (5.5.38)$$

This multiplicativity property of the phase space density has an important interpretation. We found before in section 5.1 that two random variables are statistically independent (meaning knowledge of one tells you nothing about the value of the other) if and only if their joint probability distribution is given by the product of their individual distributions. So, the multiplicativity of the phase space density for non-interacting systems means that the statistical mechanics of non-interacting systems are statistically independent. Conceptually, this is absolutely necessary. If two systems which had never interacted were not statistically independent then measurements about one system would allow you to learn about the other. In contradiction, if the two had never interacted the properties of one by definition cannot have influenced the other. Their independence is necessary for consistency. The independence of non-interacting system is in fact such a basic requirement that we could just as well have used it as our starting point. It is the interactions of systems that make them not independent. Interactions make correlations! This will be a recurring theme going forward.

Let us see how far the independence of non-interacting systems can get us. We know from equation (5.4.8) that any system allowed to evolve for long enough will approach (in time average) a distribution which is a function of only the conserved quantities of that system. From equation (5.5.32) we know we can express the set of conserved quantities of a system so that they are all extensive. So, if system 1 is allowed to evolve for a sufficiently long time it will approach some phase space density:

$$\bar{f}_1(Q_1, P_1) = F(G_1(Q_1, P_1), \dots, G_K(Q_1, P_1)). \quad (5.5.39)$$

If an identical system, system 2, is allowed to evolve in the same way it will approach some phase space density:

$$\bar{f}_2(Q_2, P_2) = F(G_1(Q_2, P_2), \dots, G_K(Q_2, P_2)). \quad (5.5.40)$$

The function F is the same between the two systems if they are prepared identically. If these two subsystems do not interact then the combined system will approach the phase space density:

$$\bar{f}(Q_1, Q_2, P_1, P_2) = F(G_1(Q_1, P_1) + G_1(Q_2, P_2), \dots, G_K(Q_1, P_1) + G_K(Q_2, P_2)) \quad (5.5.41)$$

where we have used the extensivity of the conserved quantities. The function F is again the same if they are prepared identically. Then, the condition of statistical independence demands:

$$\bar{f}(Q_1, Q_2, P_1, P_2) = \bar{f}(Q_1, P_1) \bar{f}(Q_2, P_2) \quad (5.5.42)$$

Letting $\vec{G}_1 = (G_1(Q_1, P_1), \dots, G_K(Q_1, P_1))$ and $\vec{G}_2 = (G_1(Q_2, P_2), \dots, G_K(Q_2, P_2))$ and expressing $\bar{f}$ in terms of F we have that F must satisfy:

$$F(\vec{G}_1 + \vec{G}_2) = F(\vec{G}_1) F(\vec{G}_2). \quad (5.5.43)$$

This is now a constraint on the form of the function F . Differentiating both sides with respect to G_{2a} :

$$\frac{\partial F}{\partial G_{2a}}(\vec{G}_1 + \vec{G}_2) = \frac{\partial F}{\partial G_{2a}}(\vec{G}_2) F(\vec{G}_1). \quad (5.5.44)$$

On the left, a G_{2a} derivative is the same as a G_{1a} derivative as the left hand side only depends on the sum $\vec{G}_1 + \vec{G}_2$. So:

$$\frac{\partial F}{\partial G_{1a}}(\vec{G}_1 + \vec{G}_2) = \frac{\partial F}{\partial G_{2a}}(\vec{G}_2) F(\vec{G}_1). \quad (5.5.45)$$

Now evaluating both sides at $\vec{G}_2 = 0$:

$$\frac{\partial F}{\partial G_{1a}}(\vec{G}_1) = \frac{\partial F}{\partial G_a}(0)F(\vec{G}_1). \quad (5.5.46)$$

Define the β -vector:

$$\beta^a = -\frac{\partial F}{\partial G_a}(0). \quad (5.5.47)$$

Then, this differential equation becomes:

$$\frac{\partial F}{\partial G_a}(\vec{G}) = -\beta^a F(\vec{G}) \quad (5.5.48)$$

$$\implies F(G) = \frac{e^{-\beta^a G_a}}{Z} \quad (5.5.49)$$

where Z is independent of G . Using that the phase space density must integrate to 1 over the whole phase space we can determine Z :

$$\int_{\mathbb{P}} \bar{f}(Q, P|\beta) d\mathbb{P} = \int_{\mathbb{P}} \frac{e^{-\beta^a G_a(Q, P)}}{Z} d\mathbb{P} \stackrel{!}{=} 1 \quad (5.5.50)$$

$$\implies Z = \int_{\mathbb{P}} e^{-\beta^a G_a(Q, P)} d\mathbb{P}. \quad (5.5.51)$$

Hence, this Z is a generalized partition function and the equilibrium phase space density is:

$$\bar{f}(Q, P|\beta) = \frac{e^{-\beta^a G_a(Q, P)}}{Z} \quad (5.5.52)$$

where instead of an exponential of the energy with a single parameter β the exponential is a sum over all of the extensive conserved quantities of the system with an associated β^a to each. This distribution is known as the generalized canonical ensemble or generalized Boltzmann distribution. Because the energy is one of the extensive conserved quantities, in order to reduce this distribution to the typical canonical ensemble we simply need to take all of the β^a not associated with the energy to be 0. Equivalently, this is done by requiring that each of the other extensive conserved quantities has a uniform distribution for a given value of the energy, which is what we assumed anyway when deriving the microcanonical ensemble before. Thus, the canonical ensemble can be understood as the only possible distribution which is the result of long term time evolution, makes non-interacting systems statistically independent, and only depends on the coordinates and momenta through the energy. In some cases this third assumption can reasonably be relaxed in which case this generalized Boltzmann distribution is the correction distribution to use.

Whenever a system's properties are described by the (potentially generalized) Boltzmann distribution, that system is said to be in thermodynamic equilibrium. The Boltzmann distribution is the defining distribution for what is meant by thermodynamic equilibrium. So, **a system is in thermodynamic equilibrium if it is successfully described by the distribution for thermodynamic equilibrium**. This criterion, known as Callen's Criterion, may sound circular but it is not. When trying to establish whether a system is in thermodynamic equilibrium, we view the Boltzmann distribution as having unknown parameters β, λ where λ are the parameters appearing in the Hamiltonian $\mathcal{H}$. Then, measuring the statistical properties of the system we can use known parameter estimation techniques from the mathematical theory of statistics to find "best" values for the parameters β, λ . Then, if further statistical properties of the system are correctly predicted by those now measured values of β, λ the system is said to be thermodynamic equilibrium with those given values of the parameters. If they do not predict correct further statistical properties, the system in question is not in thermodynamic equilibrium. This is also to say: **temperature is a parameter for fitting a probability distribution's expectations to experimentally measurable quantities and it only "exists" for a system when that system is in thermodynamic equilibrium**. There is no unambiguous meaning to temperature outside of thermodynamic equilibrium. Because the (generalized) Boltzmann distribution is the defining distribution for thermodynamic equilibrium, we often write:

$$f_{\text{eq}}(Q, P|\beta) = \frac{e^{-\beta^a G_a(Q, P)}}{Z} \quad (5.5.53)$$

where the subscript eq is shorthand for equilibrium.

In general the theory of statistical parameter estimation is quite sophisticated and I recommend [20], [53] for a physicist centric overview. For the basic idea of one type of parameter estimation, suppose we can

measure some random variable X of our physical system and that we do so N times, once each in N different copies of our system. Because we are using N different copies of a statistically identical system, we take each copy to be identically and independently distributed. These N measurements are called a sample. Define then the sample mean $\bar{X}$:

$$\bar{X} = \frac{1}{N} \sum_{n=1}^N X_n. \quad (5.5.54)$$

The expectation of the sample mean matches the expectation of each X_n individually:

$$\mathbb{E}(\bar{X}) = \frac{1}{N} \sum_{n=1}^N \mathbb{E}(X_n) = \frac{1}{N} \sum_{n=1}^N \mu_X = \mu_X. \quad (5.5.55)$$

Explicitly computing the variance of the sample mean:

$$\text{Var}(\bar{X}) = \mathbb{E}(\bar{X} - \mu_X)^2 = \mathbb{E} \left(\frac{1}{N} \sum_{n=1}^N (X_n - \mu_X) \right)^2 = \frac{1}{N^2} \mathbb{E} \left(\sum_{n=1}^N \sum_{k=1}^N (X_n - \mu_X)(X_k - \mu_X) \right) \quad (5.5.56)$$

$$= \frac{1}{N^2} \sum_{n=1}^N \sum_{k=1}^N \text{Cov}(X_n, X_k). \quad (5.5.57)$$

Because each X_n is independent of X_k for $n \neq k$, their correlation vanishes. However, if $n = k$, their correlation is simply the variance of X_n :

$$\text{Var}(\bar{X}) = \frac{1}{N^2} \sum_{n=1}^N \sum_{k=1}^N \delta_{nk} \text{Var}(X_n) = \frac{1}{N^2} \sum_{n=1}^N \sigma_X^2 = \frac{\sigma_X^2}{N}. \quad (5.5.58)$$

So, the variance of the sample mean gets smaller with increasing N and in fact goes to 0 as $N \rightarrow \infty$. This means that if one takes N independent samples from our system and computes the sample mean of the measured quantities, that sample mean in the large N limit converges to the expectation μ_X (as it does not vary from it at all in that limit due to its variance going to 0). The expectation μ_X can be computed as a function of the parameters of our distribution and so in the large data limit we can measure $\bar{X}$ experimentally and equate it to μ_X computed theoretically to infer values of the underlying distribution parameters. We need to do this for enough different quantities like X in order to fully determine the parameters of the distribution. This is a very frequentist way of thinking, which is often valid in statistical mechanics where we have a great number of essentially interchangeable particles to sample from.

At finite data, the variance of $\bar{X}$ is non-zero and so it is important to have a way to quantify our typical error. We know from our previous interpretations of the mean and variance that μ_X is the best constant representative value for $\bar{X}$ and $\text{Var}(\bar{X})$ is the best constant representative value for the squared-error in representing $\bar{X}$ by μ_X . So, $\sqrt{\text{Var}(\bar{X})}$ would be a good candidate for quantifying the typical error in our approximation $\bar{X} \approx \mu_X$ made at finite N . However, we don't know $\text{Var}(\bar{X})$ unless we already know σ_X^2 . So, we also need a way to estimate σ_X^2 . This can be done using the sample variance s^2 :

$$s^2 = \frac{1}{N-1} \sum_{n=1}^N (X_n - \bar{X})^2. \quad (5.5.59)$$

For computations, it is more useful to write the sample variance as:

$$s^2 = \frac{1}{N-1} \sum_{n=1}^N (X_n - \mu_X + \mu_X - \bar{X})^2 = \frac{1}{N-1} \sum_{n=1}^N ((X_n - \mu_X)^2 - 2(X_n - \mu_X)(\bar{X} - \mu_X) + (\bar{X} - \mu_X)^2) \quad (5.5.60)$$

$$= \frac{1}{N-1} \left(\sum_{n=1}^N (X_n - \mu_X)^2 - 2N(\bar{X} - \mu_X)^2 + N(\bar{X} - \mu_X)^2 \right) \quad (5.5.61)$$

$$= \frac{1}{N-1} \left(\sum_{n=1}^N (X_n - \mu_X)^2 - N(\bar{X} - \mu_X)^2 \right). \quad (5.5.62)$$

As well, it is often useful to rewrite everything in terms of some random variables Y_n which shift away the

mean μ_X :

$$Y_n = X_n - \mu_X \implies \bar{Y} = \frac{1}{N} \sum_{n=1}^N Y_n = \bar{X} - \mu_X \quad (5.5.63)$$

$$\implies \mathbb{E}Y_n = \mathbb{E}Y = 0, \quad \mathbb{E}Y_n^2 = \sigma_X^2, \quad \mathbb{E}\bar{Y}^2 = \frac{\sigma_X^2}{N} \quad (5.5.64)$$

$$\implies s^2 = \frac{1}{N-1} \left(\sum_{n=1}^N Y_n^2 - N\bar{Y}^2 \right). \quad (5.5.65)$$

Then, the expectation of the sample variance is:

$$\mathbb{E}s^2 = \frac{1}{N-1} \left(\sum_{n=1}^N \mathbb{E}Y_n^2 - N\mathbb{E}\bar{Y}^2 \right) = \frac{1}{N-1} \left(N\sigma_X^2 - N\frac{\sigma_X^2}{N} \right) = \sigma_X^2. \quad (5.5.66)$$

So, the sample variance which can be computed only from our collected data is also an unbiased estimator of the true variance of the random variable. As well, we can compute the variance of the sample variance:

$$\text{Var}(s^2) = \mathbb{E}(s^2 - \sigma_X^2)^2 = \mathbb{E}(s^4 - 2\sigma_X^2 s^2 + \sigma_X^4) = \mathbb{E}s^4 - \sigma_X^4 \quad (5.5.67)$$

$$= \mathbb{E} \left(\frac{1}{(N-1)^2} \left(\sum_{n=1}^N Y_n^2 - N\bar{Y}^2 \right)^2 \right) - \sigma_X^4 \quad (5.5.68)$$

$$= \frac{1}{(N-1)^2} \mathbb{E} \left(\left(\sum_{n=1}^N Y_n^2 \right)^2 - 2N\bar{Y}^2 \sum_{n=1}^N Y_n^2 + N^2\bar{Y}^4 \right) - \sigma_X^4. \quad (5.5.69)$$

Let us compute these pieces individually. The first piece can be rewritten as a double sum:

$$\mathbb{E} \left(\sum_{n=1}^N Y_n^2 \right)^2 = \mathbb{E} \left(\sum_{n=1}^N \sum_{k=1}^N Y_n^2 Y_k^2 \right) = \sum_{n=1}^N \mathbb{E} \left(Y_n^2 \sum_{k=1}^N Y_k^2 \right). \quad (5.5.70)$$

The expectation in the summand here is written as a function of n but because each n is identically distributed and other than the n dependence the expression is symmetry in all of the Y_k the result of that expectation is the same for each value of n :

$$\mathbb{E} \left(\sum_{n=1}^N Y_n^2 \right)^2 = N\mathbb{E} \left(Y_1^2 \sum_{k=1}^N Y_k^2 \right) = N\mathbb{E} \left(Y_1^2 (Y_1^2 + \sum_{k=2}^N Y_k^2) \right) = N\mathbb{E}Y_1^4 + N \sum_{k=2}^N \mathbb{E}(Y_1^2 Y_k^2). \quad (5.5.71)$$

In the expectation of the product appearing here $k \neq 1$ and so Y_1 and Y_k are independent giving:

$$\mathbb{E} \left(\sum_{n=1}^N Y_n^2 \right)^2 = N\mathbb{E}Y_1^4 + N \sum_{k=2}^N \mathbb{E}(Y_1^2) \mathbb{E}(Y_k^2) = N\sigma_X^4 m_4 + N(N-1)\sigma_X^4. \quad (5.5.72)$$

Here we have used the definition of the fourth normalized central moment of X :

$$m_4 = \mathbb{E} \left(\frac{X - \mu_X}{\sigma_X} \right)^4. \quad (5.5.73)$$

The second term in equation (5.5.69) can be computed using the same symmetry argument:

$$\mathbb{E} \left(\bar{Y}^2 \sum_{n=1}^N Y_n^2 \right) = \sum_{n=1}^N \mathbb{E}(\bar{Y}^2 Y_n^2) = N\mathbb{E}(Y_1^2 \bar{Y}^2) = N\mathbb{E} \left(Y_1^2 \left(\frac{1}{N} \sum_{n=1}^N Y_n \right)^2 \right) \quad (5.5.74)$$

$$= \frac{1}{N} \mathbb{E} \left(Y_1^2 \left(Y_1 + \sum_{n=2}^N Y_n \right)^2 \right) = \frac{1}{N} \mathbb{E} \left(Y_1^4 + 2Y_1^3 \sum_{n=2}^N Y_n + Y_1^2 \sum_{n=2}^N \sum_{k=2}^N Y_n Y_k \right) \quad (5.5.75)$$

$$= \frac{1}{N} (\mathbb{E}Y_1^4 + 2(N-1)\mathbb{E}(Y_1^3 Y_2) + (N-1)\mathbb{E}(Y_1^2 Y_2^2)) = \frac{1}{N} (m_4 \sigma_X^4 + (N-1)\sigma_X^4). \quad (5.5.76)$$

Finally then the third term can be computed as:

$$\mathbb{E}\bar{Y}^4 = \mathbb{E} \left(\frac{1}{N} \sum_{n=1}^N Y_n \bar{Y}^3 \right) = \frac{1}{N} N\mathbb{E}(Y_1 \bar{Y}^3) = \mathbb{E} \left(Y_1 \left(Y_1 + \sum_{n=2}^N Y_n \right)^3 \right) \quad (5.5.77)$$

$$= \mathbb{E} \left(Y_1^4 + 3Y_1^3 \sum_{n=2}^N Y_n + 3Y_1^2 \left(\sum_{n=2}^N Y_n \right)^2 + Y_1 \left(\sum_{n=2}^N Y_n \right)^3 \right) = m_4 \sigma_X^4 + 0 + 3\sigma_X^2 \mathbb{E} \left(\sum_{n=2}^N Y_n \right)^2 + 0 \quad (5.5.78)$$

$$= m_4 \sigma_X^4 + 3\sigma_X^2 \mathbb{E} \left(\sum_{n=2}^N \sum_{k=2}^N Y_n Y_k \right) = m_4 \sigma_X^4 + 3(N-1)\sigma_X^4. \quad (5.5.79)$$

Putting all of these together then gives a variance:

$$\text{Var}(s^2) = \frac{\sigma_X^4}{N} \left(m_4 - \frac{N-3}{N-1} \right). \quad (5.5.80)$$

So, for large N the variance of s^2 limits toward 0 as well. Consequently, for large data (large N) s^2 is a very good representative for the variance σ_X^2 and so we can use $\frac{s^2}{N}$ to estimate the typical error in our approximation of $\mu_X \approx \bar{X}$. $\bar{X}$ and s^2 can be determined only from the sample of measured values of X and so are experimentally measurable. Because their values (for large amount of data) are determined by the theory, they provide a link to compare theory with experiment.

The reasoning given around $\bar{X}$ and s^2 require us to measure a property X of N independent and identically distributed instances of a system. Realistically, in statistical mechanics we often do not set up the same system multiple times to measure it. More practically, if we have a large system consisting of many smaller identical subsystems which have such weak interactions with each other that for our purposes we may treat the interaction as negligible then each copy of the subsystem is like an identically and independent instance of the “same” random variable, since they are all taken to be identical subsystems. If we can then measure a property of one of the subsystems and then take another measurement of another one of the subsystems without knowing which copy we are measuring, it is like we are taking an identically independently distributed sample. For example, in a bag of colored marbles each marble has a definite property (the color) and pulling a marble out of the bag and looking at the color measures that property. Replacing the marble back into the bag, shaking the bag, and then selecting another marble allows one to take another data point from the bag in an identical and independently distributed way to the first measurement. For a box of gas, if we have a wall which is able to sense impacts of the gas molecules onto that wall, each impact acts as a measurement of the position (and potentially the velocity, depending on what the wall can register) of a gas molecule. As the molecules fly around they are like the marbles replacing themselves into the bag as the particular identity of any specific gas molecule is not tracked. Thus, while each gas molecule has definite properties, the data registered onto the detector from each molecule is an identically independently distributed random variable relative to the other data points.

Certainly not every system under all circumstances in the long run reaches the Boltzmann distribution. We can only be confident the Boltzmann distribution will be valid for a system in the long run if we have prepared it so that non-interacting subsystems are statistically independent and all extensive conserved quantities are uniformly distributed at fixed energy (or we can take the generalized Boltzmann distribution if this third condition is not true). This is as much a condition on our preparation of the system as the system itself. It so happens that these conditions on preparation are typically reasonable for experiment and this is why the Boltzmann distribution is so often useful. There are some classes of systems (called ergodic) who’s time averaged behavior do evolve toward the Boltzmann distribution very precisely for wide classes of initial conditions but not all systems are so. Precisely speaking, no system is ever likely to be exactly described by the Boltzmann distribution or equivalently exactly in thermodynamic equilibrium. Instead, thermodynamic equilibrium is an approximate idealization which is useful for the time-averaged behavior of systems which are experimentally consistent with its restrictions within a given experimental tolerance.

In defining the partition function and the Boltzmann distribution, we have of course presumed that it is possible to do so. The Hamiltonians we have dealt with so far have not been bounded above, and this is the typical case in life (arbitrarily high energies exist). In order for the partition function to exist, the integrand $e^{-\beta \mathcal{H}}$ must decay to 0 far out in the phase space so that the integral converges. For $\mathcal{H}$ which go to ∞ as we go far out into the phase space (which are all the Hamiltonians we have considered so far) this means that we need $\beta \mathcal{H} \rightarrow \infty$ or equivalently $\beta > 0$. That is, **every system with Hamiltonian unbounded from above must have nonnegative temperature**. Alternatively, if we had a Hamiltonian which was not bounded from below then we would need $\beta < 0$ in order for the partition function to converge. So, every system with a Hamiltonian unbounded from below must have a nonpositive temperature. Consequently, a system comprised of two subsystems, one with unbounded above Hamiltonian and the other with unbounded

below, can never reach thermodynamic equilibrium. Because thermodynamic equilibrium is observed as a general phenomenon, all temperatures everywhere must be either all positive or all negative. By convention they are all positive (if we had them all negative, we could use a negative α in (5.2.62) to make them all positive and so the boundedness below of the energy is a standard convention). Therefore, going forward we will use that the existence of thermodynamic equilibrium places a fundamental restriction on the Hamiltonian to be bounded below.

Because the Hamiltonian must be bounded below, the temperature of any system in equilibrium is nonnegative. It is interesting to see the properties of a system in the low temperature limit $T \rightarrow 0$. Let E_0 be the greatest lower bound of the Hamiltonian. That is, E_0 is the greatest real number so that $\mathcal{H} \geq E_0$ everywhere. This E_0 is called the “ground state energy” of the Hamiltonian. Then:

$$f_{\text{eq}}(Q, P|T) = \frac{e^{-\frac{\mathcal{H}-E_0}{T}}}{e^{\frac{E_0}{T}} Z}. \quad (5.5.81)$$

For (Q, P) so that $\mathcal{H} > E_0$, in the limit $T \rightarrow 0^+$ the expression $\frac{\mathcal{H}-E_0}{T} \rightarrow \infty$ and so $f_{\text{eq}} \rightarrow 0$. For (Q, P) so that $\mathcal{H} = E_0$, f_{eq} is proportional to a constant independent of (Q, P) . So, in the $T \rightarrow 0^+$ limit the Boltzmann distribution approaches a uniform distribution on the region of the phase space with the ground state energy and becomes 0 everywhere else:

$$\lim_{T \rightarrow 0} f_{\text{eq}}(Q, P|T) = \frac{1}{g(E_0)} \delta(\mathcal{H}(Q, P) - E_0). \quad (5.5.82)$$

Alternatively, in the high temperature limit $T \rightarrow \infty$ the term $\frac{\mathcal{H}}{T} \rightarrow 0$ and so the Boltzmann distribution becomes a uniform distribution over the entire phase space.

Theorem 5.4: Canonical Ensemble

In an extremely large system described by the microcanonical ensemble with weak interactions between a particular subsystem with Hamiltonian $\mathcal{H}$ and the rest of system, the marginal phase space density for the subsystem is given by the canonical ensemble:

$$f_{\text{canon}}(Q, P) = \frac{e^{-\frac{\mathcal{H}(Q, P)}{T}}}{Z(T)} \quad (5.5.83)$$

where T , the temperature of the system, is a distribution parameter for the subsystem which characterizes the average energy per effective harmonic oscillator degree of freedom for the full system and $Z(T)$, the partition function, is a normalization factor fixed by:

$$Z(T) = \int_{\mathbb{P}} e^{-\frac{\mathcal{H}}{T}} d\mathbb{P}. \quad (5.5.84)$$

Here the greater large system is called the thermal bath for the subsystem. A sufficiently large system then acts as a bath for itself when considering any particular subsystem in relation to the full system. This is only exactly true for an infinitely large system defined in the thermodynamic limit. Formally, this is the limit in which all extensive quantities of the system are scaled to infinity while keeping all of the intensive quantities of the system fixed.

The canonical ensemble is a special case of the generalized canonical ensemble. The generalized canonical ensemble is the generic distribution for the time averaged behavior of a system for which the noninteracting subsystems within the full system are statistically independent. Explicitly it is given by:

$$f_{\text{eq}}(Q, P) = \frac{e^{-\beta^a G_a(Q, P)}}{Z(\beta)} \quad (5.5.85)$$

where $G_a(Q, P)$ are the extensive conserved quantities of the system, β^a are distribution parameters and $Z(\beta)$, the generalized partition function, is a normalization factor fixed by:

$$Z(\beta) = \int_{\mathbb{P}} e^{-\beta^a G_a} d\mathbb{P}. \quad (5.5.86)$$

In order for a system to reach thermodynamic equilibrium, its Hamiltonian must either be bounded from below or above. If it does so with nonnegative temperature, its Hamiltonian must be bounded below.

Readers comparing to a source written in SI units will encounter a constant k_B known as the Boltzmann constant in the definition of temperature (and later into the definition of entropy). Historically, the concept of temperature was introduced before its theoretical origins and connection to energy were understood. Consequently, it was initially believed to need its own units of measurement as it was unclear how to relate it to existing units. This led to the historical artifact of introducing k_B which is a conversion factor to convert between the introduced unit for temperature, which in SI units is called the Kelvin and written K, and the pre-existing unit for energy from mechanics, which in SI units is called the Joule and written J but is the same as $\frac{\text{kg m}^2}{\text{s}^2}$. The unit of the Kelvin is defined by choosing the value of $k_B = 1.380649 \times 10^{-23} \frac{\text{J}}{\text{K}}$. There is no theoretical or experimental need to introduce separate units for temperature; the existence of the unit of the Kelvin is purely an accident of history. To compare with someone using the Kelvin, simply introduce powers of k_B to convert units of Joules to Kelvin. Please understand that k_B is not a fundamental constant of the universe, simply a historical conversion factor between different units which takes an arbitrary exactly defined value. There is no experiment to measure k_B because there is nothing to measure³.

The units of temperature are an enormous headache for communication purposes. The historical metric units of degrees Celsius were set so that the boiling point of water at standard pressure ($101325 \frac{\text{kg}}{\text{m s}^2}$, essentially the air pressure at sea level on Earth) was 100°C and the freezing point of water at the same pressure was 0°C . Consequently, it is possible to have negative degrees Celsius for temperatures, unlike an absolute temperature scale which we always use for T and which is never negative for systems with Hamiltonians unbounded above (basically everything real). The degree Celsius is related to the Kelvin by an offset so that a temperature in Celsius is equal to the temperature in Kelvin minus the numerical value 273.15. So, $0\text{K} = -273.15^\circ\text{C}$. Because the Boltzmann constant is defined to take an exact value, 0°C and 100°C no longer exactly give the freezing/boiling points of water but they are close enough for essentially all purposes. To see the social function of having different units of temperature it is interesting to look at typical human values. Barring the most extreme weather conditions, ordinary human life takes place between -50°C and 50°C with (at least by my standards) comfortable room temperature at about 20°C . In Kelvin these estimates are about 223K to 323K with comfort at 293K. In Joules $= \frac{\text{kg m}^2}{\text{s}^2}$, these would be $3.08 \times 10^{-21}\text{J}$ to $4.46 \times 10^{-21}\text{J}$ with comfort at $4.05 \times 10^{-21}\text{J}$. Thus, in Joules human relevant temperatures are a bit of a mouthful. But, at the level of basic theory, introducing a separate unit of temperature is strictly unnecessary. We will establish how to measure temperature experimentally in 5.11.

The fact that we need the Hamiltonian to be bounded below for thermodynamic equilibrium to exist at positive temperature when combined with special relativity actually implies that mass must be nonnegative. Let $\mathcal{H}$ and $\vec{p}$ be the energy and linear momentum of a relativistic free particle. Then, because $(\mathcal{H}, \vec{p})^\mu$ are the components of a 4-vector, the combination $\mathcal{H}^2 - |\vec{p}|^2$ is automatically Lorentz invariant. Because the particle is free, it also has spacetime translational symmetry and so $\mathcal{H}^2 - |\vec{p}|^2$ is a Lorentz invariant constant (as it cannot depend on $t, \vec{x}$ due to the translational symmetry). Let m^2 be the magnitude of that constant and let σ_1 be the sign of that constant so that:

$$\mathcal{H}^2 - |\vec{p}|^2 = \sigma_1 m^2 \implies \mathcal{H} = \sigma_2 \sqrt{\sigma_1 m^2 + |\vec{p}|^2} \quad (5.5.87)$$

where σ_2 is either ± 1 . The symbol m here is defined to be nonnegative (because only $m^2 = |\mathcal{H}^2 - |\vec{p}|^2|$ has been defined so far) but that symbol m has not yet earned the interpretation of mass. The velocity of the particle is then given by:

$$\dot{\vec{x}} = \frac{\partial \mathcal{H}}{\partial \vec{p}} = \frac{\sigma_2 \vec{p}}{\sqrt{\sigma_1 m^2 + |\vec{p}|^2}} = \frac{\vec{p}}{\mathcal{H}}. \quad (5.5.88)$$

Thus the speed of the particle is:

$$|\dot{\vec{x}}|^2 = \frac{|\vec{p}|^2}{\mathcal{H}^2} = 1 - \frac{\sigma_1 m^2}{\mathcal{H}^2} \quad (5.5.89)$$

which due to causality must be less than or equal to 1. Hence, causality requires $\sigma_1 = 1$ (the case that $|\dot{\vec{x}}|^2 = 1$ is covered by $m^2 = 0$). This simplifies our Hamiltonian to:

$$\mathcal{H} = \sigma_2 \sqrt{m^2 + |\vec{p}|^2} \quad (5.5.90)$$

This Hamiltonian is bounded below if and only if $\sigma_2 = 1$, and so:

$$\mathcal{H} = \sqrt{m^2 + |\vec{p}|^2}. \quad (5.5.91)$$

³Any experiment which purports to measure k_B is really just calibrating the conversion between two devices which were designed to use different units of energy from each other.

The nonrelativistic limit of this Hamiltonian then gives:

$$\mathcal{H} = m + \frac{|\vec{p}|^2}{2m} + \mathcal{O}(p^4) \quad (5.5.92)$$

where the symbol m now appearing is both guaranteed to be positive and corresponds to the mass in the Galilean Lagrangian.

Exercises

Problem 5.28: ★ Equipartition Theorem. Let x_k be the variables (both Q 's and P 's) in a system's Hamiltonian and consider a Hamiltonian which is a sum of N square terms:

$$\mathcal{H} = \sum_{k=1}^N a_k x_k^2$$

for some coefficients a_k . Show that the expected energy for this system in the canonical ensemble is:

$$E = \frac{NT}{2}.$$

Thus each variable which only enters the Hamiltonian quadratically contributes $\frac{T}{2}$ to the expected energy (this is known as the equipartition theorem).

Problem 5.29: Relationship between the partition function and density of states. Show that the partition function and density of states of a system are related by the Laplace transform, with β as the Laplace transform variable:

$$Z(\beta) = \int_{-\infty}^{\infty} e^{-\beta E} g(E) dE.$$

Problem 5.30: Simple Polarization Model. Consider an electric dipole with moment of inertia I and dipole moment magnitude $\wp$ able to rotate with spherical coordinates (θ, φ) placed in an external electric field of magnitude E aligned in the z -direction. Then, just as in problem 3.68, the Lagrangian for this single dipole is:

$$\mathcal{L} = \frac{1}{2}I(\dot{\theta}^2 + \dot{\varphi}^2 \sin^2 \theta) + \wp E \cos \theta.$$

(a) Show that the Hamiltonian for the dipole is:

$$\mathcal{H} = \frac{p_\theta^2}{2I} + \frac{p_\varphi^2}{2I \sin^2 \theta} - \wp E \cos \theta$$

and that its partition function is:

$$Z = \frac{2IT^2}{\hbar^2 \wp E} \sinh\left(\frac{\wp E}{T}\right).$$

(b) Show that the expected dipole moment for the single dipole is:

$$\mathbb{E}\vec{\wp} = \left(\frac{\wp}{\tanh\left(\frac{\wp E}{T}\right)} - \frac{T}{E} \right) \frac{\vec{E}}{E} = \frac{\wp^2}{3T} \vec{E} + \mathcal{O}(E^3).$$

As well, show that in the low temperature limit the dipole aligns perfectly with the background electric field and that in the high temperature limit the dipole's direction is completely uniformly distributed.

(c) Suppose then that we have a material consisting of n electrically dipolar molecules per unit volume, each with the same dipole moment magnitude. Show then that this simple model predicts an electric polarization of:

$$\vec{P} = \frac{n\wp^2}{3T} \vec{E} + \mathcal{O}(E^3)$$

when an external electric field is applied to the material. Thus, show that this simple model predicts an electric susceptibility of:

$$\chi_e = \frac{n\wp^2}{3\epsilon_0 T}.$$

This model is a bit too simple to accurately predict the electric susceptibility of all materials and more detailed models exist. But, this correctly captures the basic qualitative features of how electric susceptibility depends on temperature for weak external fields and can provide reasonable quantitative estimates of the susceptibilities of some real materials.

Problem 5.31: ★ Thermodynamic Limit of Extensive Quantities. Consider a system comprised of N identical noninteracting subsystems so that the total Hamiltonian is $\mathcal{H} = \mathcal{H}_1 + \dots + \mathcal{H}_N$. Let G_k be a quantity within subsystem k which is extensive so that for the combined system $G = G_1 + \dots + G_N$.

- (a) Show that in thermodynamic equilibrium each of the G_k are statistically independent of each other.
- (b) Show that:

$$\mathbb{E}(G) = N\mathbb{E}(G_1), \quad \text{Var}(G) = N\text{Var}(G_1)$$

(assuming that $\mathbb{E}(G_1)$ and $\text{Var}(G_1)$ exist and are finite).

- (c) Show that in the thermodynamic limit $N \rightarrow \infty$ the relative uncertainty in the value of G goes to 0. That is:

$$\lim_{N \rightarrow \infty} \frac{\text{Var}(G)}{(\mathbb{E}(G))^2} = 0.$$

Thus, explain that in the thermodynamic limit $\frac{G}{N}$ effectively has a definite value given by $\mathbb{E}(G_1)$. This is how definite macroscopic properties emerge from distributions over unknown microscopic variables in the thermodynamic limit.

Problem 5.32: Coulomb Partition Function. Consider a system of two charged nonrelativistic particles interacting via the Coulomb potential so that their combined Hamiltonian is:

$$\mathcal{H} = \frac{|\vec{p}_1|^2}{2m_1} + \frac{|\vec{p}_2|^2}{2m_2} + \frac{q_1 q_2}{4\pi\epsilon_0 |\vec{x}_1 - \vec{x}_2|}.$$

Show that the partition function for this system diverges due to integrating for large $|\vec{x}_1|$ or $|\vec{x}_2|$ and that it diverges due to integrating for small $|\vec{x}_1 - \vec{x}_2|$. The first of these can be mitigated by taking the charges to be confined to a container of finite volume, which is generally physically reasonable. The second of these is a genuine problem which occurs because the Coulomb interaction is singular when the particles get too close. In order to fix this issue with the Coulomb interaction one needs to modify the potential at close distances. We know from chapter 4 that we will need to move past point particles. It turns out doing so will solve this problem at close distances. Thus, we see that a classical system of point charges interacting via electrostatics does not have a well defined partition function (and consequently, does not have a well defined thermodynamic equilibrium).

Problem 5.33: Particles in a subvolume. Consider a system of N free particles in a container of volume $\mathbb{V}$. Let $\mathbb{V}_s$ be a subvolume within the larger container and let N_s be the number of particles within that subvolume. Assume the particles are in thermodynamic equilibrium.

- (a) Let $f = \frac{\mathbb{V}_s}{\mathbb{V}}$. Show that the probability distribution for N_s is exactly the binomial distribution:

$$\text{Prob}(N_s = k) = \frac{N!}{k!(N-k)!} f^k (1-f)^{N-k}.$$

- (b) Let $n = \frac{N}{\mathbb{V}}$ be the average number density of particles in the container. Suppose we take the thermodynamic limit, keeping the number density and the subvolume $\mathbb{V}_s$ under consideration fixed as we take $N \rightarrow \infty$. Show that in this limit the probability distribution for N_s is exactly the Poisson distribution:

$$\text{Prob}(N_s = k) = \frac{e^{-n\mathbb{V}_s}}{k!} (n\mathbb{V}_s)^k.$$

Problem 5.34: Air density versus altitude. Consider a system of N massive particles in a container of cross sectional area $\mathbb{A}$ and height h in a uniform gravitational field of magnitude g pointed downward. (Let up be the positive z direction.) Show that in equilibrium the mass density of the system depends on position as:

$$\rho(\vec{x}) = e^{-\frac{mgz}{T}} \rho(0)$$

and explain why near the Earth's surface this should give a reasonable first approximation for how air density varies with altitude.

5.6 Information Theory and Entropy

Before further studying the properties of systems in thermodynamic equilibrium, we need to understand some more math. In particular, let us study the question: suppose a random variable is distributed according to some probability distribution, what is the probability of observing a particular different distribution of the results when we sample from it? Formally, let X be a random variable which has d possible outcomes (label them $1, 2, \dots, d$) with probability p_k of taking the outcome k . If we sample N times from identically independently distributed such X , we can compute the probability of getting 1 a total of n_1 times, 2 a total of n_2 times, ..., and d a total of n_d times. The probability of getting the counts $n_1, \dots, n_d$ without caring about the order the results are gotten in is the sum of the probabilities of getting those counts over all specific possible orders (each order is disjoint from the others). Because each trial is identical and independent of the other trials, the probability of getting those counts with a specific ordering does not depend on that ordering and so the probability of getting those counts is the probability of getting them in any specific order times the number of equivalent ways to reorder them. For N distinct objects there are $N!$ ways to order them. In order to cancel the over counting of the $n_1!$ ways to order the identical times $X = 1$, the $n_2!$ ways to order the identical times $X = 2$, ... there are $\frac{N!}{n_1! \dots n_d!}$ distinct ways to order the results which give the specific counts $n_1, \dots, n_d$. The probability of getting k n_k times in a row is $p_k^{n_k}$ as each trial is independent. So, the probability of getting the counts $n_1, \dots, n_d$ is given by getting p_1 n_1 times in a row, p_2 n_2 times in a row, ..., p_d n_d times in a row, all times the number of ways to reorder the results:

$$p(n_1, \dots, n_d) = \frac{N!}{n_1! \dots n_d!} p_1^{n_1} \dots p_d^{n_d}. \quad (5.6.1)$$

Here $n_1 + \dots + n_d = N$ as there were N trials taken in total. This distribution is known as the multinomial distribution. If in these N trials we have observed the counts $n_1, \dots, n_d$ we have equivalently observed the outcome k a fraction $\frac{n_k}{N}$ of the time. Thus, we take as the “observed” probabilities from this sample:

$$q_k = \frac{n_k}{N}. \quad (5.6.2)$$

Automatically, these “observed” probabilities sum to 1. Equivalently then, we say that the probability of observing the distribution $\{q_k\}$ given the true distribution $\{p_k\}$ is:

$$f(q_1, \dots, q_k) = \frac{N!}{\prod_{k=1}^d (Nq_k)!} \prod_{k=1}^d p_k^{Nq_k}. \quad (5.6.3)$$

We expect (based on frequentist thinking) that for a large number of trials the observed probabilities will converge to the true probabilities. Let us study this expression for large N to confirm this suspicion. To do so it is useful to define Sterling’s function:

$$\text{St}(N) \stackrel{\text{def}}{=} \frac{N!}{N^N e^{-N} \sqrt{2\pi N}}. \quad (5.6.4)$$

Sterling’s theorem (proven in problem 5.6) is that:

$$\lim_{N \rightarrow \infty} \text{St}(N) = 1. \quad (5.6.5)$$

Thus, we can rewrite the factorial in terms of easier functions:

$$N! = N^N e^{-N} \sqrt{2\pi N} \text{St}(N) \quad (5.6.6)$$

and in the large N limit the Sterling’s function piece will simply become 1 (in fact it approaches 1 very quickly). Explicitly using this result in equation (5.6.3):

$$f(q_1, \dots, q_k) = \frac{N^N e^{-N} \sqrt{2\pi N} \text{St}(N)}{\prod_{k=1}^d \left(N^{Nq_k} q_k^{Nq_k} e^{-Nq_k} \sqrt{2\pi Nq_k} \text{St}(Nq_k) \right)} \prod_{k=1}^d p_k^{Nq_k} \quad (5.6.7)$$

$$= \frac{N^N e^{-N} \sqrt{2\pi N} \text{St}(N)}{N^N e^{-N} (2\pi N)^{\frac{d}{2}} \prod_{k=1}^d (\text{St}(Nq_k) \sqrt{q_k})} \prod_{k=1}^d \left(\frac{p_k}{q_k} \right)^{Nq_k} \quad (5.6.8)$$

$$= \frac{\text{St}(N)}{(2\pi N)^{\frac{d-1}{2}} \prod_{k=1}^d (\text{St}(Nq_k) \sqrt{q_k})} e^{-N \sum_{k=1}^d q_k \ln \left(\frac{q_k}{p_k} \right)}. \quad (5.6.9)$$

It appears that the probability exponentially decays with N and has some nasty prefactor. Define this

quantity in the exponent:

$$\mathcal{I}(q|p) \stackrel{\text{def}}{=} \sum_{k=1}^d q_k \ln \left(\frac{q_k}{p_k} \right). \quad (5.6.10)$$

Then, we have:

$$f(q_1, \dots, q_k)^{\frac{1}{N}} = \left(\frac{\text{St}(N)}{(2\pi N)^{\frac{d-1}{2}} \prod_{k=1}^d (\text{St}(Nq_k) \sqrt{q_k})} \right)^{\frac{1}{N}} e^{-\mathcal{I}}. \quad (5.6.11)$$

In the large N limit all of the Sterling's functions become 1. The quantity $C^{\frac{1}{N}}$ goes to 1 for any constant C as $N \rightarrow \infty$. As well, the quantity $N^{\frac{1}{N}}$ also goes to 1 as $N \rightarrow \infty$ (to prove this consider the logarithm of this quantity and use l'Hopital's rule). Because of this, the entire prefactor goes to 1 as $N \rightarrow \infty$. So, in the large N limit:

$$\lim_{N \rightarrow \infty} f(q_1, \dots, q_k)^{\frac{1}{N}} = e^{-\mathcal{I}} \quad (5.6.12)$$

$$\implies \boxed{f(q_1, \dots, q_k) \sim e^{-N\mathcal{I}} \quad (\text{for large } N).} \quad (5.6.13)$$

Thus, this quantity $\mathcal{I}$ gives the rate at which it becomes increasingly unlikely to observe the data $\{q_k\}$ from the probability distribution $\{p_k\}$ as the number of trials increases. In this way $\mathcal{I}$ gives some measure of how different the apparent distribution $\{q_k\}$ is from the true distribution $\{p_k\}$. This $\mathcal{I}$ is called the “**relative information**” of q to p , the “relative entropy” of q to p , or the “Kullback-Liebler divergence” of q and p .

There are other ways in which the relative information is a good measure of distance. First, let us study its extreme values. For fixed p , the relative information is a function of the variables $q_1, \dots, q_d$. Those q_k cannot be changed independently as they must sum to 1. So, to find maxima and minima of the relative information we need to vary it subject to the constraint that these variables sum to 1. By ordinary calculus, this can be imposed with a Lagrange multiplier α . So, let us vary the quantity:

$$\mathcal{I}(q|p) = \sum_{k=1}^d q_k \ln \left(\frac{q_k}{p_k} \right) + \alpha \left(\sum_{k=1}^d q_k - 1 \right) \quad (5.6.14)$$

$$\implies \frac{\partial \mathcal{I}}{\partial \alpha} = \sum_{k=1}^d q_k - 1 \stackrel{!}{=} 0 \implies \sum_{k=1}^d q_k = 1. \quad (5.6.15)$$

$$\implies \frac{\partial \mathcal{I}}{\partial q_k} = \ln \left(\frac{q_k}{p_k} \right) + 1 + \alpha. \quad (5.6.16)$$

Because the q_k are probabilities, they lie in the range $[0, 1]$. Looking for an extreme value in that range:

$$\frac{\partial \mathcal{I}}{\partial q_k} \stackrel{!}{=} 0 \implies q_k = e^{-1-\alpha} p_k \quad (5.6.17)$$

$$\implies \sum_{k=1}^d q_k = e^{-1-\alpha} \sum_{k=1}^d p_k \implies e^{-1-\alpha} = 1 \quad (5.6.18)$$

$$\implies q_k = p_k. \quad (5.6.19)$$

Hence, the only extreme value which occurs on the inside of the region of variation is when the q and p distributions are the same. For this value the relative information vanishes:

$$\mathcal{I}(p|p) = \sum_{k=1}^d p_k \ln \left(\frac{p_k}{p_k} \right) = 0. \quad (5.6.20)$$

As well, by the second derivative test this quantity is a minimum as the second derivative matrix has positive eigenvalues:

$$\frac{\partial^2 \mathcal{I}}{\partial q_k \partial q_n} = \frac{1}{q_k} \delta_{kn}. \quad (5.6.21)$$

Consequently, the relative information is always greater than or equal to 0 and it is in fact 0 if and only if $q = p$. This reinforces the interpretation of the relative information as measuring how different q is from p as this means the most similar distribution to a given distribution is itself, with a difference of 0, and that a distribution and itself are unique in having a difference of 0. Every other distribution is more different from p

than p is from itself.

In order to see the maximum value of the relative information we will have to look at extrema on the boundary of the variation region. So, each q_k must be either 0 or 1. But, because they sum to 1 precisely one of them must be 1 and all others 0. Call the value of k for which $q_k = 1$ as k_o . Then:

$$\mathcal{I}(q|p) = \sum_{k=1}^d q_k \ln \left(\frac{q_k}{p_k} \right) = -\ln p_{k_o}. \quad (5.6.22)$$

To maximize this we simply need to take the k_o for which p_o is smallest. Thus, the maximum possible value of $\mathcal{I}$ for a given p is:

$$\mathcal{I}_{\max} = -\ln \min_k(\{p_k\}) \quad (5.6.23)$$

Again interpreting the relative information as a measure of how different two distributions are, this says that the most different distribution to a given distribution is the one in which the least likely outcome of the first distribution is in fact guaranteed to be the outcome, which also makes sense.

So, for any valid probability distributions q and p we have:

$$0 \leq \mathcal{I}(q|p) \leq -\ln \min_k(\{p_k\}) \quad (5.6.24)$$

with the lower bound satisfied if and only if $q = p$ and the upper bound satisfied if and only if $q_k = \delta_{kk_o}$ where k_o is the value of k for which p_k is minimized.

With the microcanonical ensemble we found ourselves interested in the uniform distribution (at least uniform at a given energy) and so let us look at the relative information to a uniform distribution. Then, $p_k = \frac{1}{d}$ and so:

$$\mathcal{I}(q|p) = \sum_{k=1}^d q_k \ln q_k - \sum_{k=1}^d q_k \ln \frac{1}{d} = \ln d + \sum_{k=1}^d q_k \ln q_k. \quad (5.6.25)$$

Using our upper and lower bounds on the relative information:

$$0 \leq \ln d + \sum_{k=1}^d q_k \ln q_k \leq -\ln \frac{1}{d} = \ln d \quad (5.6.26)$$

$$\implies 0 \leq -\sum_{k=1}^d q_k \ln q_k \leq \ln d. \quad (5.6.27)$$

The quantity appearing here is called the entropy $S(q)$ of the distribution q :

$$\boxed{S(q) = -\sum_{k=1}^d q_k \ln q_k} \quad (5.6.28)$$

$$\implies 0 \leq S(q) \leq \ln d. \quad (5.6.29)$$

Because the negative sign in the entropy swapped the order of the upper and lower bounds, the entropy is 0 if and only if the distribution $q_k = \delta_{nk}$ for some n and the entropy is $\ln d$ if and only if the distribution q is uniform. So, the entropy can be interpreted as how similar the distribution is to being uniform. The larger the entropy the “more uniform” the distribution is. We can see this explicitly by writing the relative information of a distribution q to the uniform distribution as:

$$S(q) + \mathcal{I}(q|\text{uniform}) = \ln d. \quad (5.6.30)$$

Entropy and the relative information both have an interpretation in terms of a way to quantify “information”. As we have said, probability is the mathematical theory of how to systematically manage incomplete information. By this we mean that some variables have unknown values. When we make a measurement we determine the value of one or more of those variables and thus gain information. Suppose we have some event A . To that event we assign the probability p intended to indicate our degree of belief that A as an event will actually occur for the real version of our system. When we measure the corresponding property of our system, A is either true or false and we learn some “amount of information”. How can we meaningfully assign a value to how much information we have learned? We can do so by requiring some basic properties. First, if A was certain to be true and so had probability 1 and then when measured it in fact was true, we have learned nothing. When A is not certain and has probability not equal to 1 then when measured to be true we have learned something. So, the information gained from measuring an event to be true must

depend in some way on the probability of that event. Let $\iota(p)$ be the information gained from an event of probability p . This reasoning says that there is such a function. Because if A is certain the information should be 0:

$$\iota(1) = 0. \quad (5.6.31)$$

Second, suppose we consider the information gained from finding out that two independent events A and B (of probabilities p_A, p_B) are both true. Because they are independent, they tell us nothing about each other and so the total information gained is simply the sum of the individual information of each. However, we could also define the event $C = A \cap B$ which then has probability p_{APB} . Then, the information gained from observing C to be true is $\iota(p_C) = \iota(p_{APB})$. As we just identified this must equal the sum of the informations from A and B individually:

$$\iota(p_{APB}) = \iota(p_A) + \iota(p_B). \quad (5.6.32)$$

This is then a general requirement on the form of the function $\iota(p)$. Differentiating both sides with respect to p_B :

$$p_A \iota'(p_{APB}) = \iota'(p_B). \quad (5.6.33)$$

Now evaluate at $p_B = 1$ and $p_A = p$:

$$p \iota'(p) = \iota'(1) \quad (5.6.34)$$

$$\implies \frac{\partial \iota}{\partial p} = \frac{\iota'(1)}{p} \quad (5.6.35)$$

$$\implies \iota(p) = \iota'(1) \ln p + C. \quad (5.6.36)$$

Because $\iota(1) = 0$ we have that $C = 0$ as well:

$$\iota(1) = \iota'(1) \ln 1 + C \stackrel{!}{=} 0 \implies C = 0 \quad (5.6.37)$$

$$\implies \iota(p) = \iota'(1) \ln p. \quad (5.6.38)$$

Third, when we make a measurement of an event we gain information and so:

$$\iota(p) \geq 0. \quad (5.6.39)$$

Because $p \leq 1$ this requires $\iota'(1) \leq 0$. Because $\iota(p) \neq 0$ for $p \neq 1$ we cannot have $\iota'(1) = 0$. So, for some positive constant α we must have:

$$\iota(p) = -\alpha \ln p. \quad (5.6.40)$$

Equivalently this can be written in terms of a logarithm of a general base as:

$$\iota(p) = -\log_{e^{\frac{1}{\alpha}}} p. \quad (5.6.41)$$

Let $b = e^{\frac{1}{\alpha}}$ be that numerical base. Then, we see that the information gained from measuring an event to be true must be:

$$\iota(p) = -\log_b p. \quad (5.6.42)$$

If $b = 2$, this information is said to be measured in “bits”. This is precisely the sense of bit used in computer science. If a variable has 2^d possibilities and nothing is known about it, each outcome would have probability 2^{-d} and so measuring any value would gain d bits of information. There are 2^d sequences of ones and zeros of length d and so the value of a variable which is valued as a d length binary sequence reveals d bits of information. While computer scientists prefer $b = 2$ for counting bits, physicists prefer $b = e$ because the natural logarithm has a nicer derivative. So, by convention we define $b = e$. The corresponding measure of information with $b = e$ is called “nats” (short for natural). The choice of base never matters as the information computed be any other base is simply proportional by the change of basis factor. So, we take the information gained from measuring an event to be true to be:

$$\iota(p) = -\ln(p). \quad (5.6.43)$$

This formula for the information immediately gives an interpretation for the relative information and the entropy. Before a property of our system is measured it is represented by a random variable X with possible outcomes $x_1, \dots, x_d$ each with some probability $p_1, \dots, p_d$. After that variable is measured and its value is learned, it is definitely given by some value x_n and so after measurement the new distribution is that it takes value x_n with probability 1. Then, the relative information between this final measured distribution $q_k = \delta_{kn}$

and the initial distribution p_k is:

$$\mathcal{I}(q|p) = \sum_{k=1}^d q_k \ln \left(\frac{q_k}{p_k} \right) = 1 \ln \left(\frac{1}{p_n} \right) = -\ln p_n = \iota(p_n). \quad (5.6.44)$$

That is, the relative information of a random variable after measuring to before measuring exactly matches the formula we derived for the information gained from measuring that event. This fact is what justifies the name “relative information” for $\mathcal{I}$. $\mathcal{I}$ essentially acts as a generalization of the ι formula to the case that the initial and final distributions (p and q) are both general. The ι formula is the information gained when the initial distribution is general and the final distribution is the random variable taking a definite value. For the entropy, we can rewrite it as:

$$S(p) = -\sum_{k=1}^d p_k \ln p_k = \sum_{k=1}^d p_k \iota(p_k) = \mathbb{E}(\iota). \quad (5.6.45)$$

Hence, the entropy of a probability distribution is precisely the average amount of information one gains by measuring a sample from that distribution. Because of this the entropy is sometimes called the “surprisal” as it is the average amount by which you will be surprised by the results of an event.

The additivity of independent events for information extends to relative information and entropy as well. Suppose we have two random variables X and Y which are independently distributed both before and after some information is learned. Then, the prior joint distribution is:

$$p(x, y) = \text{Prob}(X = x \cap Y = y) = \text{Prob}(X = x)\text{Prob}(Y = y) = p_X(x)p_Y(y) \quad (5.6.46)$$

and the joint posterior distribution is:

$$q(x, y) = \text{Prob}(X = x \cap Y = y | \text{data}) = \text{Prob}(X = x | \text{data})\text{Prob}(Y = y | \text{data}) = q_X(x)q_Y(y). \quad (5.6.47)$$

Immediately then the relative information is:

$$\mathcal{I}(q|p) = \sum_{x,y} q \ln \left(\frac{q}{p} \right) = \sum_{x,y} q_X q_Y \ln \left(\frac{q_X q_Y}{p_X p_Y} \right) = \sum_x q_X \ln \left(\frac{q_X}{p_X} \right) \sum_y q_Y + \sum_x q_X \sum_y q_Y \ln \left(\frac{q_Y}{p_Y} \right) \quad (5.6.48)$$

$$= \mathcal{I}(q_X|p_X) + \mathcal{I}(q_Y|p_Y). \quad (5.6.49)$$

Similarly the entropy of either the prior or posterior distributions satisfies:

$$S(p) = -\sum_{x,y} p \ln p = -\sum_{x,y} p_X p_Y \ln(p_X p_Y) = \sum_x p_X \ln p_X \sum_y p_Y - \sum_x p_X \sum_y p_Y \ln p_Y = S(p_X) + S(p_Y). \quad (5.6.50)$$

So far we have only considered the notion of information with discrete random variables. We have done so because the definitions and intuition are easier. However, for physics we of course typically need continuous random variables. We can understand the continuous notion of information by taking appropriate limits of the discrete case. Let X be a real valued random variable with some prior probability density function $p(x)$ and some posterior probability density function $q(x)$. Then, let X_ℓ be the discrete random variable which is equal to the greatest integer multiple value of ℓ which is less than or equal to X . Then, the probability that $X_\ell = n\ell$ is given by:

$$P_n = \text{Prob}(X_\ell = n\ell) = \text{Prob}(\ell n < X \leq \ell(n+1)) = \int_{\ell n}^{\ell(n+1)} p(x) dx. \quad (5.6.51)$$

So, the relative information gained about X_ℓ is:

$$\mathcal{I}_\ell = \sum_{n \in \mathbb{Z}} Q_n \ln \left(\frac{Q_n}{P_n} \right) = \sum_{n \in \mathbb{Z}} \int_{\ell n}^{\ell(n+1)} q(x) dx \ln \frac{\int_{\ell n}^{\ell(n+1)} q(x) dx}{\int_{\ell n}^{\ell(n+1)} p(x) dx}. \quad (5.6.52)$$

For small ℓ :

$$\int_{\ell n}^{\ell(n+1)} p(x) dx = p(\ell n)\ell + \mathcal{O}(\ell^2) \quad (5.6.53)$$

$$\implies \frac{\int_{\ell n}^{\ell(n+1)} q(x) dx}{\int_{\ell n}^{\ell(n+1)} p(x) dx} = \frac{q(\ell n)}{p(\ell n)} + \mathcal{O}(\ell). \quad (5.6.54)$$

So:

$$\mathcal{I}_\ell = \sum_{n \in \mathbb{Z}} \int_{\ell(n-\frac{1}{2})}^{\ell(n+\frac{1}{2})} q(x) \left(\ln \frac{q(\ell n)}{p(\ell n)} + \mathcal{O}(\ell) \right) dx \quad (5.6.55)$$

$$= \sum_{n \in \mathbb{Z}} \int_{\ell(n-\frac{1}{2})}^{\ell(n+\frac{1}{2})} q(x) \left(\ln \frac{q(x - \ell\%(\frac{x}{\ell}))}{p(x - \ell\%(\frac{x}{\ell}))} + \mathcal{O}(\ell) \right) dx \quad (5.6.56)$$

$$= \int_{-\infty}^{\infty} q(x) \ln \frac{q(x - \ell\%(\frac{x}{\ell}))}{p(x - \ell\%(\frac{x}{\ell}))} dx + \mathcal{O}(\ell). \quad (5.6.57)$$

Finally in the $\ell \rightarrow 0$ limit we have:

$$\mathcal{I} = \int_{-\infty}^{\infty} q(x) \ln \frac{q(x)}{p(x)} dx. \quad (5.6.58)$$

So, for continuous random variables the relative information formula generalizes quite nicely. Because the relative information is non-negative for all distributions in the discrete case, it is also non-negative in the continuous case automatically through this limiting procedure. However, there is no upper bound on the value of the continuous relative information (because $\ln d$ has gone to ∞). For multidimensional random values the relative information generalizes just as well as:

$$\boxed{\mathcal{I}[q|p] = \int_{\mathbb{R}^d} q(\vec{x}) \ln \frac{q(\vec{x})}{p(\vec{x})} d^d \vec{x}.} \quad (5.6.59)$$

This formula can be arrived at explicitly by doing a d dimensional discretization and performing the same limiting procedure we did for $d = 1$ (this d refers to the number of dimensions of integration, not the number of distinct outcomes used earlier in this section).

Suppose we define a new random variable $Y = \vec{F}(X)$ through an invertible function $\vec{F}$. Then, we know the distributions for Y are given by equation (5.1.142):

$$p_Y(\vec{y}) = \frac{p_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|}, \quad q_Y(\vec{y}) = \frac{q_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|}. \quad (5.6.60)$$

Automatically then:

$$\mathcal{I}_Y = \int_{\mathbb{R}^d} q_Y(\vec{y}) \ln \frac{q_Y(\vec{y})}{p_Y(\vec{y})} d^d \vec{y} = \int_{\mathbb{R}^d} \frac{q_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|} \ln \frac{\frac{q_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|}}{\frac{p_X(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|}} \left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right| d^d \vec{x} \quad (5.6.61)$$

$$= \int_{\mathbb{R}^d} q_X(\vec{x}) \ln \frac{q_X(\vec{x})}{p_X(\vec{x})} d^d \vec{x} = \mathcal{I}_X. \quad (5.6.62)$$

So, the continuous relative information is invariant under reparameterization. It would be quite troublesome if this weren't true; what we know about a system should not depend on how we have expressed that knowledge and so the information gained in a measurement must be independent of any invertible coordinate transformation if it is to be meaningful.

Now let us look at the continuous generalization of the entropy. Returning to the discretization X_ℓ we have:

$$S_\ell = - \sum_{n \in \mathbb{Z}} P_n \ln P_n = - \sum_{n \in \mathbb{Z}} \int_{\ell n}^{\ell(n+1)} p(x) dx \ln \left(\int_{\ell n}^{\ell(n+1)} p(x) dx \right) \quad (5.6.63)$$

$$= - \sum_{n \in \mathbb{Z}} \int_{\ell n}^{\ell(n+1)} p(x) \ln (p(n\ell)\ell + \mathcal{O}(\ell^2)) dx \quad (5.6.64)$$

$$= - \sum_{n \in \mathbb{Z}} \int_{\ell n}^{\ell(n+1)} p(x) \left(\ln \ell + \ln p \left(x - \ell\% \left(\frac{x}{\ell} \right) \right) + \mathcal{O}(\ell) \right) dx \quad (5.6.65)$$

$$= - \int_{-\infty}^{\infty} p(x) \left(\ln \ell + \ln p \left(x - \ell\% \left(\frac{x}{\ell} \right) \right) + \mathcal{O}(\ell) \right) dx. \quad (5.6.66)$$

The $\ln \ell$ term prevents the entropy from having a finite $\ell \rightarrow 0$ limit. The best one can do is define the

differential entropy by subtracting off this logarithmically divergent term:

$$S_{\text{differential}}[p] \stackrel{\text{def}}{=} \lim_{\ell \rightarrow 0^+} (\ln \ell + S_\ell) = - \int_{-\infty}^{\infty} p(x) \ln p(x) dx. \quad (5.6.67)$$

Because the differential entropy is shifted by $\ln \ell$ relative to S_ℓ and ℓ is taken to 0 while $S_\ell \geq 0$ the lower bound on the differential entropy drops to $-\infty$ (as $\ln \ell \rightarrow -\infty$) and so there is no lower bound on the differential entropy of a distribution. As well, there is no upper bound on the differential entropy of a distribution for the same reason that there was none for the relative information.

The differential entropy has a few problems. In particular, the random variable X generally has some units in physics and because the probability density integrates to a number over an interval of values of X , $p(x)$ must have units inverse to X . So, $p(x)$ is generally dimensionful and so the logarithm of $p(x)$ is not meaningful as it mixes dimensionful quantities of different powers. It is not invariant under a change of units. We can see explicitly that the differential entropy is not invariant under a change of units by using that a change of units rescales the numerical value of X . So, define the new random variable X' by:

$$X' = \alpha X \quad (5.6.68)$$

for some constant $\alpha > 0$. By the probability density change of variables formula:

$$p'(x') = \frac{p(x)}{\alpha}. \quad (5.6.69)$$

Then, the differential entropy for X' is:

$$S'[p'] = \int_{-\infty}^{\infty} p'(x') \ln p'(x') dx' = \int_{-\infty}^{\infty} \frac{p(x)}{\alpha} \ln \left(\frac{p(x)}{\alpha} \right) \alpha dx = -\ln \alpha - \int_{-\infty}^{\infty} p(x) \ln p(x) dx = \ln \alpha + S[p]. \quad (5.6.70)$$

Thus, a change of units shifts the value of the differential entropy by a constant. As such, the overall value of the differential entropy is completely meaningless. Only differences of differential entropies in which the two entropies being subtracted are computed in the same units are meaningful. This way, the $\ln \alpha$ piece would cancel between the two of them.

The unit dependence of the differential entropy is a symptom of an even larger problem. Performing the same discretization for multiple variables leads to the natural generalization for the differential entropy to d dimensions:

$$S[f] = - \int_{\mathbb{R}^d} f(\vec{x}) \ln f(\vec{x}) d^d \vec{x}. \quad (5.6.71)$$

Under a reparameterization of the probability space:

$$Y = \vec{F}(X) \quad (5.6.72)$$

we have the transformed differential entropy:

$$S'[f'] = - \int_{\mathbb{R}^d} f'(\vec{y}) \ln f'(\vec{y}) d^d \vec{y} = - \int_{\mathbb{R}^d} \frac{f(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|} \ln \left(\frac{f(\vec{x})}{\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right|} \right) \left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right| d^d \vec{x} \quad (5.6.73)$$

$$= \int_{\mathbb{R}^d} f(\vec{x}) \ln \left(\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right| \right) d^d \vec{x} - \int_{\mathbb{R}^d} f(\vec{x}) \ln f(\vec{x}) d^d \vec{x} \quad (5.6.74)$$

$$= S[f] + \int_{\mathbb{R}^d} f(\vec{x}) \ln \left(\left| \det \left(\frac{\partial \vec{y}}{\partial \vec{x}} \right) \right| \right) d^d \vec{x}. \quad (5.6.75)$$

Hence, under a general coordinate transformation the differential entropy is shifted by a term which depends both on the form of the coordinate transformation and on the underlying distribution. This issue can't be fixed by subtracting differential entropies due to the dependence on the underlying distribution. So, it seems the differential entropy is basically meaningless! How can it be in any way a useful measurement of information if its value can be made anything arbitrarily by changing coordinates and that arbitrariness cannot be canceled to give something uniquely defined? It is actually "easy" to see why differential entropy had to be such a mess. We found before that the discrete entropy is the logarithm of the size of the variable space ($\ln d$) minus the relative information a given distribution has compared to the uniform distribution. The subtraction we have performed in defining the differential entropy essentially canceled off the diverging $\ln d$ part so that the differential entropy is the limit of the negative relative information compared to the uniform distribution up to adding a finite constant. We found before that the relative information between

two distributions is coordinate invariant *if one transforms both distributions*. In computing the entropy we have essentially transformed one of the distributions in a relative information without transforming the other, the uniform distribution. Under a coordinate transformation a uniform distribution does not stay uniform and so this procedure of transforming only one of the distributions is generically meaningless.

There is exactly 1 saving reason the differential entropy is usable at all in physics. Based on the arguments made so far it seems quite a troublesome quantity. However, when we formulate the phase space density we typically do so in terms of canonical coordinates (Q, P) and only demand our formalism is invariant under canonical transformations. As shown in 1.9 under a canonical transformation the Jacobian determinant is always 1:

$$\det \left(\frac{\partial(Q', P')}{\partial(Q, P)} \right) = 1. \quad (5.6.76)$$

Then, for the canonical entropy defined in terms of the phase space density by:

$$S[f] = - \int_{\mathbb{P}} f(Q, P) \ln f(Q, P) d\mathbb{P} \quad (5.6.77)$$

we see that under a canonical transformation:

$$S'[f'] = - \int_{\mathbb{P}} f'(Q', P') \ln f'(Q', P') d\mathbb{P} = S[f] + \int_{\mathbb{P}} f(Q, P) \ln(1) d\mathbb{P} = S[f] \quad (5.6.78)$$

using equation (5.6.75). So, the entropy uniquely for a system with canonical coordinates actually is canonical transformation invariant. This is because a uniform distribution in phase space does stay uniform under a canonical transformation since the determinant of any symplectic matrix is 1. For a general system, the differential entropy is completely meaningless. However, precisely for Hamiltonian systems on phase space the argument which causes differential entropy to be meaningless does not apply. Because of this, for physics we can interpret the differential entropy meaningfully as the negative of relative information between a given distribution and a uniform distribution on phase space, up to adding a constant. In that way, the differential entropy measures how uniform the phase space density is. The more uniform the phase space density is, the higher the entropy. The more localized the phase space density, the lower the entropy.

Now we can understand why it was convenient to introduce the dimensionful factor $\hbar$ in equation (5.2.4). Doing so makes the phase space density dimensionless and so the canonical entropy defined in equation (5.6.77) only contains the logarithm of a dimensionless quantity. If the phase space density were dimensionful then by equation (5.6.70) the value of the entropy would shift additively under a change of units and the entropy itself would contain a logarithm of a dimensionful quantity, which isn't meaningful. In this way it is necessary to make the phase space density dimensionless if we have any interest in having a self-consistent unit system independent notion of entropy. After doing so, it immediately follows from the definition of the canonical entropy that it is also unitless.

Theorem 5.5: Information Theory

For discrete probability distributions p_k and q_k , the relative information of q to p defined by:

$$\mathcal{I}(q|p) = \sum_k q_k \ln \left(\frac{q_k}{p_k} \right) \quad (5.6.79)$$

characterizes the rate at which it becomes exponentially improbable to observe data with the distribution q from a source with actual distribution p . For continuous distributions the appropriate generalization for the relative information is:

$$\mathcal{I}[q|p] = \int_{\mathbb{R}^d} q(\vec{x}) \ln \frac{q(\vec{x})}{p(\vec{x})} d^d \vec{x}. \quad (5.6.80)$$

In either case the relative information is non-negative and only vanishes if the two distributions are the same. As well, it is dimensionless and invariant under a change of variables.

The entropy $S(q)$ of a discrete probability distribution is the average amount of information gained by observing the value of a random variable with that distribution and it is given by:

$$S(q) = - \sum_k q_k \ln q_k. \quad (5.6.81)$$

It is always non-negative and is only 0 in the case that the random variable is some constant with probability 1. There is no well defined continuous limit of the discrete entropy. The best one can do is introduce the differential entropy:

$$S[f] = - \int_{\mathbb{R}^d} f(\vec{x}) \ln f(\vec{x}) d^d \vec{x} \quad (5.6.82)$$

which may be negative or positive, has poorly defined units due to taking the logarithm of a dimensional quantities, and is not invariant under changes of units or variables and thus is essentially meaningless when without additional structure.

In the specific case that one is considering distributions on the phase space of a Hamiltonian system, one can meaningfully use the differential entropy:

$$S[f] = - \int_{\mathbb{P}} f(Q, P) \ln f(Q, P) d\mathbb{P} \quad (5.6.83)$$

because this expression is invariant under all coordinate transformations on the phase space. Still, it may be positive or negative.

Readers who have studied statistical mechanics before are likely to encounter a factor of k_B in front of the definition of entropy I have given. This is historical (due to the k_B in the definition of temperature), unnecessary, and generally unhelpful. We will always use entropy to mean the unitless expression as defined above.

Exercises

Problem 5.35: Information Distance. We have shown that the relative information between two distributions $q(\vec{x})$ and $p(\vec{x})$ tells us something about how different the distribution $q(\vec{x})$ is from $p(\vec{x})$. We have even said it somewhat serves as a measure of “distance” between two distributions. While this can be a useful way of thinking about relative information, it isn’t perfect. Here we will see the ways in which relative information fails to be a proper distance and identify a reasonable alternative notion of distance between probability distributions.

- We have already proven that the relative information between two distributions is nonnegative and is only 0 if the distributions are the same. This property is known as positive semidefiniteness and is certainly something we expect of a distance. However, for a distance (also called a metric) we expect the distance from p to q to be the same as the distance from q to p . This is known as the symmetry requirement. Show that this is generally not true for the relative information between q and p .
- The final defining property of distance is called the triangle inequality. For any distance function $D[q, p]$ and three distributions q, p, r they should satisfy:

$$D[q, r] + D[r, p] \geq D[q, p].$$

Show that this is not satisfied in general for the relative information.

- So, while $\mathcal{I}$ tells us how different two distributions are, it does not really measure a proper distance between them. Remember that the meaning of $\mathcal{I}(q|p)$ is that it is the rate at which it becomes exponentially less and less likely to observe the distribution q when sampling from p . For a large but finite amount of data only distributions with a small value of $\mathcal{I}$ will have any meaningful chance of being observed and so it is useful to study $\mathcal{I}$ for distributions which are near each other. Suppose that both q and p are distributions characterized by a set of parameters $\theta^1, \dots, \theta^K$ simply with different values of the parameters. That is, suppose there exists a function $m(\vec{x}|\vec{\theta})$ (called the model) so that $p(\vec{x}) = m(\vec{x}|\vec{\theta})$ and $q(\vec{x}) = m(\vec{x}|\vec{\theta} + \delta\vec{\theta})$. (An example of this would be two normal distributions with different values for their means and variances.) Show that:

$$\mathcal{I}[q|p] = g_{ab} \delta\theta^a \delta\theta^b + \mathcal{O}(\delta\theta^3)$$

where g_{ab} , called the Fisher information metric, is defined by:

$$g_{ab}(\theta) = \mathbb{E} \left(\frac{\partial \ln m(\vec{X}|\vec{\theta})}{\partial \theta^a} \frac{\partial \ln m(\vec{X}|\vec{\theta})}{\partial \theta^b} \right) = \int_{\mathbb{R}^d} \frac{1}{m} \frac{\partial m}{\partial \theta^a} \frac{\partial m}{\partial \theta^b} d^d \vec{x}.$$

Thus, the Fisher information characterizes the relative information for nearby distributions. Show that g_{ab} is a positive semidefinite symmetric matrix.

- (d) Show that if new parameters are defined: $\vec{\theta}' = \vec{\theta}'(\vec{\theta})$ then the Fisher metric for the new parameters g'_{ab} is related to the Fisher metric for the old parameters by:

$$g'_{ab}(\theta') = \frac{\partial \theta^c}{\partial \theta'^a} \frac{\partial \theta^d}{\partial \theta'^b} g_{cd}(\theta).$$

- (e) Consider the space of distributions which are given by $m(\vec{x}|\vec{\theta})$ for different values of the $\vec{\theta}$. Define the line element on this space by the Fisher information metric:

$$ds^2 = g_{ab} d\theta^a d\theta^b.$$

Show that this arclength is invariant under changes of the definition of the parameters as in the previous part.

- (f) Consider a path through the space of distributions characterized by a one parameter family of values of $\vec{\theta}$: $\vec{\theta}(\lambda)$ where λ runs from 0 to 1. Explain that the arclength of such a path is then given by:

$$S[\vec{\theta}] = \int_0^1 \sqrt{g_{ab} \frac{d\theta^a}{d\lambda} \frac{d\theta^b}{d\lambda}} d\lambda.$$

Show if holding the endpoints fixed (and thus the initial and final distributions fixed) one varies this arclength and requires its variation to be zero the resulting path will be the path of shortest arclength between the endpoints. Then, show that this shortest distance, called the information distance between that initial and final distribution, satisfies positive semidefiniteness, symmetry, and the triangle inequality and thus is a mathematically proper notion of distance. The use of information distance as an actual distance on the space of distributions leads to the mathematical field of information geometry.

- (g) Consider a normal distribution with mean μ and variance $\frac{\nu^2}{2}$ for a parameter $\nu > 0$. Show that the Fisher information metric and information line element for the normal distribution are then:

$$g_{ab} = \frac{2}{\nu^2} \delta_{ab}, \quad ds^2 = \frac{2}{\nu^2} (d\mu^2 + d\nu^2).$$

- (h) Let (μ_0, ν_0) and (μ_1, ν_1) be the values of (μ, ν) for two different normal distributions and let $\mu(\lambda)$ and $\nu(\lambda)$ by the paths implied by the stationary variation of the action in part (e). Show that they satisfy:

$$\frac{d}{d\lambda} \left(\frac{1}{\nu} \frac{\dot{\mu}}{\sqrt{\dot{\mu}^2 + \dot{\nu}^2}} \right) = 0, \quad \frac{d}{d\lambda} \left(\frac{1}{\nu} \frac{\dot{\nu}}{\sqrt{\dot{\mu}^2 + \dot{\nu}^2}} \right) = -\frac{\sqrt{\dot{\mu}^2 + \dot{\nu}^2}}{\nu^2}$$

(where dots indicate λ derivatives). Finally then, solve these equations to find the information distance between normal distributions (warning: it is gross).

Problem 5.36: Jeffrey's prior.

- (a) As mentioned in problem 5.14, Jeffrey's prior is a common formal rule for selecting a prior distribution when one doesn't know what to take. Suppose we have a distribution $f(\vec{x}|\vec{\theta})$ with parameters $\vec{\theta}$ for which we would like to have a distribution so that we can apply Bayes' Theorem when collecting data about this system. To do so we need a prior distribution. Jeffrey's prior is to take the Fisher information metric g_{ab} and use its determinant as:

$$f(\vec{\theta}) = A \sqrt{\det g(\vec{\theta})}$$

where A is a normalization factor so that f integrates to 1. Show that under a change of parameters $\vec{\theta}' = \vec{\theta}'(\vec{\theta})$ Jeffrey's prior transforms correctly for a pdf (this is why Jeffrey's prior is a common choice; it does not have a preferred coordinate system). This property at least makes Jeffrey's prior superior to just assuming a uniform distribution and pretending that it is "uninformative". Jeffrey's prior is not the only choice of prior with the correct transformation property⁴ and so it is not the only reasonable formal rule. Remember, there is no such thing as an "uninformative" or "objective" prior.

- (b) Consider a Bernoulli distribution with unknown success probability $\wp$. Show that Jeffrey's prior for this parameter is:

$$f(\wp) = \frac{1}{\pi} \frac{1}{\sqrt{\wp(1-\wp)}}.$$

(with $0 \leq \wp \leq 1$). Compare this to problem 5.14(c).

⁴Later when we do general relativity we will see that out of a metric we can define coordinate invariant quantities out of its derivatives, such as the Ricci scalar, and so we could equally well take a prior which is a function of those scalars.

- (c) Consider a Poisson distribution with unknown μ . Show that Jeffrey's prior for this parameter is:

$$f(\mu) = \frac{A}{\sqrt{\mu}}$$

with $\mu \geq 0$ and show that there is no real value of A so that $f(\mu)$ is properly normalized. Thus, Jeffrey's prior can sometimes produce "improper" priors, meaning priors which cannot be normalized properly. However, show that after sampling N iid Poisson distribution samples and receiving values $n_1, \dots, n_N$ the posterior distribution is:

$$f(\mu | \text{Data}) = \frac{N^{N\bar{n} + \frac{1}{2}}}{\Gamma(N\bar{n} + \frac{1}{2})} \mu^{N\bar{n} - \frac{1}{2}} e^{-N\mu}$$

with $\bar{n}$ the sample mean of the trials. Thus, the improper normalization disappears once data is collected and the posterior is just a Gamma distribution.

5.7 The Second Law of Thermodynamics

Now that we understand that (continuous or differential) entropy is meaningful only for systems in canonical coordinates, let us study some properties of entropy in such systems. Suppose we have a system composed of two subsystems (these subsystems are allowed to interact): $(Q, P) = (Q_1, Q_2, P_1, P_2)$. Then, the combined system has some phase space density $f(Q, P)$ and the two subsystems have marginal phase space densities:

$$f_1(Q_1, P_1) = \int_{\mathbb{P}_2} f(Q_1, Q_2, P_1, P_2) \frac{d^{d_2} Q_2 d^{d_2} P_2}{(2\pi\hbar)^{d_2}}, \quad f_2(Q_2, P_2) = \int_{\mathbb{P}_1} f(Q_1, Q_2, P_1, P_2) \frac{d^{d_1} Q_1 d^{d_1} P_1}{(2\pi\hbar)^{d_1}}. \quad (5.7.1)$$

As well, they have associated entropies:

$$S[f] = - \int_{\mathbb{P}} f \ln f d\mathbb{P}, \quad S_1[f_1] = - \int_{\mathbb{P}_1} f_1 \ln f_1 d\mathbb{P}_1, \quad S_2[f_2] = - \int_{\mathbb{P}_2} f_2 \ln f_2 d\mathbb{P}_2. \quad (5.7.2)$$

We found before that when two subsystems are independent, the entropy of their combined system is equal to the sum of their individual entropies. This is not true when the systems are not independent. If the subsystems 1 and 2 were independent, they would have distribution:

$$f_{\text{indep}}(Q_1, Q_2, P_1, P_2) = f_1(Q_1, P_1) f_2(Q_2, P_2). \quad (5.7.3)$$

Let us look at the difference between the sum of subsystem entropies and the combined system entropy in general (we know it vanishes in the case of independence):

$$S_1 + S_2 - S = - \int_{\mathbb{P}_1} f_1 \ln f_1 d\mathbb{P}_1 - \int_{\mathbb{P}_2} f_2 \ln f_2 d\mathbb{P}_2 + \int_{\mathbb{P}} f \ln f d\mathbb{P} \quad (5.7.4)$$

$$= - \int_{\mathbb{P}} f \ln f_1 d\mathbb{P} - \int_{\mathbb{P}} f \ln f_2 d\mathbb{P} + \int_{\mathbb{P}} f \ln f d\mathbb{P} \quad (5.7.5)$$

$$= \int_{\mathbb{P}} f \ln \left(\frac{f}{f_1 f_2} \right) d\mathbb{P} = \int_{\mathbb{P}} f \ln \left(\frac{f}{f_{\text{indep}}} \right) d\mathbb{P} \quad (5.7.6)$$

$$= \mathcal{I}(f|f_{\text{indep}}). \quad (5.7.7)$$

So, the difference between the sum of subsystem entropies and the combined system entropy is in fact the relative information between the actual joint distribution and the hypothetical joint distribution if the two subsystems were independent. As we have already proven, relative information is always non-negative and is only 0 when the two distributions are the same. So, we see:

$$S_1 + S_2 - S = \mathcal{I}(f|f_{\text{indep}}) \geq 0 \quad (5.7.8)$$

$$\implies \boxed{S \leq S_1 + S_2} \quad (5.7.9)$$

with equality holding if and only if the two subsystems are actually independent. Because of this, entropy is said to be sub-additive. Entropy adds in the case of two systems being independent. In any other case, the combined system has less entropy than the sum of the entropies of the individual systems. Viewing entropy as the average amount of information gained from measuring the exact state of a system, this makes perfect sense. When two systems are independent their informations add because they tell you nothing about each other. When the two systems are not independent, there are non-trivial correlations between them and so each system contains some information about the other. Thus, the entropy of system 1 contains all of the information of system 1 and some of the information of system 2. Simply adding to that the entropy of system 2 then double counts the information shared between the two systems. so, $S_1 + S_2$ must be greater than the actual information S .

We have said before interactions cause correlations. Interactions breaks independence. We can see this explicitly in equation (5.2.55). Suppose we begin a system comprised of two subsystems so that initially the two subsystems are statistically independent:

$$f(0, Q, P) = f_1(0, Q_1, P_1) f_2(0, Q_2, P_2). \quad (5.7.10)$$

The general solution to the Liouville equation for a Hamiltonian system is:

$$f(t, Q, P) = f(0, U^{-1}(t, Q, P)) \quad (5.7.11)$$

where the function U is the time evolution map for the underlying equations of motion. Then, combining this with initial independence we have:

$$f(t, Q_1, Q_2, P_1, P_2) = f_1(0, U_1^{-1}(t, Q_1, Q_2, P_1, P_2)) f_2(0, U_2^{-1}(t, Q_1, Q_2, P_1, P_2)). \quad (5.7.12)$$

If the subsystem 1 components of the time evolution map U depend on Q_2 or P_2 or vice versa then this expression is not a product of the form $f_1(1, Q_1, P_1)f_2(t, Q_2, P_2)$. The time evolution map, being derived directly from solving the equations of motion, depends on the coordinates of the other system if and only if the equations of motion do. Thus, if there is any interaction between the two systems (meaning their equations of motion depend on each other), the phase space density of the full system cannot maintain the statistical independence of the two systems in time. Again, interactions cause correlations. This has important consequences for the entropy which we will get to momentarily.

Let us look at the time evolution of the entropy in a Hamiltonian system subject to external forces. For compactness of notation let us adopt the $\phi = (Q, P)$ notation used in section 5.2. Due to allowing the presence of external forces, the equations of motion will be:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{H}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{H}}{\partial Q^a} + F_a^{\text{ext}}. \quad (5.7.13)$$

Then, the Liouville equation and entropy for this system are given by:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \phi^a}(fV^a) = 0, \quad S[f] = - \int_{\mathbb{P}} f \ln f \mathbb{P}. \quad (5.7.14)$$

The time derivative of the entropy then gives (using that the phase space density must go to 0 far out in the phase space):

$$\frac{dS}{dt} = - \int_{\mathbb{P}} \frac{\partial f}{\partial t} (\ln f + 1) d\mathbb{P} = \int_{\mathbb{P}} \frac{\partial}{\partial \phi^a}(fV^a)(\ln f + 1) d\mathbb{P} \quad (5.7.15)$$

$$= - \int_{\mathbb{P}} fV^a \frac{\partial}{\partial \phi^a} (\ln f + 1) d\mathbb{P} = - \int_{\mathbb{P}} fV^a \frac{1}{f} \frac{\partial f}{\partial \phi^a} d\mathbb{P} \quad (5.7.16)$$

$$= \int_{\mathbb{P}} f \frac{\partial V^a}{\partial \phi^a} d\mathbb{P} = \mathbb{E} \left(\frac{\partial V^a}{\partial \phi^a} \right). \quad (5.7.17)$$

So, the rate of change of entropy is just the expectation of the divergence of the phase space velocity. This has a nice interpretation. By equation (5.2.36) the Jacobian that relates the evolved coordinates to the initial conditions on phase space satisfies:

$$\frac{d}{dt} \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right) = \frac{\partial V^a}{\partial \phi^a} \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right). \quad (5.7.18)$$

Then, because the rate of change of the total entropy is the expectation of the divergence, we can define the point-wise rate of entropy production as:

$$\frac{ds}{dt}(t, \phi) = \frac{\partial V^a}{\partial \phi^a} \implies \frac{dS}{dt} = \mathbb{E} \left(\frac{ds}{dt} \right). \quad (5.7.19)$$

The Jacobian then evolves as:

$$\frac{d}{dt} \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right) = \frac{ds}{dt} \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right) \quad (5.7.20)$$

$$\implies \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right) = e^{s(t)-s(0)} = e^{\Delta s}. \quad (5.7.21)$$

The phase space volume element of the evolved coordinates is related to the volume element of the initial coordinates by the Jacobian change of variables formula:

$$\boxed{d\mathbb{P}(t) = \det \left(\frac{\partial \phi(t)}{\partial \phi(0)} \right) d\mathbb{P}(0) = e^{\Delta s} d\mathbb{P}(0).} \quad (5.7.22)$$

So, the change in entropy of a blob of initial conditions in phase space gives the amount which one must exponentiate to get the change in volume of the blob during its evolution. In this way, we can see more clearly that increasing entropy means spreading out the phase space density more uniformly across phase space and decreasing entropy means accumulating the phase space density in a smaller region. This is exactly what we would expect from our previous analysis that entropy is larger the closer a distribution is to being uniform.

Now let us explicitly put in our equations of motion into the rate of change of entropy:

$$\frac{dS}{dt} = \mathbb{E} \left(\frac{\partial}{\partial Q^a} \left(\frac{\partial \mathcal{H}}{\partial P_a} \right) + \frac{\partial}{\partial P_a} \left(-\frac{\partial \mathcal{H}}{\partial Q^a} + F_a^{\text{ext}} \right) \right) \quad (5.7.23)$$

$$\Rightarrow \boxed{\frac{dS}{dt} = \mathbb{E} \left(\frac{\partial F_a^{\text{ext}}}{\partial P_a} \right)}. \quad (5.7.24)$$

Hence, we see that in the absence of external forces the entropy is constant. That is, **the entropy of any isolated Hamiltonian system is conserved. The entropy of the whole universe as one system then is exactly constant.**

Suppose we take two initially independent systems and allow them to interact with no external forces from outside of these two systems. Then, their initial combined entropy S is:

$$S(0) = S_1(0) + S_2(0) \quad (5.7.25)$$

due to their independence. Once the systems have interacted they are no longer statistically independent. But, it is still possible to define their marginal distributions and compute their individual entropies $S_1(t)$ and $S_2(t)$. However, due to sub-additivity of the entropy their sum will exceed the actual entropy of the combined system for $t > 0$:

$$S_1(t) + S_2(t) \geq S(t) \quad (5.7.26)$$

with equality holding if and only if there is no interaction (as only then is independence maintained). Then, because the combined system is an isolated Hamiltonian system we have that the full system entropy is conserved:

$$S_1(t) + S_2(t) \geq S(t) = S(0) = S_1(0) + S_2(0) \quad (5.7.27)$$

$$\Rightarrow S_1(t) - S_1(0) + S_2(t) - S_2(0) \geq 0 \quad (5.7.28)$$

$$\Rightarrow \boxed{\Delta S_1 + \Delta S_2 \geq 0} \quad (5.7.29)$$

with equality holding if and only if there is no interaction. Thus, in any interaction between two initially independent subsystems the sum of their subsystem entropies increases. This is known as the **second law of thermodynamics**.

It is important to note that the second law of thermodynamics absolutely does **NOT** say that the entropy of any system can only increase, nor does it say that the entropy of the universe can only increase (these are common errors). The entropy of any particular system can increase or decrease due to the influence of external forces. The entropy of the whole universe is guaranteed to be exactly constant because there are no forces external to it by definition. The second law of thermodynamics says that when two initially independent subsystems interact the sum of their individual entropies increases. Due to the interaction, the sum of subsystem entropies after the interaction is not the entropy of the full system. Treating the sum of subsystem entropies as the full entropy, as we have seen, assumes that the two systems are statistically independent and thus throws away any information about their correlations. If we are unaware of the details of the interaction between the two systems, then the precise correlations which develop between them are beyond us. So, we may only be able to compute their individual properties and not their correlations. In only being able to do so we have access to less than the full information of the system and thus the amount of information we stand to learn by measuring the system increased. This is the real meaning to the second law of thermodynamics. All of this is to say that the second law of thermodynamics is not actually a law of physics. It is not the output of any particular theory. The second law of thermodynamics is a mathematical theorem about Hamiltonian systems that applies when the initial subsystems are statistically independent. It basically amounts to the fact **when we neglect the correlations which develop between systems as they interact we lose information**.

Using our established reasoning that a large system of many identical constituents allows us to treat each constituent as a sample of the same sort of underlying random variable, the entropy of such a system is a measure of how spread out the different conditions of the constituents are. If all of the gas molecules in a box are very close to each other moving with the same momentum, then sampling over them one will find that the phase space density is very sharply peaked near those values of position and momentum and so the entropy of the distribution will be very low. If instead the gas fills the box and all of the molecules are moving in their own different directions the phase space density will be meaningfully different from 0 in a much larger region of phase space and so the entropy of the distribution will be much higher. Because of this you will sometimes hear “entropy is a measure of disorder”, but I don’t find this very helpful. Much more precisely, entropy is a measure of uniformity. The more uniform a distribution is the higher the entropy. The more sharp and narrow a distribution is, the lower the entropy.

Because entropy is a measure of uniformity and the microcanonical ensemble is exactly a uniform

distribution at fixed energy, the microcanonical ensemble is the distribution of maximum entropy at a fixed exact energy. Let us see this formally. Suppose we consider a phase space density $f(Q, P)$ which is only non-zero for (Q, P) for which $\mathcal{H}(Q, P) = E$. Then, for some function $F(Q, P)$:

$$f(Q, P) = F(Q, P)\delta(E - \mathcal{H}(Q, P)). \quad (5.7.30)$$

Because $f(Q, P)$ must integrate to 1:

$$\int_{\mathbb{P}} f(Q, P) d\mathbb{P} = \int_{\mathbb{P}} F(Q, P)\delta(E - \mathcal{H}(Q, P)) d\mathbb{P} = \int_{\mathcal{H}=E} F(Q, P) d\mathbb{P}|_{\mathcal{H}=E} = 1 \quad (5.7.31)$$

where the last integral is just a short hand for indicating we are only integrating over the region of phase space on which $\mathcal{H} = E$. Then, the entropy of such a distribution is:

$$S[f] = - \int_{\mathbb{P}} f \ln f d\mathbb{P} \quad (5.7.32)$$

$$= - \int_{\mathbb{P}} (F(Q, P)\delta(E - \mathcal{H}(Q, P)) \ln F(Q, P) + F(Q, P)\delta(E - \mathcal{H}(Q, P)) \ln(\delta(E - \mathcal{H}(Q, P)))) d\mathbb{P} \quad (5.7.33)$$

$$= - \int_{\mathcal{H}=E} F(Q, P) \ln F(Q, P) d\mathbb{P}|_{\mathcal{H}=E} - \int_{\mathcal{H}=E} F(Q, P) \ln \delta(0) d\mathbb{P}|_{\mathcal{H}=E} \quad (5.7.34)$$

$$= S_{\mathcal{H}=E}[F] - \ln \delta(0). \quad (5.7.35)$$

The quantity $\delta(0)$ is of course divergent and an artifact of the continuous limits involved in defining the differential entropy. We see that the divergent term here is independent of F and so entropy differences for different F will cancel this nasty piece. Maximizing $S[f]$ is then equivalent to maximizing the much more well-defined $S_{\mathcal{H}=E}[F]$.

To maximize $S_{\mathcal{H}=E}[F]$ we can simply vary the entropy and find its maximum using the calculus of variations. However, we have the constraint that F integrates to 1 over the phase space at energy E and so we must include a Lagrange multiplier α to enforce this constraint:

$$S_{\mathcal{H}=E} = - \int_{\mathcal{H}=E} F \ln F d\mathbb{P}|_{\mathcal{H}=E} + \alpha \left(1 - \int_{\mathcal{H}=E} F d\mathbb{P}|_{\mathcal{H}=E} \right). \quad (5.7.36)$$

The variation of this with respect to α gives the constraint:

$$\frac{\partial S_{\mathcal{H}=E}}{\partial \alpha} = 1 - \int_{\mathcal{H}=E} F d\mathbb{P}|_{\mathcal{H}=E} \stackrel{!}{=} 0 \quad (5.7.37)$$

and the variation of this with respect to F will maximize the entropy:

$$\frac{\delta S_{\mathcal{H}=E}}{\delta F} = -\ln F - 1 - \alpha \stackrel{!}{=} 0 \implies F = e^{-1-\alpha}. \quad (5.7.38)$$

Hence, to extremize the entropy F must be a constant and thus we have a uniform distribution over the phase space of fixed energy. To verify this is a maximum we should use the second derivative test:

$$\frac{\delta^2 S_{\mathcal{H}=E}}{\delta F(Q, P) \delta F(Q', P')} = -\frac{1}{F} \delta(Q - Q') \delta(P - P'). \quad (5.7.39)$$

This is a linear operator with negative eigenvalues and so the entropy is maximized. As expected then, the microcanonical ensemble is the maximum entropy distribution at fixed energy.

The canonical ensemble is the distribution of a system's degrees of freedom in the thermodynamic limit of that system having finite expected energy while being in a large bath so that the total system is in microcanonical ensemble. Let us study the maximum entropy distribution for a given fixed expected energy. Then, we have two Lagrange multipliers α and β , one to enforce that the f should integrate to 1 and one to enforce that the expected energy is E . The entropy functional is then:

$$S[f] = - \int_{\mathbb{P}} f \ln f d\mathbb{P} + \alpha \left(1 - \int_{\mathbb{P}} f d\mathbb{P} \right) + \beta \left(E - \int_{\mathbb{P}} f \mathcal{H} d\mathbb{P} \right). \quad (5.7.40)$$

The variation of this with respect to α just guarantees that the phase space density integrates to 1:

$$\frac{\partial S}{\partial \alpha} = 1 - \int_{\mathbb{P}} f d\mathbb{P} \stackrel{!}{=} 0 \quad (5.7.41)$$

and the variation of this with respect to β just guarantees that the expected energy is E :

$$\frac{\partial S}{\partial \beta} = E - \int_{\mathbb{P}} f \mathcal{H} d\mathbb{P} \stackrel{!}{=} 0. \quad (5.7.42)$$

Then, the variation with respect to f gives:

$$\frac{\delta S}{\delta f} = -\ln f - 1 - \alpha - \beta \mathcal{H} \stackrel{!}{=} 0 \quad (5.7.43)$$

$$\implies f(Q, P) = e^{-1-\alpha} e^{-\beta \mathcal{H}}. \quad (5.7.44)$$

Again the second variation of the entropy gives:

$$\frac{\delta^2 S}{\delta f(Q, P) \delta f(Q', P')} = -\frac{1}{f(Q, P)} \delta(Q - Q') \delta(P - P') \quad (5.7.45)$$

which is again a negative operator. Thus, the maximum entropy distribution at fixed expected energy is an exponential of the Hamiltonian. That is precisely the canonical ensemble! Both the microcanonical and canonical ensembles can be understood as the maximum entropy distributions consistent with their respective conditions (fixed exact energy, fixed expected energy).

Finally, as you might expect, the generalized Boltzmann distribution is also the maximum entropy distribution consistent with its conditions. If we have fixed expectations of extensive conserved quantities G_a :

$$\mathcal{G}_a = \int_{\mathbb{P}} G_a(Q, P) f(Q, P) d\mathbb{P} \quad (5.7.46)$$

then the appropriate entropy functional is:

$$S[f] = - \int_{\mathbb{P}} f \ln f d\mathbb{P} + \alpha \left(1 - \int_{\mathbb{P}} f d\mathbb{P} \right) + \beta^a \left(\mathcal{G}_a - \int_{\mathbb{P}} G_a f d\mathbb{P} \right). \quad (5.7.47)$$

The α and G_a variations just impose our various constraints and the f variation derives the generalized Boltzmann distribution:

$$\frac{\delta S}{\delta f} = -\ln f - 1 - \alpha - \beta^a G_a \stackrel{!}{=} 0 \quad (5.7.48)$$

$$\implies f(Q, P) = e^{-1-\alpha} e^{-\beta^a G_a}. \quad (5.7.49)$$

So, incredibly, all of the distributions we have associated with the equilibrium behavior of statistical mechanical systems are in fact the maximum entropy distributions consistent with their defining properties. Thus, entropy provides another way to uniquely characterize thermodynamic equilibrium. A system is in thermodynamic equilibrium if it is in the maximum entropy distribution consistent with the constraints upon it. This characterization of thermodynamic equilibrium only relies on entropy differences (as the maximum value has a positive difference with any other value when subtracted from it) and so cancels the unit dependence of the absolute value of the entropy.

It may be surprising that we can simultaneously have it be true that the entropy of an isolated system is exactly conserved and that the appropriate phase space density to use for a system in equilibrium is the distribution of maximum entropy. How can an isolated system approach this maximum entropy distribution if it will always follow a path along which its entropy is conserved? There are some key subtleties here which led to significant confusion in the early days of statistical mechanics. It is absolutely true that the exact phase space density of a classical system follows the Liouville equation and that for an isolated system using Hamilton's equations one can quickly prove that the entropy of that exact instantaneous phase space density is conserved. That is:

$$\frac{d}{dt} S[f] = -\frac{d}{dt} \int_{\mathbb{P}} f \ln f d\mathbb{P} = 0. \quad (5.7.50)$$

However, when we are describing a system in equilibrium we are not using its instantaneous phase space density f , we are using its time averaged phase space density $\bar{f}$ as defined in equation (5.4.2). This is because the underlying phase space has many microscopic variables which evolve very quickly on experimentally relevant timescales and so the experimentally relevant phase space density is the one which averages over that microscopic time evolution. Then, we have found that in the thermodynamic limit that the system is very large the only distribution with the right statistical properties⁵ to serve as this time averaged experimentally effective distribution is the generalized canonical ensemble/Boltzmann distribution. That distribution is the distribution of maximum entropy with given fixed expectations for the extensive conserved quantities of the

⁵Specifically, the generalized Boltzmann distribution is the only distribution which is a function of conserved quantities only (so is a legitimate time averaged distribution) and for which dynamically independent systems are statistically independent (because it factorizes over extensive conserved quantities).

system. With that distribution as $\bar{f}$, its entropy is:

$$S[\bar{f}] = - \int_{\mathbb{P}} \bar{f} \ln \bar{f} d\mathbb{P} \quad (5.7.51)$$

and it is maximized. This entropy in general is not the same value as the constant value $S[f]$ as the system evolves. These two are not the same because the operation of time averaging the distribution and taking the logarithm in the entropy formula do not commute. So, it is **NOT** typically the case that in the long run the phase space density f converges to the equilibrium distribution f_{canon} . Instead, the correct statement is that the time averaged expectation values of functions on phase space computed with respect to f converge to the expectation values computed using f_{canon} . Consequently, under this time averaging, f_{canon} can be used as the experimentally relevant effective phase space density. The germ of this thinking is contained in the simplest example: the harmonic oscillator. Imagine a harmonic oscillator which we start precisely with energy E . It automatically from its equations of motion will whirl around a circle in phase space (if one scales the Q and P axes appropriately) with radius determined by E . Instantaneously, the harmonic oscillator is at a definite point $(Q(t), P(t))$ and its phase space density is a Dirac delta at that point so $S[f]$ is arbitrarily low. However, if the frequency of the harmonic oscillator is very high then the relevant experimental quantity is its time averaged phase space density. Its time averaged phase space density is a uniform distribution on the circle it travels on and so $\bar{f}$ has a much higher entropy than f itself, even though $S[f]$ is exactly constant.

To avoid confusion, it is helpful to clearly distinguish between the entropy $S[f]$ of the full phase space density f and the entropy $S[f_{\text{sub}}]$ of some marginal or representative distribution f_{sub} of some subset of interesting variables. Whenever there may be doubt, one should call $S[f]$ the full system entropy as it is the entropy of the full system's phase space density. Similarly, one should call $S[f_{\text{sub}}]$ the coarse grained entropy as it is the entropy of only a coarser imperfect statistical representation of the system. The coarse grained entropy only has any meaning when one clearly specifies what the coarse graining is (what variables did you lose) and it only has any use when your choice of coarse graining is relevant for your experimental scenario.

The second law of thermodynamics only shows precisely that when two statistically independent system are brought together to interact, the sum of their subsystem entropies will increase. However, in applications one is likely to assume that over each interval of time of interaction between two macroscopic systems, the sum of the subsystem entropies of those systems will increase. This is subtly different, because after the two systems have interacted for one second, they are no longer statistically independent during the second second of their interaction. Yet, practically it is most often still a good assumption that their subsystem entropy total will increase during that second second. The reason for this is that while correlations do develop between the degrees of freedom of the two macroscopic systems, if the systems are very macroscopic then the time scale over which those correlations begin to matter is very long compared to the time scale over which the leading order interaction (in which they are still treated as independent) develops. Because of this, the second law of thermodynamics can typically be applied instantaneously during the interactions of macroscopic objects to extremely good approximation.

Theorem 5.6: Second Law of Thermodynamics

The entropy of an isolated system is exactly constant. In the presence of external forces, the rate of change of the entropy of a system is:

$$\frac{dS}{dt} = \mathbb{E} \left(\frac{\partial F_a^{\text{ext}}}{\partial P_a} \right). \quad (5.7.52)$$

When two initially independent systems interact, the sum of their individual system entropies (**NOT** the full entropy of the combined system) is non-decreasing. That sum will increase if there is any interaction and it will remain constant if and only if there is no interaction:

$$\Delta S_1 + \Delta S_2 \geq 0. \quad (5.7.53)$$

The phase space density of thermodynamic equilibrium is the phase space density of maximum entropy consistent with the constraints defining that equilibrium (fixed exact energy in the case of microcanonical, fixed expected energy in the case of canonical, fixed expected extensive conserved quantities in the case of generalized canonical). That is, in equilibrium:

$$\delta S = 0, \quad \delta^2 S \leq 0 \quad (5.7.54)$$

among all variations of the phase space density which preserve the constraints of that equilibrium.

The common confusion around whether the second law of thermodynamics is about the entropy of the instantaneous phase space density of the full system or about the sum of subsystem entropies for the time averaged phase space densities of those subsystems has historically led to other further points of confusion, such as Loschmidt's paradox. Loschmidt's paradox is that many systems in physics which microscopically have time reversal symmetry (such as charges interacting with electromagnetism) macroscopically lead to some behavior which is not time reversal symmetric (such as Ohm's law); how can the effective theory of Ohm's law not have the underlying symmetries of the full theory? The answer lies in the fact that not all degrees of freedom are present in Ohm's law and so the same words "time reversal" are being used for actually two different meanings. It is absolutely true that the full theory of charges interacting with electromagnetism has time reversal symmetry (and this fact is not changed later on when more complicated physics is considered at more microscopic levels; electromagnetism by all experimental evidence truly does have time reversal symmetry). However, when averaging is performed over the countless microscopic variables (the positions and velocities of each particle) in a wire to derive Ohm's law, the resultant theory has far fewer variables (like the spatially averaged current density). The microscopic theory has time reversal symmetry under time reversing *everything* about the microscopic system. The macroscopic theory does not have time reversal symmetry under time reversing *only the macroscopic variables*. In fact, if one is careful the macroscopic theory does have time reversal symmetry under time reversing everything in the same way as the microscopic theory. This is exactly analogous to the example in section 1.2 about two blocks attached by a spring on a table. The system only has translational symmetry (in this case time reversal symmetry) if you consider the *whole* system. If you only translate (or time reverse) part of the system, you don't have symmetry. Thus, there is no actual contradiction in Loschmidt's paradox. If degrees of freedom are averaged out in a symmetry breaking way, the resultant effective theory will have that symmetry be broken.

Another common historical concept which causes confusion when first learning statistical mechanics is the Maxwell Demon. The Maxwell Demon is a hypothetical being who can systematically control the interaction of two systems (such as moving a wall between two containers of gas) with such precision that the demon could cause violations of the second law of thermodynamics. In the gas example, if the demon opened and closed the wall quickly the demon could make sure that all faster than average gas molecules end up on one side of the wall while all slower than average molecules end up on the other side of the wall. The entropy of each of the two gases is then lower than when they were mixed because their momentum distributions are less uniform. There are two conjugate ways in which this is not a violation of the second law of thermodynamics. First, because this is now a system of interacting demon, gas 1, and gas 2 it is necessary to consider the interactions of these three subsystems, not just the two gases, when using the second law of thermodynamics. Thus, it is okay if the individual subsystem entropies of the gases decrease provided the entropy of the demon overcompensates this change. (This is necessarily mathematically true by the proof given leading to equation (5.7.29). One may worry how to apply a proof written for 2 systems to 3 systems; simply take one of the systems in the 2 system proof to be a composition of 2 systems which are initially independent and it immediately generalizes.) So, the thought experiment of the Maxwell Demon does not actually cause issue if we take the positions of the molecules in the gases to be microscopic and thus need a phase space density and also use an appropriate phase space density for the variables in the system of the demon. Alternatively, if we take that the Maxwell Demon has such perfect control over the wall between the gases and knowledge of the velocities of individual molecules so that the demon can make decisions about when to raise and lower the wall, then to the demon the molecular velocities are not microscopic at all. To the demon, all of the variables of the gas are macroscopic quantities described by ordinary classical mechanics with no phase space density and there is no notion of entropy nor second law of thermodynamics to violate. In short, if the gas degrees of freedom are microscopic the demon's entropy will increase to compensate the amount decrease in gas entropy; if the gas degrees of freedom are macroscopic there is no notion of entropy to worry about. The second law of thermodynamics as derived in equation (5.7.29) is just a basic mathematical fact about any Hamiltonian system divided into interacting subsystems. Any demonic thought experiment one contrives will inevitably yield to it, if analyzed in enough detail.

There is another subtle issue regarding thermodynamic equilibrium which is often confused. There is a theorem of Hamiltonian systems known as Poincare Recurrence which states that in any Hamiltonian system with bounded dynamics, if the system exists in some open set in phase space at one time and leaves that open set later, then it will return to that open set infinitely many times as time passes. Because of this, in

many physical systems, if one waits extremely long the system will return to being arbitrarily close to where it was at any earlier time. However, this recurrence time is typically inconceivably irrelevantly impossibly large, so that this doesn't matter experimentally. Poincare Recurrence means that systems do not really approach thermodynamic equilibrium in the long run exactly. Instead, it is more correct to say that over long periods of time, systems spend the significant majority of that time in states consistent with thermodynamic equilibrium.

Exercises

Problem 5.37: Entropy and the normal distribution. Using the calculus of variations and method of Lagrange multipliers, show that the distribution $f(x)$ for a real valued random variable X with the highest entropy at fixed mean μ and variance σ^2 is the normal distribution.

5.8 Thermal Quasidynamics

Suppose we have a system consisting of macroscopic degrees of freedom (Q, P) and microscopic degrees of freedom (q, p) . Then, because the (q, p) degrees of freedom are microscopic and evolve on much shorter time scales, their values will fluctuate quickly and so it is most appropriate to describe their uncertain experimental values through a time averaged phase space density. As macroscopic degrees of freedom, we will typically assume that Q and P evolve so slowly that we can treat them as effectively constant on the time scale of evolution of (q, p) . This is known as the quasidynamic approximation. In the quasidynamic approximation, we then assume that the (q, p) variables have reached thermodynamic equilibrium at fixed (Q, P) . In this perspective, the Hamiltonian $\mathcal{H}(Q, q, P, p)$ essentially treats the phase space as (q, p) with (Q, P) fixed as parameters for the purposes of thermodynamics. Then, (q, p) are distributed at fixed (Q, P) by the Boltzmann distribution:

$$f(q, p|Q, P, T) = \frac{e^{-\beta\mathcal{H}(Q, q, P, p)}}{Z}. \quad (5.8.1)$$

The partition function is given by:

$$Z(T, Q, P) = \int_{\mathbb{P}} e^{-\beta\mathcal{H}(Q, q, P, p)} \frac{d^d q d^d p}{(2\pi\hbar)^d}. \quad (5.8.2)$$

Given this, how do we expect Q and P to evolve? We can simply compute their expected time evolution using Hamilton's equations:

$$\mathbb{E} \left(\frac{dQ^a}{dt} \right) = \int_{\mathbb{P}} f \frac{\partial \mathcal{H}}{\partial P_a} \frac{d^d q d^d p}{(2\pi\hbar)^d} = \int_{\mathbb{P}} \frac{e^{-\beta\mathcal{H}}}{Z} \frac{\partial \mathcal{H}}{\partial P_a} \frac{d^d q d^d p}{(2\pi\hbar)^d} \quad (5.8.3)$$

$$= -\frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial P_a} \int_{\mathbb{P}} e^{-\beta\mathcal{H}} \frac{d^d q d^d p}{(2\pi\hbar)^d} = \frac{T}{Z} \frac{\partial Z}{\partial P_a} \quad (5.8.4)$$

$$= \frac{\partial}{\partial P_a} (-T \ln Z) \quad (5.8.5)$$

$$\mathbb{E} \left(\frac{dP_a}{dt} \right) = - \int_{\mathbb{P}} f \frac{\partial \mathcal{H}}{\partial Q^a} \frac{d^d q d^d p}{(2\pi\hbar)^d} = - \int_{\mathbb{P}} \frac{e^{-\beta\mathcal{H}}}{Z} \frac{\partial \mathcal{H}}{\partial Q^a} \frac{d^d q d^d p}{(2\pi\hbar)^d} \quad (5.8.6)$$

$$= -\frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial Q^a} \int_{\mathbb{P}} e^{-\beta\mathcal{H}} \frac{d^d q d^d p}{(2\pi\hbar)^d} = -\frac{T}{Z} \frac{\partial Z}{\partial Q^a} \quad (5.8.7)$$

$$= -\frac{\partial}{\partial Q^a} (-T \ln Z). \quad (5.8.8)$$

So, both the expected evolution of Q and P can be written as derivatives of the function:

$$\boxed{\mathcal{F}(T, Q, P) \stackrel{\text{def}}{=} -T \ln Z.} \quad (5.8.9)$$

This function is called the Free Energy of Helmholtz Free Energy of the system. Because temperature is intensive and the partition function is multiplicative, the logarithm of Z and consequently the free energy are both extensive. Then, the expected time evolution of Q and P satisfy:

$$\mathbb{E} \left(\frac{dQ^a}{dt} \right) = \frac{\partial \mathcal{F}}{\partial P_a}, \quad \mathbb{E} \left(\frac{dP_a}{dt} \right) = -\frac{\partial \mathcal{F}}{\partial Q^a}. \quad (5.8.10)$$

These are called Ralston's equations of motion. They look quite like Hamilton's equations with the free energy acting as the effective Hamiltonian in equilibrium. However, we have only found the expected evolution of Q and P . Because their exact evolution depends on q and p , there is a difference between the exact and expected values of the evolution of Q and P . The expected evolution is only a good representative of the actual evolution if the variances involved are small. Let us compute the variances of a single Q and P . Then, the variance of the velocity of Q is:

$$\text{Var}(\dot{Q}) = \mathbb{E} \left(\frac{\partial \mathcal{H}}{\partial P} \right)^2 - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 = \int_{\mathbb{P}} \frac{e^{-\beta\mathcal{H}}}{Z} \left(\frac{\partial \mathcal{H}}{\partial P} \right)^2 d\mathbb{P} - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 \quad (5.8.11)$$

$$= \frac{1}{Z} \int_{\mathbb{P}} \frac{\partial \mathcal{H}}{\partial P} \frac{\partial}{\partial P} \left(-\frac{1}{\beta} e^{-\beta\mathcal{H}} \right) d\mathbb{P} - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 \quad (5.8.12)$$

$$= -T \frac{\partial}{\partial P} \left(\int_{\mathbb{P}} \frac{\partial \mathcal{H}}{\partial P} \frac{e^{-\beta \mathcal{H}}}{Z} d\mathbb{P} \right) + T \int_{\mathbb{P}} \frac{\partial^2 \mathcal{H}}{\partial P^2} f d\mathbb{P} + T \frac{\partial}{\partial P} \left(\frac{1}{Z} \right) \int_{\mathbb{P}} \frac{\partial \mathcal{H}}{\partial P} e^{-\beta \mathcal{H}} d\mathbb{P} - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 \quad (5.8.13)$$

$$= -T \frac{\partial}{\partial P} \mathbb{E} \left(\frac{\partial \mathcal{H}}{\partial P} \right) + T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}}{\partial P^2} \right) - \frac{T}{Z^2} \frac{\partial Z}{\partial P} Z \mathbb{E} \left(\frac{\partial \mathcal{H}}{\partial P} \right) - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 \quad (5.8.14)$$

$$= -T \frac{\partial^2 \mathcal{F}}{\partial P^2} + T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}}{\partial P^2} \right) + \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 - \left(\frac{\partial \mathcal{F}}{\partial P} \right)^2 \quad (5.8.15)$$

$$= T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}}{\partial P^2} \right) - T \frac{\partial^2 \mathcal{F}}{\partial P^2}. \quad (5.8.16)$$

The corresponding calculation of the variance of the rate of change of momentum gives:

$$\text{Var}(\dot{P}) = T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}}{\partial Q^2} \right) - T \frac{\partial^2 \mathcal{F}}{\partial Q^2}. \quad (5.8.17)$$

The action of a system is extensive (because the actions of non-interacting systems are additive). By the Hamilton Jacobi conditions we have that the momentum is given in terms of the canonical action by:

$$P_a = \frac{\partial S_c}{\partial Q^a}. \quad (5.8.18)$$

If the coordinate Q is intensive then its corresponding momentum is the derivative of an extensive quantity with respect to an intensive quantity and so is extensive. Alternatively, if a coordinate is extensive then its corresponding momentum is the derivative of an extensive quantity with respect to an extensive quantity and so is intensive. Hence, if a coordinate is intensive/extensive its conjugate momentum has the opposite property. We can then always use the canonical transformation $Q' = P$, $P' = -Q$ to swap these properties at will so that we fix the coordinates to be intensive and the conjugate momenta to be extensive. With extensivity, we have that under a scaling transformation in which we consider N copies of our system:

$$Q' = Q, \quad P' = NP. \quad (5.8.19)$$

As well, the Hamiltonian and free energy are extensive and so:

$$\mathcal{H}' = N\mathcal{H}, \quad \mathcal{F}' = N\mathcal{F}. \quad (5.8.20)$$

(The extensivity of the free energy follows from the multiplicativity of the partition function in (5.5.37).) Under this transformation the relative fluctuations scale as:

$$\frac{\text{Var}(\dot{Q}')}{(\mathbb{E}\dot{Q}')^2} = \frac{T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}'}{\partial P'^2} \right) - T \frac{\partial^2 \mathcal{F}'}{\partial P'^2}}{\left(\frac{\partial \mathcal{F}'}{\partial P'} \right)^2} = \frac{1}{N} \frac{\text{Var}(\dot{Q})}{(\mathbb{E}\dot{Q})^2} \quad (5.8.21)$$

$$\frac{\text{Var}(\dot{P}')}{(\mathbb{E}\dot{P}')^2} = \frac{T \mathbb{E} \left(\frac{\partial^2 \mathcal{H}'}{\partial Q'^2} \right) - T \frac{\partial^2 \mathcal{F}'}{\partial Q'^2}}{\left(\frac{\partial \mathcal{F}'}{\partial Q'} \right)^2} = \frac{1}{N} \frac{\text{Var}(\dot{P})}{(\mathbb{E}\dot{P})^2}. \quad (5.8.22)$$

Hence, in the thermodynamic limit of large N , the relative fluctuations go to 0 and the expectations of the velocities become completely representative of the actual dynamics. The thermodynamic limit being necessary reflects the fact that we are considering Q and P which are macroscopic variables and so they have to be macroscopic with respect to something. Together we have that, in the thermodynamic limit and quasidynamic approximation the macroscopic variables evolve according to:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{F}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{F}}{\partial Q^a}. \quad (5.8.23)$$

The computation which derived this assumed the full dynamics were given by the underlying Hamiltonian $\mathcal{H}$. In the presence of external forces there would have been another term in equation (5.8.6) for those forces. In general, there may be microscopic external forces $F_{ma}(t, T, Q, q, P, p)$ and macroscopic external forces $F_{Ma}(t, T, Q, P)$ on the system. The macroscopic external forces are written to not depend on q, p because I have assumed their expectation over q, p has already been taken. Repeating the steps for equations (5.8.3) to (5.8.8) then gives:

$$\frac{dQ^a}{dt} = \frac{\partial \mathcal{F}}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial \mathcal{F}}{\partial Q^a} + F_{Ma}(t, T, Q, P). \quad (5.8.24)$$

These are not a complete set of equations of motion because they do not specify the behavior of the temperature T with time. In order to make them a complete set of equations of motion, we need some way of

specifying the evolution of $T(t)$. To do so, it turns out to be easier to look at the behavior of the entropy in time. The entropy of the Boltzmann distribution is given by:

$$S = - \int_{\mathbb{P}} f \ln f d\mathbb{P} = - \int_{\mathbb{P}} f \ln \left(\frac{e^{-\beta\mathcal{H}}}{Z} \right) d\mathbb{P} = \beta \int_{\mathbb{P}} f \mathcal{H} d\mathbb{P} + \ln Z \int_{\mathbb{P}} f d\mathbb{P} \quad (5.8.25)$$

$$= \beta E + \ln Z. \quad (5.8.26)$$

Written in terms of temperature and the free energy:

$$TS = E + T \ln Z = E - \mathcal{F}. \quad (5.8.27)$$

As well, recall equation (5.5.23). Then:

$$E = -\frac{\partial}{\partial \beta} \ln Z = T^2 \frac{\partial}{\partial T} \ln Z = T^2 \frac{\partial}{\partial T} \left(-\frac{\mathcal{F}}{T} \right) = T^2 \left(\frac{\mathcal{F}}{T^2} - \frac{1}{T} \frac{\partial \mathcal{F}}{\partial T} \right) = \mathcal{F} - T \frac{\partial \mathcal{F}}{\partial T}. \quad (5.8.28)$$

Relating back to the entropy we have:

$$TS = \mathcal{F} - T \frac{\partial \mathcal{F}}{\partial T} - \mathcal{F} = -T \frac{\partial \mathcal{F}}{\partial T} \quad (5.8.29)$$

$$\implies \boxed{S = -\frac{\partial \mathcal{F}}{\partial T}}. \quad (5.8.30)$$

Hence, the entropy of the distribution of our microscopic variables is very nicely computed from the free energy. Equation (5.8.27) can also be rewritten as:

$$E = \mathcal{F} + TS. \quad (5.8.31)$$

Computed from the partition function, we have found $\mathcal{F}$ to be a function of T, Q, P . Computed from equation (5.8.30), the entropy is then also written as a function of T, Q, P . If equation (5.8.30) is invertible in how it relates S to T then we can use it to define $T(S, Q, P)$ as the temperature which when fed into equation (5.8.30) produces the S appearing on the left hand side. Then, this relationship between E and $\mathcal{F}$ in equation (5.8.31) performs a Legendre transformation from T dependence to S dependence. We can see this by looking at the total differential:

$$dE = d\mathcal{F} + TdS + SdT = \frac{\partial \mathcal{F}}{\partial T} dT + \frac{\partial \mathcal{F}}{\partial Q^a} dQ^a + \frac{\partial \mathcal{F}}{\partial P_a} dP_a + TdS - \frac{\partial \mathcal{F}}{\partial T} dT \quad (5.8.32)$$

$$\implies dE = TdS + \frac{\partial \mathcal{F}}{\partial Q^a} dQ^a + \frac{\partial \mathcal{F}}{\partial P_a} dP_a \quad (5.8.33)$$

$$\implies \frac{\partial E}{\partial S} = T, \quad \frac{\partial E}{\partial Q^a} = \frac{\partial \mathcal{F}}{\partial Q^a}, \quad \frac{\partial E}{\partial P_a} = \frac{\partial \mathcal{F}}{\partial P_a}. \quad (5.8.34)$$

So, the expected energy is naturally written as a function of S, Q, P after the Legendre transformation. That is, the detailed expression for the Legendre transformation is:

$$\boxed{E(S, Q, P) = \mathcal{F}(T, Q, P) + TS}. \quad (5.8.35)$$

Then, because the Q and P derivatives of $\mathcal{F}$ and E match (where the $\mathcal{F}$ derivatives are taken at fixed T and the E derivatives are taken at fixed S) we have:

$$\frac{dQ^a}{dt} = \frac{\partial E}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial E}{\partial Q^a} + F_{Ma}(t, S, Q, P). \quad (5.8.36)$$

From equation (5.7.24), we already know how to compute the rate of change of the entropy:

$$\frac{dS}{dt} = \mathbb{E} \left(\frac{\partial F_{ma}}{\partial p_a} \right) \quad (5.8.37)$$

where F_{ma} are the microscopic external forces acting on our system (the macroscopic external forces do not contribute because the macroscopic variables are not averaged over, they are fixed parameters from the perspective of the microscopic variables). This expression can be written quite nicely as:

$$\frac{dS}{dt} = \mathbb{E} \left(\frac{\partial F_{ma}}{\partial p_a} \right) = \int_{\mathbb{P}} \frac{e^{-\beta\mathcal{H}}}{Z} \frac{\partial F_{ma}}{\partial p_a} d\mathbb{P} = \frac{1}{Z} \int_{\mathbb{P}} \left(\frac{\partial}{\partial p_a} (e^{-\beta\mathcal{H}} F_{ma}) - F_{ma} \frac{\partial}{\partial p_a} e^{-\beta\mathcal{H}} \right) d\mathbb{P} \quad (5.8.38)$$

$$= -\frac{1}{Z} (-\beta) \int_{\mathbb{P}} F_{ma} \frac{\partial \mathcal{H}}{\partial p_a} e^{-\beta\mathcal{H}} d\mathbb{P} = \frac{1}{T} \mathbb{E} (F_{ma} \dot{q}^a). \quad (5.8.39)$$

Comparing to equation (5.3.8) we see then that in the quasidynamic approximation the rate of change of

entropy is exactly related to the rate of heat flow into the system. The heat flow into a system is called the heat current $\Phi(t, S, Q, P)$ (it may also be written in terms of temperature by using $T = T(S, Q, P)$ to get $\Phi(t, T, Q, P)$):

$$\boxed{T \frac{dS}{dt} = \frac{dQ}{dt} \stackrel{\text{def}}{=} \Phi(t, S, Q, P).} \quad (5.8.40)$$

Then, the full equations of motion for a quasidynamic system are given in terms of the expected energy E by:

$$\boxed{\frac{dQ^a}{dt} = \frac{\partial E}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial E}{\partial Q^a} + F_{Ma}(t, S, Q, P), \quad \frac{\partial E}{\partial S} \frac{dS}{dt} = \Phi(t, S, Q, P).} \quad (5.8.41)$$

In order to specify the dynamics of a quasidynamic system then we need to specify the external forces on its macroscopic variables as well as the heat current into the system. This is quite a significant simplification as in the case of the exact underlying dynamics we needed to specify all of the microscopic external forces as well. All of that incredibly large number of intricate forces has been reduced in the quasidynamic approximation to just needing the heat current.

With our complete set of equations of motion, the energy of the system now changes in time as:

$$\frac{dE}{dt} = \frac{\partial E}{\partial S} \frac{dS}{dt} + \frac{\partial E}{\partial Q^a} \frac{dQ^a}{dt} + \frac{\partial E}{\partial P_a} \frac{dP_a}{dt} \quad (5.8.42)$$

$$= \Phi + \frac{\partial E}{\partial Q^a} \frac{\partial E}{\partial P_a} + \frac{\partial E}{\partial P_a} \left(F_{Ma} - \frac{\partial E}{\partial Q^a} \right) \quad (5.8.43)$$

$$= \Phi + F_{Ma} \dot{Q}^a \quad (5.8.44)$$

$$= \frac{dQ}{dt} + \frac{dW}{dt} \quad (5.8.45)$$

which simply recovers the first law of thermodynamics by using the definitions of heat and work established in section 5.3. So, the entropy equation of motion for a quasidynamic system is simply the necessary equation of motion required by the first law of thermodynamics (and in turn, by energy conservation).

Thus, from an underlying Hamiltonian for interacting microscopic variables with some macroscopic variables we can compute the partition function Z by equation (5.8.2) for the system in quasidynamic equilibrium, valid whenever the microscopic variables reach thermodynamic equilibrium on time scales much shorter than the time scale on which the macroscopic variables change. From the partition function we can compute the free energy $\mathcal{F}$ by equation (5.8.9). From the free energy $\mathcal{F}$ we can Legendre to compute the expected energy $E(S, Q, P)$ by equation (5.8.35). Then, the combination of that expected energy and whatever macroscopic external forces and heat current act on the system determines the dynamics of the entropy and the macroscopic variables of the system by Ralston's equations of motion, equation (5.8.41). These have the expected energy acting as the effective Hamiltonian and the entropy evolving according to the first law of thermodynamics.

There is another useful way to formulate the quasidynamic equations of motion. Define $\mathcal{P}$, the power delivered to the system. For an isolated system then $\mathcal{P} = 0$ due to energy conservation. In terms of $\mathcal{P}$ the entropy evolution becomes:

$$\mathcal{P} = \frac{dE}{dt} = \frac{dW}{dt} + \frac{dQ}{dt} = F_{Ma} \dot{Q}^a + \Phi \quad (5.8.46)$$

$$\implies T \frac{dS}{dt} = \mathcal{P} - F_{Ma} \dot{Q}^a. \quad (5.8.47)$$

Now consider the action:

$$\mathcal{S} = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - E(Q, P, S) \right) dt \quad (5.8.48)$$

(we use $\mathcal{S}$ to avoid confusion with S , the entropy). Under general variations (including variations of the entropy) which keep the boundary conditions on Q fixed:

$$\delta \mathcal{S} = \int_{t_0}^{t_f} \left(-\dot{P}_a \delta Q^a + \dot{Q}^a \delta P_a - \frac{\partial E}{\partial Q^a} \delta Q^a - \frac{\partial E}{\partial P_a} \delta P_a - \frac{\partial E}{\partial S} \delta S \right) dt. \quad (5.8.49)$$

We can see that if we define the variations of the entropy to satisfy:

$$T \delta S = -F_{Ma} \delta Q^a \quad (5.8.50)$$

then the result is that the stationary variation of the action $\mathcal{S}$ produces the quasidynamic equations of motion for (Q, P) :

$$\delta\mathcal{S}|_{T\delta S=-F_{Ma}\delta Q^a} \stackrel{!}{=} 0 \implies \dot{Q}^a = \frac{\partial E}{\partial P_a}, \quad \dot{P}_a = -\frac{\partial E}{\partial Q^a} + F_{Ma} \quad (5.8.51)$$

and the entropy equation of motion is specified by supplying the power function $\mathcal{P}(t)$. In this alternative formulation we essentially have a nonholonomic constraint on the variations of the entropy and it induces the correct evolution of (Q, P) . It makes perfect sense why we have a nonholonomic variational condition. In averaging out the microscopic coordinates to produce the quasidynamic equations of motion we have essentially performed a version of the top-down effective theory thinking in section 2.7 and thus naturally produce a system with hysteresis. We are lucky that all of that hysteresis can be isolated to path dependent (nonholonomic) variations of the entropy. Because for an isolated system $\mathcal{P} = 0$, the entropy evolution in that case is determined by energy conservation.

When using this entropy varied formulation it is useful to define the effective Q^a derivative Δ which accounts for the associated variation of the entropy. For a general quantity $A(t, S, Q, P)$:

$$\frac{\Delta A}{\Delta Q^a} = \frac{\partial A}{\partial Q^a} + \frac{\delta S}{\delta Q^a} \frac{\partial A}{\partial S} = \frac{\partial A}{\partial Q^a} - \frac{F_{Ma}}{T} \frac{\partial A}{\partial S}. \quad (5.8.52)$$

Then, the time derivative of A is:

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{\partial A}{\partial S} \frac{dS}{dt} + \frac{\partial A}{\partial Q^a} \dot{Q}^a + \frac{\partial A}{\partial P_a} \dot{P}_a \quad (5.8.53)$$

$$= \frac{\partial A}{\partial t} + \frac{\mathcal{P}}{T} \frac{\partial A}{\partial S} - \frac{1}{T} \frac{\partial A}{\partial S} F_{Ma} \dot{Q}^a + \frac{\partial A}{\partial Q^a} \frac{\partial E}{\partial P_a} - \frac{\partial A}{\partial P_a} \frac{\partial E}{\partial Q^a} + \frac{\partial A}{\partial P_a} F_{Ma} \quad (5.8.54)$$

$$= \frac{\partial A}{\partial t} + \frac{\mathcal{P}}{T} \frac{\partial A}{\partial S} + \frac{\Delta A}{\Delta Q^a} \frac{\partial E}{\partial P_a} - \frac{\partial A}{\partial P_a} \frac{\Delta E}{\Delta Q^a}. \quad (5.8.55)$$

The first two terms represent the explicit time dependence of A and how it is driven due to the power function, which are analogous to the explicit time dependent term in equation (1.4.24). The remaining structure defines the effective quasidynamic Poisson bracket:

$$\{A, B\}_S \stackrel{\text{def}}{=} \frac{\Delta A}{\Delta Q^a} \frac{\partial B}{\partial P_a} - \frac{\partial A}{\partial P_a} \frac{\Delta B}{\Delta Q^a} = \left(\frac{\partial A}{\partial Q^a} - \frac{F_{Ma}}{T} \frac{\partial A}{\partial S} \right) \frac{\partial B}{\partial P_a} - \frac{\partial A}{\partial P_a} \left(\frac{\partial B}{\partial Q^a} - \frac{F_{Ma}}{T} \frac{\partial B}{\partial S} \right). \quad (5.8.56)$$

Theorem 5.7: Quasidynamic Equations of Motion

In the thermodynamic limit of a system with macroscopic variables (Q, P) interacting with microscopic variables (q, p) described by the Hamiltonian $\mathcal{H}(Q, q, P, p)$, the microscopic variables are described by the canonical ensemble:

$$f(q, p|T, Q, P) = \frac{e^{-\beta\mathcal{H}(Q, q, P, p)}}{Z} \quad (5.8.57)$$

with the partition function given by:

$$Z(T, Q, P) = \int_{\mathbb{P}} e^{-\beta\mathcal{H}(Q, q, P, p)} \frac{d^d q d^d p}{(2\pi\hbar)^d}. \quad (5.8.58)$$

In terms of the Free Energy $\mathcal{F}$ defined by:

$$\mathcal{F}(T, Q, P) = -T \ln Z \quad (5.8.59)$$

the entropy of the system can be computed by:

$$S(T, Q, P) = -\frac{\partial \mathcal{F}}{\partial T} \quad (5.8.60)$$

and the expected energy of the system can be computing using the Legendre transform:

$$E(S, Q, P) = \mathcal{F}(T, Q, P) + TS \quad (5.8.61)$$

$$\implies T(S, Q, P) = \frac{\partial E}{\partial S}. \quad (5.8.62)$$

Then, the equations of motion for Q, P are given by Hamilton's equations (including any present

external forces) treating the expected energy as the Hamiltonian:

$$\frac{dQ^a}{dt} = \frac{\partial E}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial E}{\partial Q^a} + F_{Ma}(t, S, Q, P) \quad (5.8.63)$$

and the equation of motion for the entropy is given by the first law of thermodynamics:

$$\frac{dE}{dt} = \frac{dW}{dt} + \frac{dQ}{dt} \implies T \frac{dS}{dt} = \frac{dQ}{dt} = \Phi(t, S, Q, P) \quad (5.8.64)$$

where $\Phi(t, S, Q, P)$ is the rate of heat transfer to the system.

Equivalently, if $\mathcal{P}$ is the power delivered to the system the equations of motion for the system are given by requiring the stationary variation of the action:

$$\mathcal{S} = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - E(Q, P, S) \right) dt \quad (5.8.65)$$

under general variations of Q, P and constrained variations of the entropy which satisfy:

$$T\delta S + F_{Ma}\delta Q^a = 0. \quad (5.8.66)$$

The evolution of the entropy is given by the first law of thermodynamics:

$$T \frac{dS}{dt} + F_{Ma} \dot{Q}^a = \mathcal{P}. \quad (5.8.67)$$

Using this entropy-varied formulation, the effective Poisson bracket is:

$$\{A, B\}_S = \frac{\Delta A}{\Delta Q^a} \frac{\partial B}{\partial P_a} - \frac{\partial A}{\partial P_a} \frac{\Delta B}{\Delta Q^a} = \left(\frac{\partial A}{\partial Q^a} - \frac{F_{Ma}}{T} \frac{\partial A}{\partial S} \right) \frac{\partial B}{\partial P_a} - \frac{\partial A}{\partial P_a} \left(\frac{\partial B}{\partial Q^a} - \frac{F_{Ma}}{T} \frac{\partial B}{\partial S} \right). \quad (5.8.68)$$

Exercises

Problem 5.38: ★ No Classical Magnetization. Consider a system of N point charges each of mass m and charge q subject to an external constant magnetic field. Show by direct integration that in both the relativistic and nonrelativistic case the partition function for the system of charges does not depend on that magnetic field at all and thus in thermodynamic equilibrium there is no effect of an external magnetic field on point charges. This fact prevents any explanation based in point particles of the macroscopic magnetic properties of matter.

Problem 5.39: ★ Heating up a table. Consider a mass m moving on a table experiencing kinetic friction with friction coefficient μ as it slides on a table. Suppose that the table and surface of the mass are both at temperature T and that the internal energy of the table and mass system in thermodynamic equilibrium is CT for a constant C and that the table is always in thermodynamic equilibrium so that the quasidynamic equations of motion apply.

(a) Explain that the total energy of the mass and table system is given by:

$$E = \frac{1}{2}m\dot{x}^2 + CT$$

and that the position of the mass and temperature of the system evolve in time as the object slides (to the right) by:

$$m\ddot{x} = -\mu mg, \quad C\dot{T} = \mu mg\dot{x}.$$

(b) Suppose the mass is initially moving with velocity v . Show then that as the mass comes to a stop the change in temperature of the system is:

$$\Delta T = \frac{mv^2}{2C}.$$

5.9 Quasistatics and Thermodynamic Potentials

There is a further approximation which is often useful for studying thermodynamics known as the quasistatic approximation. The quasistatic approximation is the approximation that in addition to the quasidynamic approximation the macroscopic variables Q and P have velocities which are so small that they can instantaneously be approximated as 0. That is, the quasistatic approximation is the dual approximation that the microscopic variables are always in equilibrium and the macroscopic variables change arbitrarily slowly. Then, we must have:

$$\dot{Q}^a = \frac{\partial E}{\partial P_a} \approx 0, \quad \dot{P}_a = -\frac{\partial E}{\partial Q^a} + F_{Ma} \approx 0 \implies F_{Ma} \approx \frac{\partial E}{\partial Q^a}. \quad (5.9.1)$$

Consequently, the total derivative of the expected energy becomes in this approximation:

$$dE = \frac{\partial E}{\partial S} dS + \frac{\partial E}{\partial Q^a} dQ^a + \frac{\partial E}{\partial P_a} dP_a = T dS + F_{Ma} dQ^a + 0 = T dS + dW. \quad (5.9.2)$$

For quasistatic processes then we can identify using the first law of thermodynamics:

$$\boxed{dQ = T dS = \frac{\partial E}{\partial S} dS, \quad dW = F_{Ma} dQ^a = \frac{\partial E}{\partial Q^a} dQ^a.} \quad (5.9.3)$$

By equation (5.9.1) we see that in the quasistatic approximation $\frac{\partial E}{\partial P_a} = 0$ and so the expected energy becomes a function of the entropy and the coordinates only. As well, in the quasistatic approximation the external forces can be computed from the expected energy (as their value is fixed by equation (5.9.1) in order to preserve the quasistatic property).

One of the possible coordinates for a thermodynamic system is the number of microscopic constituents comprising that system (for a box of gas, the number of gas molecules). We call that coordinate N and its associated external force μ the (total) chemical potential. We will explicitly pull that coordinate out of further coordinate sums going forward. Because the number of constituents of a system is extensive and the energy is extensive, by equation (5.9.1) the chemical potential is intensive. It is often nice to distinguish between coordinates which are extensive and coordinates which are intensive. Suppose we have organized all of our coordinates in a way so that they are either intensive or extensive. The intensive coordinates we will write as x^a and their external forces as F_a (as they are automatically extensive). The extensive coordinates we will write as X^a and their external forces as f_a (as they are automatically intensive). (Do not confuse the symbol f_a , the external macroscopic force on extensive variable X^a , with the phase space density f .) Then, expanding out (5.9.2) in terms of these coordinates we have introduced we have that for quasistatic processes:

$$\boxed{dE(S, N, X, x) = T dS + \mu dN + f_a dX^a + F_a dx^a} \quad (5.9.4)$$

$$\implies T = \frac{\partial E}{\partial S}, \quad \mu = \frac{\partial E}{\partial N}, \quad f_a = \frac{\partial E}{\partial X^a}, \quad F_a = \frac{\partial E}{\partial x^a}. \quad (5.9.5)$$

This is often known as the “fundamental thermodynamic relation”. Recalling that the free energy is the Legendre transformation of the energy with respect to entropy/temperature:

$$\boxed{\mathcal{F}(T, N, X, x) = E(S, N, X, x) - TS} \quad (5.9.6)$$

$$\implies d\mathcal{F}(T, N, X, x) = T dS + \mu dN + f_a dX^a + F_a dx^a - T dS - S dT \quad (5.9.7)$$

$$\implies \boxed{d\mathcal{F}(T, N, X, x) = -S dT + \mu dN + f_a dX^a + F_a dx^a} \quad (5.9.8)$$

$$\implies S = -\frac{\partial \mathcal{F}}{\partial T}, \quad \mu = \frac{\partial \mathcal{F}}{\partial N}, \quad f_a = \frac{\partial \mathcal{F}}{\partial X^a}, \quad F_a = \frac{\partial \mathcal{F}}{\partial x^a}. \quad (5.9.9)$$

One could also Legendre transform with respect to any combination of the coordinates and so if there are d such coordinates there are 2^{d+1} functions related by Legendre transformation to the energy which can all recover all of the thermodynamic information. These functions, including the energy and the free energy, are all called thermodynamic potentials. Of this large space of potentials, there are four of particular interest for most applications. We have already identified two: the expected energy and the free energy. The other two are known as the Gibbs energy and the enthalpy. The Gibbs energy G is defined by Legendre transforming the free energy with respect to all of the extensive coordinates:

$$\boxed{G \stackrel{\text{def}}{=} \mathcal{F} - f_a X^a} \quad (5.9.10)$$

$$\implies dG = -SdT + \mu dN + f_a dX^a + F_a dx^a - f_a dX^a - X^a df_a \quad (5.9.11)$$

$$\implies \boxed{dG(T, N, x, f) = -SdT + \mu dN + F_a dx^a - X^a df_a} \quad (5.9.12)$$

$$\implies S = -\frac{\partial G}{\partial T}, \quad \mu = \frac{\partial G}{\partial N}, \quad F_a = \frac{\partial G}{\partial x^a}, \quad X^a = -\frac{\partial G}{\partial f_a}. \quad (5.9.13)$$

So, the Gibbs energy is a function only 1 extensive quantity, the constituent number N . The Gibbs energy is the difference between extensive quantities and so it is automatically extensive. The enthalpy H is defined as the same Legendre transformation but of the energy:

$$\boxed{H \stackrel{\text{def}}{=} E - f_a X^a} \quad (5.9.14)$$

$$\implies dH = TdS + \mu dN + f_a dX^a + F_a dx^a - f_a dX^a - X^a df_a \quad (5.9.15)$$

$$\implies \boxed{dH(S, N, x, f) = TdS + \mu dN + F_a dx^a - X^a df_a} \quad (5.9.16)$$

$$\implies T = \frac{\partial H}{\partial S}, \quad \mu = \frac{\partial H}{\partial N}, \quad F_a = \frac{\partial H}{\partial x^a}, \quad X^a = -\frac{\partial H}{\partial f_a}. \quad (5.9.17)$$

The enthalpy is also automatically extensive from its definition as the difference of extensive quantities.

Because the Gibbs energy after the Legendre transformation is written in terms of T, N, x, f , we have:

$$\mu(T, N, x, f) = \frac{\partial G}{\partial N}. \quad (5.9.18)$$

However, the chemical potential is intensive. So, under a scaling of the extensive quantities of the system by a factor α :

$$N' = \alpha N, \quad \mu' = \mu. \quad (5.9.19)$$

To make this consistent with the formula derived for the chemical potential we have:

$$\mu(T, \alpha N, x, f) = \mu(T, N, x, f). \quad (5.9.20)$$

Differentiating both sides with respect to α at $\alpha = 1$ then gives:

$$N \frac{\partial \mu}{\partial N}(T, N, x, f) = 0 \quad (5.9.21)$$

$$\implies \frac{\partial \mu}{\partial N}(T, N, x, f) = 0 \quad (5.9.22)$$

$$\implies \mu = \mu(T, x, f). \quad (5.9.23)$$

Hence, the chemical potential does not actually depend on N when written in terms of T, x, f . Then, integrating the relationship between μ and G we have:

$$\mu(T, x, f) = \frac{\partial G}{\partial N}(T, N, x, f) \quad (5.9.24)$$

$$\implies G(T, N, x, f) = \mu(T, x, f)N + G(T, 0, x, f). \quad (5.9.25)$$

The extensivity of G requires:

$$G(T, \alpha N, x, f) = \alpha G(T, N, x, f) \quad (5.9.26)$$

$$\implies G(T, 0, x, f) = 0G(T, N, x, f) = 0. \quad (5.9.27)$$

So, the Gibbs energy is given in terms of the chemical potential and constituent number as:

$$\boxed{G(T, N, x, f) = N\mu(T, x, f).} \quad (5.9.28)$$

Hence, the (total) chemical potential of a thermodynamic system fully determines its Gibbs energy and so by Legendre transformation determines all of the other thermodynamic potentials and consequently all of the thermodynamic properties of the system. Computing the derivatives of G in terms of the chemical potential then gives:

$$S = \frac{\partial G}{\partial T} = N \frac{\partial \mu}{\partial T}, \quad F_a = \frac{\partial G}{\partial x^a} = N \frac{\partial \mu}{\partial x^a}, \quad X^a = -\frac{\partial G}{\partial f_a} = -N \frac{\partial \mu}{\partial f_a}. \quad (5.9.29)$$

This allows us to express the following relationships in terms of purely intensive quantities:

$$\mu(T, x, f) = \frac{\partial G}{\partial N}, \quad \frac{S}{N} = \frac{\partial \mu}{\partial T}(T, x, f) \quad (5.9.30)$$

$$\frac{F_a}{N} = \frac{\partial \mu}{\partial x^a}(T, x, f), \quad \frac{X^a}{N} = -\frac{\partial \mu}{\partial f_a}(T, x, f). \quad (5.9.31)$$

These equations are called the **equations of state** of the thermodynamic system. We see that if there are d coordinates (x, X) then there are $d + 2$ equations of state for the system. We can see that the equations of state determine all of the intensive quantities of the thermodynamic system in terms of the $d + 1$ quantities (T, x, f) . The system then has the single overall scale N to set the size of the system.

Due to the equality of mixed partial derivatives, there are many seemingly non-trivial equivalences that can be written between thermodynamic quantities. For example, taking equation (5.9.5):

$$\frac{\partial T}{\partial x^a}(S, N, X, x) = \frac{\partial^2 E}{\partial S \partial x^a}(S, N, X, x) = \frac{\partial F_a}{\partial S}(S, N, X, x). \quad (5.9.32)$$

The equality of these partial derivatives is one of many such relations. For any thermodynamic potential one can produce such a relation, called a Maxwell relation, by taking the mixed partial of that potential with respect to any two of its variables and expressing that mixed partial in the two different possible ways as derivatives of one of its first derivatives. These Maxwell relations predict relationships often between directly measurable quantities and so while (given a thermodynamic potential) they are theoretically trivial they are experimentally useful.

Theorem 5.8: Quasistatic Processes

For a quasidynamic system with velocities $\dot{Q}^a$ and $\dot{P}_a$ so slow that we can always instantaneously approximate them to 0, the expected energy becomes only a function of the entropy and the coordinates $E(S, N, X, x)$ where x^a are the intensive coordinates, X^a are the extensive coordinates except the number of constituents in the system, and N is the number of constituents of the system. In this approximation, the temperature T , chemical potential μ , extensive external forces F_a , and intensive external forces f_a are given by the fundamental thermodynamic relation:

$$dE(S, N, X, x) = TdS + \mu dN + f_a dX^a + F_a dx^a. \quad (5.9.33)$$

Similarly, all of these quantities can be computed using various Legendre transformations of the energy such as the Free Energy $\mathcal{F}$, the Gibbs Energy G , or the Enthalpy H :

$$\mathcal{F}(T, N, X, x) = E(S, N, X, x) - TS \quad (5.9.34)$$

$$\implies d\mathcal{F} = -SdT + \mu dN + f_a dX^a + F_a dx^a \quad (5.9.35)$$

$$G(T, N, x, f) = \mathcal{F}(T, N, X, x) - f_a X^a \quad (5.9.36)$$

$$\implies dG = -SdT + \mu dN - X^a df_a + F_a dx^a \quad (5.9.37)$$

$$H(S, N, x, f) = E(S, N, X, x) - f_a X^a \quad (5.9.38)$$

$$\implies dH = TdS + \mu dN - f_a dX^a + F_a dx^a. \quad (5.9.39)$$

For a system of N identical constituents, the Gibbs energy is given in terms of the chemical potential by:

$$G(T, N, x, f) = N\mu(T, x, f) \quad (5.9.40)$$

and all of the intensive quantities of the system are determined by the equations of state:

$$\mu(T, x, f) = \frac{\partial G}{\partial N}, \quad \frac{S}{N} = \frac{\partial \mu}{\partial T}(T, x, f) \quad (5.9.41)$$

$$\frac{F_a}{N} = \frac{\partial \mu}{\partial x^a}(T, x, f), \quad \frac{X^a}{N} = -\frac{\partial \mu}{\partial f_a}(T, x, f). \quad (5.9.42)$$

5.9.1 Identical Particles and Boltzmann Statistics

We will often consider systems which consist of many “identical” particles/microscopic constituents. By identical here we do not simply mean that these particles have a Hamiltonian which is symmetric under

interchanging them but also that any interaction which could be performed with these particles also is symmetric under interchanging them. Consequently, no experiment could be performed which identifies “which” particle you are looking at. To make this more concrete, for all mechanical purposes a red ball and a blue ball have the same Hamiltonian. However, under the electromagnetic interaction they do not; one reflects red light while the other reflects blue. So, they can be distinguished by some interaction. Identical particles are ones for which no such interaction could possibly be produced. We believe by a combination of experimental evidence and theoretical reasons which we will discuss in Part II that all the electrons in the universe are indistinguishable from each other. This property is not specific to electrons. Really, we believe all particles of the same “particle species” are indistinguishable by any experiment. When discussing identical particles there is an intrinsic redundancy in the phase space. For two identical particles with coordinates and momenta (Q_1, P_1) and (Q_2, P_2) respectively the points (Q_1, P_1, Q_2, P_2) and (Q_2, P_2, Q_1, P_1) in phase space are actually the same point. They are the same because they are related by interchanging the particles and that interchange is not a physical symmetry but a bookkeeping relabeling of the data of the problem; it changes nothing because the particles are the same. It does not matter which particle we call particle 1 and which one we call particle 2. Consequently, if we do not account for this interchange then we are double-counting points in phase space.

When we have N identical particles the phase space of the N of them is simply given by the coordinates $(Q_1, P_1, \dots, Q_N, P_N)$ but where all $N!$ reorderings of these coordinates are treated equally. The arguments leading to the canonical ensemble are unchanged and so:

$$f_{\text{canon}} = \frac{e^{-\beta\mathcal{H}}}{Z} \quad (5.9.43)$$

where the partition function gives the normalization:

$$Z = \int e^{-\beta\mathcal{H}} d\mathbb{P}. \quad (5.9.44)$$

However, the phase space integral here is only over the phase space of the identical particles. The volume of any region of the identical particle phase space is $\frac{1}{N!}$ the volume of the corresponding volume of the phase space if the particles were treated as distinguishable, due to the $N!$ over counting of the different orderings. So:

$$Z_N^{\text{identical}} = \int e^{-\beta\mathcal{H}} d\mathbb{P}_{\text{identical}} = \frac{1}{N!} \int e^{-\beta\mathcal{H}} d\mathbb{P}_{\text{distinct}} = \frac{Z_N^{\text{distinct}}}{N!} \quad (5.9.45)$$

When we have N distinct particles the phase space of the N of them is simply given by the coordinates $(Q_1, P_1, \dots, Q_N, P_N)$. If these particles are not interacting and each particle has partition function Z_1 then by equation (5.5.37) the partition function for the N of them together is:

$$Z_N^{\text{distinct}} = Z_1^N. \quad (5.9.46)$$

For N noninteracting identical particles then:

$$Z_N = \frac{Z_1^N}{N!} \quad (5.9.47)$$

Classical identical particles thus combine partition functions with this factor of $N!$. Anything which does so is said to satisfy “Boltzmann statistics”.

At the theoretical level in classical physics, every different object has independent mass, charge, and other values of parameters in the action. Of course macroscopically several different species of materials are observable, leading to shared properties among different objects (lead exists and different blocks of pure lead under the same thermodynamic conditions will have the same density, for example). Microscopically, this is due to the fact that there are apparently identical atoms coming in only very limited varieties comprising macroscopic objects. At the level of classical physics, it is unexplained why such thing as identical atoms exist (underlying this are the questions like why does every proton have the same mass, why does every neutron have the same mass?). There is an explanation, but we will have to wait until Part II to understand it.

Identical particles give another way to understand in what sense distributions are considered in statistical mechanics. We can view each particle as an experimental trial with a definite (likely unknown state) thus described by a phase space density which is a Dirac delta in phase space. Then, the average behavior of all of the N particles is given by $\frac{1}{N}$ times the sum over each particle’s delta. This gives the effective single particle phase space density. When the number of particles is very large, this phase space density effectively smoothens out (in terms of its behavior when integrating against functions that do not vary quickly on the

scale of the interparticle separation) and so we can define a reasonably smooth function $f(t, Q, P)$ describing the single particle phase space density. Each particle interacts with all of the other particles and so effectively is in a bath provided by those other particles. Thus, under reasonable considerations we can argue that $f(t, Q, P)$ when time-averaged should approach the canonical ensemble.

5.9.2 Example: Nonrelativistic Ideal Gases

The simplest state of matter to describe is the gas. An Ideal Gas is a system of identical particles with no interactions between the particles beyond the amount necessary to bring them into thermodynamic equilibrium. Real gases do include some small interactions between the particles but are often approximately correctly described by the ideal gas. Let us suppose we have N identical nonrelativistic particles with positions $\vec{x}_1(t), \dots, \vec{x}_N(t)$ moving in a container of volume $\mathbb{V}$. These particles may have some internal degrees of freedom $\mathbf{q}, \mathbf{p}$ each. For example, a molecule may have some spin degrees of freedom to rotate about its center of mass or some vibrational degrees of freedom to expand and contract. In any case, we will assume these internal degrees of freedom have been defined so that they are unchanged by translations, boosts, or rotations of the overall system. Each particle then will contribute $\frac{|\vec{p}_k|^2}{2m} + h(\mathbf{q}_k, \mathbf{p}_k)$ to the free Hamiltonian where $h(\mathbf{q}, \mathbf{p})$ is whatever the free Hamiltonian happens to be for the particle internal degrees of freedom. Because we assume there are no interparticle interactions on our ideal gas, the free Hamiltonian is the total Hamiltonian. h cannot depend on the positions or momenta of the particles due to translational symmetry and Galilean boost symmetry. As well, we will assume that the internal degrees of freedom have a quadratic free Hamiltonian (this is automatically true or at least can be made true for many common types of internal degrees of freedom such as vibrational or spin modes) and that that Hamiltonian is bounded below (which should be believable by the logic of section 5.5). By theorem 1.14 any such quadratic Hamiltonian can, through a canonical transformation, be put in the form:

$$h(\mathbf{q}, \mathbf{p}) = \sum_{j=1}^{d_1} \left(\frac{(\mathbf{p}^j)^2 + \omega_j^2 (\mathbf{q}^j)^2}{2} \right) \quad (5.9.48)$$

where $\omega_j \geq 0$. Here there are d_1 coordinate pairs of internal degrees of freedom per particle. Some of these ω_j may be 0. Let there be d_2 coordinate pairs with non-zero ω_j . Then, there are $d \stackrel{\text{def}}{=} d_1 + d_2$ quadratic terms in the free Hamiltonian of each particle's internal degrees of freedom. With this the full Hamiltonian becomes:

$$\mathcal{H} = \sum_{k=1}^N \left(\frac{|\vec{p}_k|^2}{2m} + \sum_{j=1}^{d_1} \left(\frac{(\mathbf{p}_k^j)^2 + \omega_j^2 (\mathbf{q}_k^j)^2}{2} \right) \right). \quad (5.9.49)$$

To study the thermodynamics of the ideal gas we will need the partition function which from equation (5.9.47) we can get from the single particle partition function. It is appropriate to use equation (5.9.47) because each gas molecule, being of the same species, is identical to all the others and so we should use Boltzmann statistics. Let us we define the internal coordinates so that the last $d_1 - d_2$ of them are the ones which have vanishing ω_j and so that each $\mathbf{q}^j$ with vanishing ω_j is allowed to be in a range 0 to ℓ_j for some constants ℓ_j . Then, the single particle partition function is:

$$Z_1 = \int_{\mathbb{P}_1} e^{-\beta \mathcal{H}_1} d\mathbb{P}_1 \quad (5.9.50)$$

$$= \int_{\mathbb{R}^3 \mathbb{V} \mathbb{R}^{2d_1} \mathbb{R}^{d_2}} \int_0^{\ell_1} \dots \int_0^{\ell_{d_1-d_2}} e^{-\frac{\beta}{2m} |\vec{p}|^2 - \beta \sum_{j=1}^{d_1} \left(\frac{(\mathbf{p}^j)^2 + \omega_j^2 (\mathbf{q}^j)^2}{2} \right)} \frac{d\mathbf{q}^1 d\mathbf{p}^1}{2\pi\hbar} \dots \frac{d\mathbf{q}^{d_1} d\mathbf{p}^{d_1}}{2\pi\hbar} \frac{d^3 \vec{x} d^3 \vec{p}}{(2\pi\hbar)^3} \quad (5.9.51)$$

$$= \int_{\mathbb{R}^3} e^{-\frac{\beta |\vec{p}|^2}{2m}} \frac{d^3 \vec{p}}{(2\pi\hbar)^3} \int_{\mathbb{V}} d^3 \vec{x} \left(\prod_{j=1}^{d_2} \int_{\mathbb{R}} e^{-\frac{\beta (\mathbf{p}^j)^2}{2}} \frac{d\mathbf{p}^j}{2\pi\hbar} \int_{\mathbb{R}} e^{-\frac{\beta \omega_j^2 (\mathbf{q}^j)^2}{2}} d\mathbf{q}^j \right) \left(\prod_{j=d_2+1}^{d_1} \int_{\mathbb{R}} e^{-\frac{\beta (\mathbf{p}^j)^2}{2}} \frac{d\mathbf{p}^j}{2\pi\hbar} \int_0^{\ell_j} d\mathbf{q}^j \right) \quad (5.9.52)$$

$$= \left(\frac{mT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \mathbb{V} \left(\prod_{j=1}^{d_2} \frac{T}{\hbar\omega_j} \right) \left(\prod_{j=d_2+1}^{d_1} \ell_j \sqrt{\frac{T}{2\pi\hbar^2}} \right) \quad (5.9.53)$$

$$= (2\pi)^{d_2} \frac{\prod_{j=d_2+1}^{d_1} \ell_j}{\hbar^{3+d_1} \prod_{j=1}^{d_2} \omega_j} m^{\frac{3}{2}} \left(\frac{T}{2\pi} \right)^{\frac{3+d}{2}} \mathbb{V}. \quad (5.9.54)$$

The complicated prefactor here is just a constant multiplier which will end up dropping out of calculations of experimentally meaningful quantities. For the sake of brevity, let us define the constant κ by:

$$\kappa \stackrel{\text{def}}{=} \left(\frac{(2\pi)^{d_2}}{\hbar^{3+d_1}} \frac{\prod_{j=d_2+1}^{d_1} \ell_j}{\prod_{j=1}^{d_2} \omega_j} m^{\frac{3}{2}} \right)^{\frac{2}{3+d}} \quad (5.9.55)$$

$$\implies Z_1 = \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \mathbb{V} \quad (5.9.56)$$

$$\implies Z_N = \frac{Z_1^N}{N!} = \frac{1}{N!} \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2} N} \mathbb{V}^N. \quad (5.9.57)$$

The N particle free energy before taking the thermodynamic limit then is:

$$\mathcal{F}_N = -T \ln Z_N = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \mathbb{V} \right) + T \ln N!. \quad (5.9.58)$$

Recalling the definition of Sterling's function:

$$\mathcal{F}_N = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \mathbb{V} \right) + NT \ln \left(\sqrt{2\pi N} N^N e^{-N} \text{St}(N) \right) \quad (5.9.59)$$

$$\implies \frac{\mathcal{F}_N}{N} = -T \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{\mathbb{V}}{N} \right) + \frac{T}{N} \ln \left(\sqrt{2\pi N} \text{St}(N) \right) - T. \quad (5.9.60)$$

The total volume of two adjacent containers is the sum of their volumes and so volume is extensive. Then, in the thermodynamic limit the intensive quantities T , $\frac{\mathcal{F}}{N}$, $\frac{\mathbb{V}}{N}$ are held fixed and N is taken to infinity. Actually performing this limit we have:

$$\frac{\mathcal{F}}{N} = -T \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{\mathbb{V}}{N} \right) - T. \quad (5.9.61)$$

Thus, for a nonrelativistic ideal gas the free energy is:

$$\boxed{\mathcal{F} = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{\mathbb{V}}{N} \right) - NT.} \quad (5.9.62)$$

We can see that in the notation of equation (5.9.4), there are no x coordinates and the only X coordinate is $\mathbb{V}$. We can find a nice interpretation for the thermodynamic force f conjugate to $\mathbb{V}$ by equation (5.9.5). In order change the volume of the container, one will have to apply a force to container walls. The work element done on the container wall when an external force $\vec{F}_{\text{ext}}$ is applied to it causing a displacement $d\vec{x}$ of the wall is:

$$dW = \vec{F}_{\text{ext}} \cdot d\vec{x}. \quad (5.9.63)$$

Let the wall have surface area $\mathbb{A}$ and outward pointing normal vector $\vec{\ell}$. Only forces into the wall will cause the wall to compress and so the compressing force will be:

$$\vec{F}_{\text{ext}} = -F_{\text{ext}} \vec{\ell} \quad (5.9.64)$$

where $F_{\text{ext}} = |\vec{F}_{\text{ext}}|$. Pressure is defined as the force into a surface per unit surface area. Therefore, the externally applied pressure due to this external force is:

$$p_{\text{ext}} = -\frac{\vec{\ell} \cdot \vec{F}_{\text{ext}}}{\mathbb{A}} = \frac{F_{\text{ext}}}{\mathbb{A}}. \quad (5.9.65)$$

Then, the work element becomes:

$$dW = -p_{\text{ext}} \mathbb{A} \vec{\ell} \cdot d\vec{x}. \quad (5.9.66)$$

The change in volume of the container due to the compression is given by:

$$d\mathbb{V} = \mathbb{A} \vec{\ell} \cdot d\vec{x}. \quad (5.9.67)$$

Thus, we have that the work done on a container when an external pressure is applied to change the volume

of that container is:

$$dW = -p_{\text{ext}}dV. \quad (5.9.68)$$

By comparing with equation (5.3.12) we see that treating the volume of the container as a macroscopic coordinate leads to $-p_{\text{ext}}$ being its canonically conjugate force. Consequently, the quantity $-\frac{\partial E}{\partial V}$ defines the internal pressure of the gas. For quasistatic processes the internal and external pressures will match by equation (5.9.1) however in general they will not. The internal pressure is often just written p whereas the external pressure is written p_{ext} . This gives us:

$$\boxed{p = -\frac{\partial E}{\partial V}}. \quad (5.9.69)$$

Thus, $-p$ is the conjugate to V . Comparing equations (5.9.5) and (5.9.9) allows us to identify that p can equivalently be computed by:

$$p = -\frac{\partial \mathcal{F}}{\partial V}. \quad (5.9.70)$$

Now we can compute all of the thermodynamic properties of the ideal gas. The entropy is:

$$S = -\frac{\partial \mathcal{F}}{\partial T} = N \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{V}{N} \right) + \frac{5+d}{2} N. \quad (5.9.71)$$

This is called the Sackur-Tetrode formula. The internal pressure is:

$$p = -\frac{\partial \mathcal{F}}{\partial V} = \frac{NT}{V} \implies \boxed{pV = NT}. \quad (5.9.72)$$

This is called the ideal gas law. It was discovered experimentally before it had a theoretical foundation. The chemical potential is:

$$\mu = \frac{\partial \mathcal{F}}{\partial N} = -T \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{V}{N} \right) = -T \ln \left(\left(\frac{\kappa}{2\pi} \right)^{\frac{3+d}{2}} \frac{T^{\frac{5+d}{2}}}{p} \right). \quad (5.9.73)$$

Finally, the expected energy E is:

$$E = \mathcal{F} + TS = \frac{3+d}{2} NT. \quad (5.9.74)$$

Every variable which enters the Hamiltonian only quadratically and is allowed to take any real value contributes $\frac{T}{2}$ to the expected energy (the equipartition theorem) which is directly reflected in this expression for the expected energy.

The parameter d which corresponds to the number of internal variables which enter the Hamiltonian quadratically per particle appears in most of the thermodynamic relations above, but it is a bit disconnected from direct experimental practice. Instead, it is common to write the above expressions in terms of an alternate parameter called the adiabatic ratio γ which is directly related to d but more obviously measurable. Suppose our gas undergoes a quasistatic process in which no heat is added to it (such a process is called adiabatic, which is an unfortunate overlap of language with the use of the word adiabatic in adiabatic invariants which are unrelated). Then, by the first law of thermodynamics, equation (5.9.68), and equation (5.9.3):

$$dE = -pdV. \quad (5.9.75)$$

Using equations (5.9.72) and (5.9.74):

$$dE = d \left(\frac{3+d}{2} NT \right) = d \left(\frac{3+d}{2} pV \right) = \frac{3+d}{2} pdV + \frac{3+d}{2} Vdp = -pdV \quad (5.9.76)$$

$$\implies \frac{dp}{p} + \frac{5+d}{3+d} \frac{dV}{V} = 0 \quad (5.9.77)$$

$$\implies pV^{\frac{5+d}{3+d}} = \text{Constant}. \quad (5.9.78)$$

Thus defining the adiabatic ratio γ :

$$\gamma = \frac{5+d}{3+d} \quad (5.9.79)$$

$$\implies pV^\gamma = \text{Constant} \quad (5.9.80)$$

for processes in which no heat is supplied to the gas. This γ is more experimentally directly accessible because one can measure the initial volume and pressure of the gas $(\mathbb{V}_0, p_0)$ and the final volume and pressure of the gas $(\mathbb{V}_f, p_f)$ directly. If one's experiment is so that the process connecting these two states does not involve any appreciable heat transfer to the gas we will have:

$$p_f \mathbb{V}_f^\gamma = p_0 \mathbb{V}_0^\gamma \quad (5.9.81)$$

$$\implies \gamma = \frac{\ln p_f - \ln p_0}{\ln \mathbb{V}_f - \ln \mathbb{V}_0}. \quad (5.9.82)$$

Thus, γ can be easily determined. Then, the chemical potential can be written:

$$\mu = -\frac{T}{\gamma - 1} \ln \left(\frac{\kappa}{2\pi} \left(\frac{T}{p} \right)^\gamma \right) \quad (5.9.83)$$

and using equations (5.9.41) and (5.9.42) all of the thermodynamic properties of the gas can be computed from this chemical potential.

Exercises

Problem 5.40: Maxwell Speed Distribution. Consider a gas of N identical nonrelativistic particles each of mass m in a volume $\mathbb{V}$ in thermodynamic equilibrium at temperature T . Show that the pdf for the speed v of any particle in the gas is given by the Maxwell speed distribution:

$$f(v) = \sqrt{\frac{m^3}{2\pi T^3}} v^2 e^{-\frac{mv^2}{2T}} \vartheta(v).$$

Problem 5.41: Massless Ideal Gas. Consider a gas of N identical relativistic particles each of mass 0 in a volume $\mathbb{V}$ so that the single particle Hamiltonian is simply $\mathcal{H} = c|\vec{p}|$.

(a) Show that the partition function for single particle is:

$$Z_1 = \frac{\mathbb{V} T^3}{\pi^2 \hbar^3 c^3}.$$

(b) Show that in the thermodynamic limit the free energy of the system becomes:

$$\mathcal{F} = -NT - NT \ln \left(\frac{\mathbb{V} T^3}{\pi^2 \hbar^3 c^3 N} \right).$$

Thus explain that a relativistic massless ideal gas is thermodynamically just like a nonrelativistic ideal gas with $d = 3$.

(c) Show that the speed distribution for the massless gas is what you should expect:

$$f(v) = \delta(v - c) \vartheta(v).$$

Problem 5.42: ★ Lorentz Invariance of the Phase Space Density. Consider a relativistic free particle of mass m . For the purposes of this question you can work in one spatial dimension for simplicity, but the result is independent of this simplification. For this question we will use $c = 1$ units.

(a) Show that the solution to the equations of motion for the particle is:

$$x(t) = x(0) - t \frac{p(0)}{\sqrt{m^2 + p(0)^2}}, \quad p(t) = p(0).$$

Use this to show that the solution to the Liouville equation for the particle is:

$$f(t, x, p) = f \left(0, x + t \frac{p}{\sqrt{m^2 + p^2}}, p \right).$$

(b) Consider a Lorentz boost of the system by a velocity v . Let $X'(t')$ and $P'(t')$ indicate the Lorentz transformed position and momentum of the particle viewed as random variables. Explain that the transformed phase space density for the particle is:

$$f'(t', x', p') = \mathbb{E}((2\pi\hbar)\delta(x' - X'(t'))\delta(p' - P'(t'))).$$

Using the properties of the Dirac delta and the solutions to the equations of motion, show:

$$\delta(x' - X'(t')) = \frac{E'}{E} \delta \left(X(0) - \frac{E'x' - P'(t')t'}{E} \right), \quad \delta(p' - P'(t')) = \frac{E}{E'} \delta \left(P(0) - \gamma(p' - v\sqrt{p'^2 + m^2}) \right)$$

where:

$$E = \sqrt{|\vec{P}(t)|^2 + m^2}, \quad E' = \sqrt{|\vec{P}'(t')|^2 + m^2}.$$

- (c) With the above results demonstrate that the phase space density is Lorentz invariant:

$$f'(t', x', p') = f(t, x, p)$$

where t', x', p' are related to t, x, p exactly as usual by Lorentz transformation. Explain how this result could have been anticipated using our established results about canonical transformations and their effect on the phase space volume measure. Explain how a corresponding calculation can be performed to demonstrate that the phase space density of a Galilean particle is Galilean invariant.

Problem 5.43: ★ Relativistic Ideal Gas. Consider a gas of N identical relativistic particles with no internal degrees of freedom each of mass m in a volume $\mathbb{V}$.

- (a) Show that the partition function for single particle is:

$$Z_1 = \frac{cm^2\mathbb{V}T}{2\pi^2\hbar^3} K_2\left(\frac{mc^2}{T}\right)$$

where the modified Bessel functions of the second kind $K_\alpha(x)$ are defined by:

$$K_\alpha(x) = \int_0^\infty e^{-x \cosh t} \cosh(\alpha t) dt.$$

- (b) Show that in the thermodynamic limit the free energy of the system becomes:

$$\mathcal{F} = -NT - NT \ln \left(\frac{cm^2\mathbb{V}T}{2\pi^2\hbar^3 N} K_2\left(\frac{mc^2}{T}\right) \right).$$

- (c) Show that in the low temperature limit $T \ll mc^2$ this free energy precisely reproduces the nonrelativistic gas free energy:

$$\mathcal{F} = -NT - NT \ln \left(\frac{\mathbb{V}}{N} \left(\frac{mT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \right) + mc^2 N$$

with appropriate energy shift due to the difference in the inclusion of the mc^2 rest energy in the relativistic versus nonrelativistic Hamiltonian. To do this the large argument behavior of $K_\alpha(x)$ will be helpful:

$$K_\alpha(x) = \sqrt{\frac{\pi}{2x}} e^{-x} \left(1 + \mathcal{O}\left(\frac{1}{x}\right) \right).$$

- (d) Show that in the high temperature limit $T \gg mc^2$ this free energy precisely reproduces the massless gas free energy:

$$\mathcal{F} = -NT - NT \ln \left(\frac{\mathbb{V}T^3}{\pi^2\hbar^3 c^3 N} \right).$$

To do this the small argument behavior of $K_\alpha(x)$ will be helpful:

$$K_\alpha(x) = \frac{\Gamma(\alpha)}{2} \left(\frac{2}{x} \right)^\alpha (1 + \mathcal{O}(x)).$$

- (e) Show that the speed distribution for the relativistic gas is:

$$f(v) = \frac{m}{cTK_2\left(\frac{mc^2}{T}\right)} \gamma^5 v^2 e^{-\frac{\gamma mc^2}{T}}.$$

This is known as the Jüttner speed distribution.

- (f) Let $f_0^{(3)}(\vec{p}_0)$ be the probability distribution of the momentum 3-vector $\vec{p}_0$ of a single particle in the frame of the box. For the rest of this question we will use $c = 1$ units. Show that:

$$f_0^{(3)}(\vec{p}_0) = \frac{e^{-\beta\sqrt{|\vec{p}_0|^2 + m^2}}}{4\pi m^2 T K_2\left(\frac{m}{T}\right)}.$$

Show that this is the average rest frame of the box (meaning that the expectation of the particle 3-velocity is 0 in this frame) and the center of momentum frame of the system (meaning that the expectation of the particle 3-momentum is 0 in this frame).

- (g) Let $f^{(3)}(\vec{p})$ be the distribution of the momentum 3-vector $\vec{p}$ of a single particle in a general frame Lorentz boosted by a velocity $\vec{v}$ from the frame of the box. Show that:

$$f^{(3)}(\vec{p}) = \frac{\sqrt{|\vec{p}_0|^2 + m^2}}{\sqrt{|\vec{p}|^2 + m^2}} f_0^{(3)}(\vec{p}_0).$$

where $\vec{p}$ is related to $\vec{p}_0$ as usual through a Lorentz boost by $\vec{v}$.

- (h) Define the quantity $f^{(4)}(\vec{p})$ by:

$$f^{(4)}(\vec{p}) = 2\sqrt{|\vec{p}|^2 + m^2} f^{(3)}(\vec{p}).$$

Show that the expectation of a function g of momentum can be computed by:

$$\mathbb{E}(g) = \int_{\mathbb{R}^3} g(\vec{p}) f^{(4)}(\vec{p}) \frac{d^3\vec{p}}{2\sqrt{|\vec{p}|^2 + m^2}}$$

and that the integral measure:

$$d\Pi(\vec{p}) = \frac{d^3\vec{p}}{2\sqrt{|\vec{p}|^2 + m^2}}$$

is Lorentz invariant. This Lorentz invariant integral measure will be useful for us in many different contexts.

- (i) Let u^μ be the 4-velocity of a particular frame relative to the box's frame and let $p^\mu = (\sqrt{|\vec{p}|^2 + m^2}, \vec{p})^\mu$ be the usual 4-momentum vector of the particle. Show that $f^{(4)}(\vec{p})$ is given by:

$$f^{(4)}(\vec{p}) = \frac{|u \cdot p|}{2\pi m^2 T K_2\left(\frac{m}{T}\right)} e^{\frac{u \cdot p}{T}}.$$

Thus using this distribution with the Lorentz invariant measure $d\Pi(\vec{p})$ and defining the temperature T to be Lorentz invariant this gives the appropriate momentum distribution for a particle in thermodynamic equilibrium in an arbitrary reference frame. (There has historically been some confusion on the Lorentz transformation property of temperature. The temperature T above is the temperature in the center of momentum frame and in order to determine what temperature is in another frame one has to define what is meant by temperature in a general frame. The coefficients $\beta^\mu = \frac{u^\mu}{T}$ form a 4-vector as seen in the exponential and $T = \frac{1}{-\beta^\mu \beta_\mu}$ which we take to be the definition of the temperature in a general frame, thus making it Lorentz invariant by definition. We will always use this definition.)

- (j) Show that for a function $g(\vec{p})$:

$$\int_{\mathbb{R}^3} g(\vec{p}) d\Pi(\vec{p}) = \int_{\mathbb{R}^4} g(\vec{p}) \vartheta(p^0) \delta(p^2 + m^2) d^4p$$

where on the right hand side p^0 is added as an independent integration variable. Show that the sign of p^0 is Lorentz invariant when p^μ on the right hand side is Lorentz transformed as a 4-vector. Thus, define the “positive energy on shell Dirac delta”:

$$\delta_+(p^2 + m^2) = \vartheta(p^0) \delta(p^2 + m^2) = \vartheta(p^0) \delta(|\vec{p}|^2 + m^2 - (p^0)^2)$$

and explain that it is Lorentz invariant. Finally then, show that expectations of functions of momenta can be written in an explicitly Lorentz invariant way as:

$$\mathbb{E}(g) = \int_{\mathbb{R}^4} g(p) f^{(4)}(p) \delta_+(p^2 + m^2) d^4p.$$

- (k) Let $\mathcal{U}(T)$ be the expected energy of a particle in the box rest frame. Show that in a general frame with 4-velocity u^μ the expected momentum of the distribution is given by:

$$\mathbb{E}(p^\mu) = \mathcal{U}(T) u^\mu.$$

Problem 5.44: Oscillating piston. Consider N gas particles of mass m and adiabatic ratio γ in a cylinder with cross sectional area A and a piston of mass M sitting atop the column of gas. We assume that the gas cannot escape from under the piston. Let z be the height the piston sits above the base of the column and P be the conjugate momentum to z (with p the pressure of the gas). Assume quasidynamics apply.

- (a) Assume that as the piston moves there is no heat transfer between it and the gas. Show that the entropy of the gas is constant and that as the piston moves pV^γ is constant. Show that the combined energy of

the gas piston system is:

$$E = \frac{P^2}{2M} + Mgz + \frac{NT}{\gamma - 1}$$

and that the equation of motions for the system are:

$$M\ddot{z} = p\mathbb{A} - Mg, \quad \frac{d}{dt}(pz^\gamma) = 0.$$

- (b) Show explicitly that the energy in the previous part can be written as:

$$E = \frac{P^2}{2M} + Mgz + \left(\frac{\ell}{z}\right)^{\gamma-1}$$

where ℓ is a constant determined by the microscopic properties of the gas, N , and the constant entropy S of the gas. Show that this form is appropriate for use with the quasidynamic equations of motion and that it reproduces those found in part (a).

- (c) Show that the mechanical equilibrium pressure of the gas is:

$$p = \frac{Mg}{\mathbb{A}}.$$

Suppose that the piston is sitting at rest at a height h . Show that for small deviations from that equilibrium height the system oscillates with angular frequency ω given by:

$$\omega^2 = \frac{\gamma g}{h}.$$

- (d) Assume that as the piston moves it experiences a damping force of $-\kappa\dot{z}$ from heat transfer with the piston. Show that the expression for the total energy is unchanged but the equations now become:

$$M\ddot{z} + \kappa\dot{z} = p\mathbb{A} - Mg, \quad \gamma p\dot{z} + \dot{p}z = \frac{\kappa(\gamma - 1)}{\mathbb{A}}\dot{z}^2.$$

5.10 Thermodynamic Processes and Stability

Let us now study the process of what happens when two thermodynamic systems are brought together to interact. There are many different important classes of such processes and these different classes of processes can be enforced by different experimental setups. One important class is the class of reversible processes. A process is reversible whenever the change in the entropy of system 1 plus the change in the entropy of system 2 is 0. That is:

$$\Delta S_1 + \Delta S_2 = 0 \iff \text{reversible.} \quad (5.10.1)$$

By the logic of section 5.7, no interacting process can be exactly reversible. But, we can sometimes take a process to be at least approximately reversible. The reason for the name reversible is because the sum of entropy changes when independent systems are brought together is guaranteed to be greater than or equal to 0 by the second law of thermodynamics, the only possible value of the change of entropy sum in a process which is allowed by that process and the inverse of that process (its reverse) is 0. Any process which is not reversible is called irreversible.

Another important class is the class of adiabatic processes. A process is adiabatic whenever there is no heat transfer between the systems. That is, in an adiabatic process:

$$dQ_1 = dQ_2 = 0 \iff \text{adiabatic.} \quad (5.10.2)$$

Importantly, reversibility and adiabaticity are completely independent concepts. There are reversible processes which are adiabatic, reversible processes which are not adiabatic, irreversible processes which are adiabatic, and irreversible processes which are not adiabatic. As well, it should be made clear that this adiabatic is not the same as the adiabatic used in the term “adiabatic invariant” defined in section 1.14. This adiabatic means no transfer of heat. The adiabatic invariants are quantities which change extremely slowly as a system is perturbed. They are simply unrelated⁶.

We have already introduced the idea of a quasistatic process. A system undergoes a quasistatic process if instantaneously at all points in the process the conditions in equation (5.9.1) hold (so that the system can be treated as “instantaneously in equilibrium”):

$$dQ = \frac{\partial E}{\partial S} dS, \quad F_{Ma} = \frac{\partial E}{\partial Q^a} \iff \text{quasistatic.} \quad (5.10.3)$$

Again, this is a completely distinct descriptor from reversible or adiabatic.

It is also common to consider isentropic processes. A system undergoes an isentropic process if in that process the system’s entropy does not change:

$$dS = 0 \iff \text{isentropic.} \quad (5.10.4)$$

This is distinct from reversible in which two systems interacted and the sum of their entropies did not change. In a reversible process the individual systems may have changing entropies, it is just the sum which cancels. For an isentropic process and individual system’s entropy does not change.

Another class is the class of isothermal processes. A system undergoes an isothermal process if in that process the system’s temperature does not change:

$$dT = 0 \iff \text{isothermal.} \quad (5.10.5)$$

In generalization of this, it is common to consider processes in which any thermodynamic variable x, X or thermodynamic force F, f is held constant. So, one may consider an “iso- x ”, “iso- X ”, “iso- F ”, or “iso- f ” process as any one which keeps a particular such variable or force constant:

$$dx^a = 0 \iff \text{iso-}x^a \quad (5.10.6)$$

$$dX^a = 0 \iff \text{iso-}X^a \quad (5.10.7)$$

$$dF_a = 0 \iff \text{iso-}F_a \quad (5.10.8)$$

$$df_a = 0 \iff \text{iso-}f_a. \quad (5.10.9)$$

Under different circumstances systems may be able to exchange different kinds of conserved quantities with each other and so there is vocabulary for that too. As always, a system is called isolated if it does not interact with anything outside of itself at all. As such, the Hamiltonian of that system describes its full

⁶They are not *completely* unrelated but they are certainly distinct. If a system is only perturbed slowly (adiabatically in the classical sense) then it can often be easier to ensure that no or negligible heat is transferred (adiabatic in the thermodynamic sense).

dynamics and all quantities to be conserved by that Hamiltonian are in fact conserved for that system. A system is called open if it does interact with some variables external to itself. Consequently, an open system may not have conserved quantities. If an open system conserves how many particles of each species are present within it, it is called thermodynamically closed. Otherwise, it is called thermodynamically open.

Let us now look at the most basic of thermodynamic processes between two systems: composition. Consider two thermodynamic systems which have the same coordinates X and are brought from being initially independent and individually in equilibrium into contact with each other and allowed to interact extremely weakly. We will assume all of the coordinates appearing in the energy are extensive by definition. If a coordinate x were not extensive we could simply define $X = Nx$ to be a new extensive coordinate and express the Hamiltonian in terms of it. In that way, we can always guarantee that this is possible. Now that we have $E(S, N, X)$ we can invert it to find $S(E, N, X)$. Then, in the limit of weak interactions all of the extensive quantities of the two systems including the entropy simply add in thermodynamic equilibrium and so:

$$E = E_1 + E_2, \quad S = S_1 + S_2, \quad N = N_1 + N_2, \quad X^a = X_1^a + X_2^a. \quad (5.10.10)$$

The total entropy is then:

$$S(E_1, E_2, N_1, N_2, X_1, X_2) = S_1(E_1, N_1, X_1) + S_2(E_2, N_2, X_2). \quad (5.10.11)$$

When the combined system has reached equilibrium the variation of the total entropy consistent with all of the constraints must vanish so as to be a maximum. So:

$$dS = \frac{\partial S_1}{\partial E_1} dE_1 + \frac{\partial S_1}{\partial N_1} dN_1 + \frac{\partial S_1}{\partial X_1^a} dX_1^a + \frac{\partial S_2}{\partial E_2} dE_2 + \frac{\partial S_2}{\partial N_2} dN_2 + \frac{\partial S_2}{\partial X_2^a} dX_2^a \stackrel{!}{=} 0. \quad (5.10.12)$$

All of the conserved extensive quantities then constrain the variations as:

$$dE_1 + dE_2 = 0, \quad dN_1 + dN_2 = 0, \quad dX_1^a + dX_2^a = 0 \quad (5.10.13)$$

$$\Rightarrow dS = \left(\frac{\partial S_1}{\partial E_1} - \frac{\partial S_2}{\partial E_2} \right) dE_1 + \left(\frac{\partial S_1}{\partial N_1} - \frac{\partial S_2}{\partial N_2} \right) dN_1 + \left(\frac{\partial S_1}{\partial X_1^a} - \frac{\partial S_2}{\partial X_2^a} \right) dX_1^a \stackrel{!}{=} 0. \quad (5.10.14)$$

If the systems are allowed to exchange all extensive quantities through interactions then the remaining variations are unconstrained and so in order for this to vanish for all allowed variations we must have:

$$\frac{\partial S_1}{\partial E_1} = \frac{\partial S_2}{\partial E_2}, \quad \frac{\partial S_1}{\partial N_1} = \frac{\partial S_2}{\partial N_2}, \quad \frac{\partial S_1}{\partial X_1^a} = \frac{\partial S_2}{\partial X_2^a}. \quad (5.10.15)$$

We can compute these partial derivatives explicitly from the total differential of E :

$$dE = TdS + \mu dN + f_a dX^a \quad (5.10.16)$$

$$\Rightarrow dS = \frac{1}{T} dE - \frac{\mu}{T} dN - \frac{f_a}{T} dX^a \quad (5.10.17)$$

$$\Rightarrow \frac{\partial S}{\partial E} = \frac{1}{T}, \quad \frac{\partial S}{\partial N} = -\frac{\mu}{T}, \quad \frac{\partial S}{\partial X^a} = -\frac{f_a}{T}. \quad (5.10.18)$$

Then, our equilibrium conditions become:

$$\frac{1}{T_1} = \frac{1}{T_2}, \quad -\frac{\mu_1}{T_1} = -\frac{\mu_2}{T_2}, \quad -\frac{f_{1a}}{T_1} = -\frac{f_{2a}}{T_2} \quad (5.10.19)$$

$$\Rightarrow T_1 = T_2, \quad \mu_1 = \mu_2, \quad f_{1a} = f_{2a}. \quad (5.10.20)$$

Thus, when two systems are put into contact the equilibrium state they will reach is when all of the intensive quantities conjugate to exchangeable extensive quantities of those two systems match.

In performing this calculation for equilibrium we required the variation of the entropy to vanish. However, we found earlier in 5.6 that equilibrium is given by the state of maximum entropy consistent with the constraints on a system. So, we now need to guarantee that this stationary point we have identified is in fact a maximum. This must mean that the entropy function $S(E, N, X)$ evaluated at the total quantities is greater than or equal to the sum of entropies of the individual systems for any way of apportioning the extensive quantities among those systems. That is, for all $\delta E, \delta N, \delta X^a$:

$$S(E, N, X) \geq S\left(\frac{E}{2} + \delta E, \frac{N}{2} + \delta N, \frac{X}{2} + \delta X\right) + S\left(\frac{E}{2} - \delta E, \frac{N}{2} - \delta N, \frac{X}{2} - \delta X\right). \quad (5.10.21)$$

Because this must hold for each E, N, X it must also hold at $2E, 2N, 2X$:

$$S(2E, 2N, 2X) \geq S(E + \delta E, N + \delta N, X + \delta X) + S(E - \delta E, N - \delta N, X - \delta X). \quad (5.10.22)$$

On the left hand side we can use the extensivity condition:

$$S(2E, 2N, 2X) = 2S(E, N, X) \quad (5.10.23)$$

to arrive at:

$$2S(E, N, X) \geq S(E + \delta E, N + \delta N, X + \delta X) + S(E - \delta E, N - \delta N, X - \delta X). \quad (5.10.24)$$

Because this condition is true for all $\delta E, \delta N, \delta X^a$ it is also true for $\varepsilon \delta E, \varepsilon \delta N, \varepsilon \delta X^a$ where ε is some real parameter. Then:

$$S(E + \varepsilon \delta E, N + \varepsilon \delta N, X + \varepsilon \delta X) - S(E, N, X) + S(E - \varepsilon \delta E, N - \varepsilon \delta N, X - \varepsilon \delta X) - S(E, N, X) \leq 0. \quad (5.10.25)$$

If we now divide by ε^2 and take the limit $\varepsilon \rightarrow 0$ using l'Hopital's rule twice (with the shorthand $\phi = (E, N, X)$):

$$\lim_{\varepsilon \rightarrow 0} \frac{S(E + \varepsilon \delta E, N + \varepsilon \delta N, X + \varepsilon \delta X) - S(E, N, X) + S(E - \varepsilon \delta E, N - \varepsilon \delta N, X - \varepsilon \delta X) - S(E, N, X)}{\varepsilon^2} \leq 0 \quad (5.10.26)$$

$$\implies \lim_{\varepsilon \rightarrow 0} \frac{S(\phi + \varepsilon \delta \phi) - S(\phi) + S(\phi - \varepsilon \delta \phi) - S(\phi)}{\varepsilon^2} \leq 0 \quad (5.10.27)$$

$$\implies \lim_{\varepsilon \rightarrow 0} \frac{\delta \phi^a \frac{\partial S}{\partial \phi^a}(\phi + \varepsilon \delta \phi) - \delta \phi^a \frac{\partial S}{\partial \phi^a}(\phi - \varepsilon \delta \phi)}{2\varepsilon} \leq 0 \quad (5.10.28)$$

$$\implies \lim_{\varepsilon \rightarrow 0} \frac{\delta \phi^a \delta \phi^b \frac{\partial^2 S}{\partial \phi^a \partial \phi^b}(\phi + \varepsilon \delta \phi) + \delta \phi^a \delta \phi^b \frac{\partial^2 S}{\partial \phi^a \partial \phi^b}(\phi - \varepsilon \delta \phi)}{2} \leq 0 \quad (5.10.29)$$

$$\implies \delta \phi^a \delta \phi^b \frac{\partial^2 S}{\partial \phi^a \partial \phi^b}(\phi) \leq 0 \quad (5.10.30)$$

$$\implies \boxed{d^2 S \leq 0}. \quad (5.10.31)$$

So, the condition of equilibrium on the entropy is that it must be a concave down function of all of its variables. This is known as the stability condition on the entropy. We generally don't work with the entropy function $S(E, N, X)$ directly and instead use one of the thermodynamic potentials. So, it is convenient to formulate this condition on the entropy in terms of the thermodynamic potentials. To do so it is easiest to start with the energy. The first and second variations of the energy are defined by:

$$dE = \left. \frac{dE}{d\varepsilon} (S + \varepsilon \delta S, N + \varepsilon \delta N, X + \varepsilon \delta X) \right|_{\varepsilon=0} \quad (5.10.32)$$

$$d^2 E = \left. \frac{d^2 E}{d\varepsilon^2} (S + \varepsilon \delta S, N + \varepsilon \delta N, X + \varepsilon \delta X) \right|_{\varepsilon=0}. \quad (5.10.33)$$

The total differential and second differential of the energy give:

$$dE = TdS + \mu dN + f_a dX^a \quad (5.10.34)$$

$$\implies d^2 E = dTdS + Td^2 S + d\mu dN + \mu d^2 N + df_a dX^a + f_a d^2 X^a. \quad (5.10.35)$$

Considering the entropy as a function of E, N, X the second variations of E, N, X are all 0 and so we have:

$$Td^2 S = -dSdT - d\mu dN - df_a dX^a. \quad (5.10.36)$$

Considering the energy as a function of S, N, X the second variations of S, N, X are all 0 and so we have:

$$d^2 E = dTdS + d\mu dN + df_a dX^a. \quad (5.10.37)$$

Thus, the second variations of the energy and entropy are related as:

$$d^2 E = -Td^2 S. \quad (5.10.38)$$

Because the entropy is concave down as a function of all of its variables, this means that the energy is a concave up (also called convex) function of all of its variables:

$$\boxed{d^2 E \geq 0}. \quad (5.10.39)$$

For many purposes, it is nice to formulate this condition in terms of the chemical potential. It is easiest to do this in terms of the Gibbs energy which is again given by:

$$G = E - TS - f_a X^a \quad (5.10.40)$$

$$\implies dG = -SdT + \mu dN - X^a df_a \quad (5.10.41)$$

$$\implies d^2G = -Sd^2T - dSdT + d\mu dN + \mu d^2N - dX^a df_a - X^a d^2f_a. \quad (5.10.42)$$

Again because G is a function of T, N, f_a , their second variations vanish and so:

$$d^2G = -dTdS - d\mu dN - dX^a df_a. \quad (5.10.43)$$

The Gibbs energy we found is related to the chemical potential by:

$$G = \mu N \quad (5.10.44)$$

$$\implies dG = Nd\mu + \mu dN \quad (5.10.45)$$

$$\implies d^2G = Nd^2\mu + 2d\mu dN + \mu d^2N. \quad (5.10.46)$$

Again $d^2N = 0$ because the Gibbs energy is written as a function of N . Equating these we have:

$$Nd^2\mu + 2d\mu dN = -dTdS + d\mu dN - dX^a df_a \quad (5.10.47)$$

$$\implies Nd^2\mu = -dTdS - d\mu dN - dX^a df_a = Td^2S \quad (5.10.48)$$

$$\implies \boxed{d^2\mu \leq 0}. \quad (5.10.49)$$

So, the condition of stability on the chemical potential is that it also must be a concave down function of all of its variables. The stability of the chemical potential is perhaps the most natural to check for many systems as the chemical potential is directly derived from the thermodynamic potentials without having to perform the nasty inverse function to compute $S(E, N, X)$.

All together then, when two systems are combined they will reach an equilibrium consistent with all of the constraints on the combined system in which the two subsystems have matching intensive quantities provided that their chemical potential is a concave down function of all of the intensive quantities of the system. What happens instead if the chemical potential is not a purely concave down function? Then, this stationary point we have found is not the maximum value of the entropy and not the stable equilibrium reached by the thermodynamic system.

5.10.1 Phase Transitions

Suppose we have derived some partition function Z (by integration over the microscopic phase space in the usual way) and from it we compute a Helmholtz energy, the expected energy, and then the entropy function $S(E, N, X)$. As was just proven, the condition of thermodynamic stability demands that this entropy function is purely concave down. The intensive thermodynamic quantities T, μ, f can be computed from the derivatives of S and then we can formulate all of the various thermodynamic potentials using the Legendre transformation. If at any point S changes concavity then one of the eigenvalues of its Hessian matrix (the matrix of second derivatives) must switch from negative to positive and thus pass through zero. Thus, the Hessian matrix loses invertibility at such a point (because in the diagonal basis the inverse just reciprocates the eigenvalues and $1/0$ is not defined). Consequently, in the neighborhood of such a point the Legendre transformation between the thermodynamic quantities cannot be completed as invertibility is lost. Normally we would invert the derivatives of S to compute the extensive quantities E, N, X in terms of the local intensive quantities T, μ, f . But, due to the loss of invertibility there will be multiple solutions (called branches) to the inversion problem. So, when concavity fails the thermodynamic system becomes inhomogeneous; some elements of the system will satisfy each different branch of the Legendre transformation.

Let there be B branches of the Legendre transformation and $\mu_b(T, f)$ be the chemical potential of branch b . Then, if the system consists of N total elements and each branch has N_b elements we have:

$$N = \sum_{b=1}^B N_b. \quad (5.10.50)$$

This mixture system will reach equilibrium at the maximum entropy state possible. By our previous reasoning this will require that all of the intensive quantities match among the branches which have nonzero N_b :

$$T_1 = \dots = T_B, \quad f_{1a} = \dots = f_{Ba}, \quad \mu_1 = \dots = \mu_B. \quad (5.10.51)$$

These different branches are called phases and whenever there is more than one nonzero N_b we have what is called phase coexistence. Phase coexistence occurs in a region of failed concavity of the entropy as that introduces the multiple branches. This can be understood graphically by plotting the entropy S versus the extensive variable Y against which it loses the property of being concave down. The entropy of the multi-branch system must be stable and thus never become concave up. So, on the plot of $S(Y)$ if one draws

the tangent line to each Y and S is always concave down, then those tangent lines will always overshoot $S(Y')$ for $Y' > Y$. If S is ever concave up then there will be a tangent line which makes contact at Y_0 and then makes contact again at a later $Y_1 > Y_0$. The system cannot always follow this naive entropy curve because it breaks the stability condition. The derivatives of the entropy give the intensive variables of the system and so when the system stops following the naive entropy curve it must leave the curve along a tangent line so as to continuously change the local quantities of the system. As well, when the system makes contact again later with the naive entropy curve it must do so along a tangent line. So, the multi-phase system must follow the particular tangent line which intersects the naive entropy curve twice rather than the underlying naive $S(Y)$ in order to preserve its concavity. In fact, this tangent line is the maximum entropy state consistent with all of the fixed extensive quantities. This linear region in the entropy is then the region of phase coexistence and one can explicitly compute the N_b at each point on the line. At one end, the system will be in a pure phase of one kind and at the other end the system will be in a pure phase of another branch. Crossing along this line is called a phase transition. This is shown graphically in 5.1

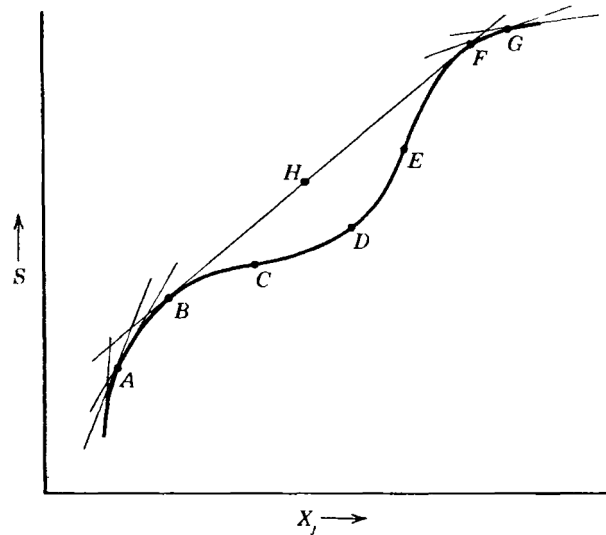


Figure 5.1: Figure taken from [13]. The thick curve represents the naive entropy curve computed from the naive partition function versus an extensive quantity X_j (which we called Y). At the points A and G the entropy is stable and the naive curve represents the actual entropy of the system in equilibrium. The curve $BCDEF$ is unstable because of the concavity of the entropy in that region. Notice that the entropy is actually still concave down at B and F . However, the tangent line at B meets the entropy curve later at F also as a tangent line (and it is the unique line which is tangent at two points). Therefore, by the argument given in the text, the entropy curve followed by the system is $ABHFG$. Between the points B and F the system is in a mixture of two phases, one phase determined by the branch at B and the other phase determined by the branch at F . The construction $ABHFG$ is called the “superior tangent envelope” of the naive entropy curve.

In general, whenever the qualitative behavior of a thermodynamic system changes as one of its parameters is changed the system is said to undergo a phase transition. So, they are quite a general phenomenon which come in many types. Unfortunately, it is very difficult to find systems (even toy models) with phase transitions that can be computed analytically and so most phase transitions are understood with computer assistance.

Theorem 5.9: Stability of Thermodynamic Equilibrium

When two systems are brought into contact, the thermodynamic equilibrium they will reach is when all of their intensive quantities which are conjugate to extensive quantities that may be exchanged between them match.

When the expected energy of a system is written in terms of extensive quantities only, it is purely a concave up function in thermodynamic equilibrium:

$$d^2E \geq 0. \quad (5.10.52)$$

Consequently, the entropy and chemical potentials written in terms of their appropriate variables after

Legendre transformations are both purely concave down functions in thermodynamic equilibrium:

$$d^2 S \leq 0, \quad d^2 \mu \leq 0. \quad (5.10.53)$$

5.10.2 Example: Van der Waals Fluid

The Ideal Gas is sometimes too ideal. By including no interparticle interactions, the ideal gas doesn't undergo any phase transitions. The Van der Waals fluid is the closest approximation to an ideal gas which intends to capture (at least qualitatively) the transition of a gas into a liquid. There are many quantitatively better models for the liquid-gas transition but they are generally significantly more complicated and rely more on the specific substance being modeled. Similarly to the ideal gas, let us suppose we have N identical nonrelativistic particles with positions $\vec{x}_1(t), \dots, \vec{x}_N(t)$ moving in a container of volume $\mathbb{V}$. These particles may still have some internal degrees of freedom $\mathbf{q}, \mathbf{p}$ each which we again assume have been defined so that they are unchanged by translations, boosts, or rotations of the overall system. Each particle will contribute $\frac{|\vec{p}_k|^2}{2m} + h(\mathbf{q}_k, \mathbf{p}_k)$. h cannot depend on the positions or momenta of the particles due to translational symmetry and Galilean boost symmetry and we still assume that the internal degrees of freedom have a quadratic free Hamiltonian that we have put in the form of equation (5.9.48). All of the interactions we studied before with Galilean symmetry (meaning electrostatics and Newtonian gravity) in chapter 3 gave that the interparticle interactions is be pairwise (meaning there are only interactions between two particles, no three particle or higher particle interactions) and that it adds a term to the Hamiltonian which only depends on $|\vec{x}_k - \vec{x}_l|$ for the two particles, not on their momenta (to establish this see problem 3.69). Then, we take the full Hamiltonian for the system of particles to be:

$$\mathcal{H} = \sum_{k=1}^N \left(\frac{|\vec{p}_k|^2}{2m} + \sum_{j=1}^{d_1} \left(\frac{(\mathbf{p}^j)^2 + \omega_j^2 (\mathbf{q}^j)^2}{2} \right) \right) + \sum_{k=1}^{N-1} \sum_{l=k+1}^N U(|\vec{x}_k - \vec{x}_l|, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l) \quad (5.10.54)$$

where U is some function called the two particle potential which characterizes the interparticle interactions. This Hamiltonian is the very same form as the theory in equation (3.4.87), with the additional possibility of internal structure and non-point-particles.

So far this is quite a generic Hamiltonian for describing nonrelativistic interactions. The specific form taken for the Van der Waals fluid is to approximate the interparticle as only depending on the distance between the particles and being an extremely strong repulsion for small distances and a weak attraction for medium to large distances. Close up this strong repulsion is modeled as a hard sphere collision like in problem 3.56, meaning that if the particles are less than a critical distance D apart the potential is taken to be arbitrarily large (∞). For distances greater than D , the potential is assumed to decay in strength with distance. This gives a potential of the form:

$$U(r, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l) = \begin{cases} \infty, & r < D \\ u_0(r), & r > D \end{cases} \quad (5.10.55)$$

where $u_0(r)$ is some function which goes to 0 sufficiently quickly for large r . We will assume that u_0 is always near enough to 0 to series expand treating it as small. Then, the partition function for the N particles is:

$$Z_N = \frac{1}{N!} \int e^{-\beta \mathcal{H}} d\mathbb{P}_{\text{distinct}}. \quad (5.10.56)$$

Everything except the potential part of the Hamiltonian integrates exactly like in the case of the ideal gas and so performing everything except the position integrals gives:

$$Z_N = \frac{1}{N!} \frac{(2\pi)^{d_2}}{\hbar^{3+d_1}} \frac{\prod_{j=d_2+1}^{d_1} \ell_j}{\prod_{j=1}^{d_2} \omega_j} m^{\frac{3}{2}} \left(\frac{T}{2\pi} \right)^{\frac{3+d}{2}} \int_{\mathbb{V}^N} e^{-\frac{\beta}{2} \sum_{k=1}^N \sum_{l=1, l \neq k}^N U(|\vec{x}_k - \vec{x}_l|)} d^3 \vec{x}_1 \dots d^3 \vec{x}_N. \quad (5.10.57)$$

Define the same constant κ as in the ideal gas and also define $\mathbb{M}$ to be the set of all points in the set $\mathbb{V}^N$ in which none of the particles are closer than D to each other. Any of the points where the particles are closer than D do not contribute to the partition function as for them the exponential immediately decays to 0. Then:

$$Z_N = \frac{1}{N!} \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2} N} \int_{\mathbb{M}} e^{-\frac{\beta}{2} \sum_{k=1}^N \sum_{l=1, l \neq k}^N u_0(|\vec{x}_k - \vec{x}_l|)} d^3 \vec{x}_1 \dots d^3 \vec{x}_N. \quad (5.10.58)$$

The remaining integration would be enormously complicated to do exactly and so instead we will approximate for small u_0 . Expanding the exponential:

$$Z_N = \frac{1}{N!} \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}N} \int_{\mathbb{M}} \left(1 - \frac{\beta}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N u_0(|\vec{x}_k - \vec{x}_l|) + \mathcal{O}(u_0^2) \right) d^3\vec{x}_1 \dots d^3\vec{x}_N. \quad (5.10.59)$$

The integral of 1 over $\mathbb{M}$ can be computed directly. Each particle occupies an effective volume of $\nu = \frac{4\pi D^3}{3}$, meaning that when a particle is placed at a point no other particle can be placed within the ball of volume ν centered around the first particle. So, the first integral over $d^3\vec{x}_1$ gives a factor $\mathbb{V}$ as it may be anywhere but the second integral over $d^3\vec{x}_2$ gives a factor $\mathbb{V} - \nu$ as the second particle cannot be placed within a distance D of the first. This pattern continues to reduce the available volume by ν for each added particle. Thus:

$$\int_{\mathbb{M}} d^3\vec{x}_1 \dots d^3\vec{x}_N = \mathbb{V}(\mathbb{V} - \nu)(\mathbb{V} - 2\nu) \dots (\mathbb{V} - (N-1)\nu) = \prod_{k=0}^{N-1} (\mathbb{V} - k\nu). \quad (5.10.60)$$

The linear in u_0 integral can approximately be computed. Due to the symmetry of renaming the particles, each term in the series contributes exactly the same amount:

$$\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \int_{\mathbb{M}} u_0(|\vec{x}_k - \vec{x}_l|) d^3\vec{x}_1 \dots d^3\vec{x}_N = \frac{N(N-1)}{2} \int_{\mathbb{M}} u_0(|\vec{x}_1 - \vec{x}_2|) d^3\vec{x}_1 \dots d^3\vec{x}_N. \quad (5.10.61)$$

The integrals over $\vec{x}_3$ through $\vec{x}_N$ are unchanged from the previous integral because the potential does not depend on them. So:

$$\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \int_{\mathbb{M}} u_0(|\vec{x}_k - \vec{x}_l|) d^3\vec{x}_1 \dots d^3\vec{x}_N = \frac{N(N-1)}{2} \left(\prod_{k=2}^{N-1} (\mathbb{V} - k\nu) \right) \int u_0(|\vec{x}_1 - \vec{x}_2|) d^3\vec{x}_1 d^3\vec{x}_2. \quad (5.10.62)$$

The remaining integration is only over all of $\mathbb{V}$ for particle 1 and all of $\mathbb{V}$ except for the volume ν around particle 1 for particle 2. We can approximately perform this integration by changing to the new variables:

$$\vec{X} = \frac{\vec{x}_1 + \vec{x}_2}{2}, \quad \vec{x} = \vec{x}_2 - \vec{x}_1 \quad (5.10.63)$$

$$\Rightarrow \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \int_{\mathbb{M}} u_0(|\vec{x}_k - \vec{x}_l|) d^3\vec{x}_1 \dots d^3\vec{x}_N = \frac{N(N-1)}{2} \left(\prod_{k=2}^{N-1} (\mathbb{V} - k\nu) \right) \int u_0(|\vec{x}|) d^3\vec{x} d^3\vec{X}. \quad (5.10.64)$$

For large volume $\mathbb{V}$ (so that effects near the boundary are small), the approximate regions of integration for the average $\vec{X}$ becomes simply the volume $\mathbb{V}$ and the region of integration for the difference $\vec{x}$ becomes distances greater than D up until the edge of the container. If the potential u_0 decays quickly enough for $r > D$, we can extend the upper distance limit to ∞ with negligible error. Then, in this approximation:

$$\int u_0(|\vec{x}|) d^3\vec{x} d^3\vec{X} \approx \mathbb{V} \int_D^\infty 4\pi r^2 u_0(r) dr. \quad (5.10.65)$$

Thus we can introduce a new parameter ε from this integral and arrive at:

$$\varepsilon = -\frac{1}{2} \int_D^\infty 4\pi r^2 u_0(r) dr \quad (5.10.66)$$

$$\Rightarrow \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \int_{\mathbb{M}} u_0(|\vec{x}_k - \vec{x}_l|) d^3\vec{x}_1 \dots d^3\vec{x}_N \approx -\frac{\varepsilon N(N-1)}{(\mathbb{V} - \nu)} \prod_{k=0}^{N-1} (\mathbb{V} - k\nu). \quad (5.10.67)$$

The potential u_0 is required to limit to 0 for large r faster than $\frac{1}{r^3}$ for this integral to converge. Returning this to equation (5.10.59) gives:

$$Z_N \approx \frac{1}{N!} \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}N} \left(\prod_{k=0}^{N-1} (\mathbb{V} - k\nu) \right) \left(1 + \frac{\beta \varepsilon N(N-1)}{(\mathbb{V} - \nu)} + \mathcal{O}(u_0^2) \right). \quad (5.10.68)$$

The higher order terms $\mathcal{O}(u_0^2)$ here in the Van der Waals approximation are assumed to be approximately

captured by exponentiation of the first term:

$$1 + \frac{\beta \varepsilon N(N-1)}{(\mathbb{V} - \nu)} + \mathcal{O}(u_0^2) = e^{\frac{\beta \varepsilon N(N-1)}{(\mathbb{V} - \nu)}} + \mathcal{O}(u_0^2) \quad (5.10.69)$$

and so using this exponential form we neglect any other higher order effects. In the Van der Waals approximation then we take the partition function to be:

$$Z_N = \frac{1}{N!} \left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}N} e^{\frac{\beta \varepsilon N(N-1)}{(\mathbb{V} - \nu)}} \left(\prod_{k=0}^{N-1} (\mathbb{V} - k\nu) \right). \quad (5.10.70)$$

Before taking the thermodynamic limit then the N particle free energy is given by:

$$\mathcal{F}_N = -T \ln Z_N = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \mathbb{V} \right) + T \ln N! - \frac{\varepsilon N(N-1)}{(\mathbb{V} - \nu)} - T \sum_{k=0}^{N-1} \ln \left(1 - k \frac{\nu}{\mathbb{V}} \right). \quad (5.10.71)$$

To take the thermodynamic limit here it is nice to introduce the number density $n = \frac{N}{\mathbb{V}}$ because it remains fixed in the limit. Then, using Sterling's function:

$$\frac{\mathcal{F}_N}{N} = -T \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{1}{n} \right) - T \ln N + \frac{T}{N} \ln(\sqrt{2\pi N} \text{St}(N) N^N e^{-N}) - \frac{\varepsilon(N-1)}{(\frac{N}{n} - \nu)} - \frac{T}{N} \sum_{k=0}^{N-1} \ln \left(1 - k \frac{n\nu}{N} \right). \quad (5.10.72)$$

In the thermodynamic limit $N \rightarrow \infty$ then:

$$\frac{\mathcal{F}}{N} = -T \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{1}{n} \right) - T - \varepsilon n - T \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=0}^{N-1} \ln \left(1 - k \frac{n\nu}{N} \right). \quad (5.10.73)$$

The limit of the sum here becomes a Riemann sum in the thermodynamic limit. Define the variable $h = \frac{k n \nu}{N}$. Then, the sum bounds are from $h = 0$ to $h = \frac{N-1}{N} n \nu$ and the increment of h per term in the sum is $\Delta h = \frac{n\nu}{N}$. Thus:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=0}^{N-1} \ln \left(1 - k \frac{n\nu}{N} \right) = \lim_{N \rightarrow \infty} \sum_{\substack{h=0 \\ \Delta h = \frac{n\nu}{N}}}^{\frac{N-1}{N} n \nu} \ln(1-h) \frac{\Delta h}{n\nu} = \int_0^{n\nu} \ln(1-h) \frac{dh}{n\nu} \quad (5.10.74)$$

$$= -1 - \frac{1 - n\nu}{n\nu} \ln(1 - n\nu). \quad (5.10.75)$$

Thus:

$$\boxed{\mathcal{F} = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{\mathbb{V}}{N} \right) - \frac{\varepsilon N^2}{\mathbb{V}} + \frac{\mathbb{V}T}{\nu} \left(1 - \frac{N\nu}{\mathbb{V}} \right) \ln \left(1 - \frac{N\nu}{\mathbb{V}} \right).} \quad (5.10.76)$$

This free energy is not the usual Van der Waals free energy but instead an “improved” expression which better captures the effects of the excluded volume from the hard spheres interaction. In order to get here we only accurately tracked the u_0 dependence to linear order in u_0 which translates to linear order in ε . Thus, this expression receives corrections $\mathcal{O}(\varepsilon^2)$ which we haven't calculated. For the purposes of studying the qualitative behavior of this free energy it is also useful to consider that typically the occupied volume $N\nu$ is very small compared to the volume of the container $\mathbb{V}$. Then, we can perform the series expansion:

$$\mathcal{F} = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \frac{\mathbb{V}}{N} \right) - \frac{\varepsilon N^2}{\mathbb{V}} - NT + \frac{N^2 T \nu}{2\mathbb{V}} + \mathcal{O}(\nu^2) + \mathcal{O}(\varepsilon^2) \quad (5.10.77)$$

$$= -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \left(\frac{\mathbb{V}}{N} - \frac{\nu}{2} \right) \right) - \frac{\varepsilon N^2}{\mathbb{V}} - NT + \mathcal{O}(\nu^2, \varepsilon^2). \quad (5.10.78)$$

The final expression for the free energy here is equivalent to our previous free energy up to order ε^2 and ν^2 and it is the standard free energy used for the Van der Waals model. Going forward we will take this free energy to be the Van der Waals (VdW) free energy by definition:

$$\boxed{\mathcal{F}_{\text{VdW}} = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{3+d}{2}} \left(\frac{\mathbb{V}}{N} - \frac{\nu}{2} \right) \right) - \frac{\varepsilon N^2}{\mathbb{V}} - NT} \quad (5.10.79)$$

because it is a good toy model to understand phase transitions, although imperfect in its ability to precisely describe real fluids. We make this simplification only because this simplified toy model is pedagogically instructive, not because it is actually a reasonable approximation to make in general from equation (5.10.76). Immediately, the pressure is given by:

$$p = -\frac{\partial \mathcal{F}}{\partial \mathbb{V}} = \frac{NT}{\mathbb{V} - \frac{\nu N}{2}} - \frac{\varepsilon N^2}{\mathbb{V}^2}. \quad (5.10.80)$$

This gives us what is commonly called the Van der Waals equation of state:

$$\left(p + \frac{\varepsilon N^2}{\mathbb{V}^2}\right) \left(\mathbb{V} - \frac{\nu N}{2}\right) = NT. \quad (5.10.81)$$

Generally we would use this to invert and compute the volume from the local intensive conditions p, T . The VdW equation of state can be rearranged to give:

$$p \left(\frac{\mathbb{V}}{N}\right)^3 - \left(\frac{\nu p}{2} + T\right) \left(\frac{\mathbb{V}}{N}\right)^2 + \varepsilon \frac{\mathbb{V}}{N} - \frac{\varepsilon \nu}{2} = 0 \quad (5.10.82)$$

which is a cubic equation for the volume in terms of the other variables. This is like the ideal gas law but with a shift in the pressure due to the interparticle attraction and a shift in the volume due to the excluded volume from the hard spheres interaction. Real cubics have either 1 or 3 real solutions (counting repeated roots with their multiplicities) and so it is possible, at least for some values of p and T , that it is not possible to perform the inversion and compute the volume from p and T . Thus, this system may have a phase transition. Because this equation only depends on the combination $\frac{\mathbb{V}}{N}$ it is nice to define the available volume per particle $\mathbb{V}_1$ (which is the reciprocal of the number density):

$$\mathbb{V}_1 \stackrel{\text{def}}{=} \frac{\mathbb{V}}{N} \quad (5.10.83)$$

$$\implies p = \frac{T}{\mathbb{V}_1 - \frac{\nu}{2}} - \frac{\varepsilon}{\mathbb{V}_1^2}. \quad (5.10.84)$$

By definition, we need $\mathbb{V} > N\nu$ so that there is any allowed region of phase space for the particles to exist in. Consequently, we only need to consider $\mathbb{V}_1 > \nu$. In order for it to be possible to invert $p(\mathbb{V}_1)$ in order to find a well defined $\mathbb{V}_1(p)$ it must be the case that no two $\mathbb{V}_1 > \nu$ produce the same p . If two such $\mathbb{V}_1$ do exist then on the interval between them the average value of the derivative $\frac{\partial p}{\partial \mathbb{V}_1}$ is necessarily 0. By the mean value theorem a continuous function hits its average value on the interval somewhere in that interval. Therefore, if $p(\mathbb{V}_1)$ is not invertible its derivative must vanish somewhere. Conversely, if that derivative does vanish somewhere then automatically in the neighborhood of that point $p(\mathbb{V}_1)$ is not invertible. So, $p(\mathbb{V}_1)$ is invertible if and only if there is no $\mathbb{V}_1$ so that $\frac{\partial p}{\partial \mathbb{V}_1}$ is 0. (This argument is simply the inverse function theorem.) That derivative is given by:

$$\frac{\partial p}{\partial \mathbb{V}_1} = -\frac{T}{(\mathbb{V}_1 - \frac{\nu}{2})^2} + \frac{2\varepsilon}{\mathbb{V}_1^3}. \quad (5.10.85)$$

Let $y > \nu$ be a value of $\mathbb{V}_1$ so that this derivative vanishes, if such a value exists. Then:

$$p \text{ not invertible} \iff \exists y > \nu \mid Ty^3 = 2\varepsilon \left(y - \frac{\nu}{2}\right)^2. \quad (5.10.86)$$

Define the function $f(y)$:

$$f(y) = Ty^3 - 2\varepsilon \left(y - \frac{\nu}{2}\right)^2. \quad (5.10.87)$$

For $T > 0$ and $\varepsilon > 0$ we have immediately that $f(\frac{\nu}{2}) > 0$ and that $f(0) < 0$. Therefore, by the intermediate value theorem $f(y)$ must always have at least one root between 0 and $\frac{\nu}{2}$. In general it is straightforward to characterize the number of real solutions to a cubic equation in a way similar to a quadratic. For a cubic equation with real coefficients:

$$ax^3 + bx^2 + cx + d = 0 \quad (5.10.88)$$

the discriminant Δ is defined by:

$$\Delta = b^2c^2 - 4ac^3 - 4b^3d - 27a^2d^2 + 18abcd. \quad (5.10.89)$$

If the discriminant is positive then the cubic has three distinct real roots, if the discriminant is 0 then the cubic has one real root of multiplicity one and one real root of multiplicity two, and if the discriminant is

negative then the cubic has only one real root. For $f(y)$ the discriminant is then:

$$\Delta = \frac{27\varepsilon^2\nu^4}{4}T\left(\frac{16\varepsilon}{27\nu} - T\right). \quad (5.10.90)$$

For $T > \frac{16\varepsilon}{27\nu}$ this discriminant is negative and so $f(y)$ has only one real solution, which we know by our previous analysis to be between 0 and $\frac{\nu}{2}$ and so it is outside of the physical region. Consequently, for $T > \frac{16\varepsilon}{27\nu}$ equation (5.10.85) has no physical values where invertibility fails, allowing the Legendre transformation to be completed. For $T < \frac{16\varepsilon}{27\nu}$ this discriminant is positive and so $f(y)$ has three real solutions, one of which is necessarily in the unphysical region by our previous analysis. At $T = \frac{16\varepsilon}{27\nu}$ we can easily factorize $f(y)$:

$$T = \frac{16\varepsilon}{27\nu} \implies f(y) = \frac{16\varepsilon}{27\nu} \left(y - \frac{3}{2}\nu\right)^2 \left(y - \frac{3}{8}\nu\right) \quad (5.10.91)$$

and so we can explicitly see that there is a double root in the physical region and a single root in the unphysical region we knew had to be there. For $T > \frac{16\varepsilon}{27\nu}$ instead of a double root in the physical region there will be two distinct roots in the physical region. It is impossible for a root to move from being greater than $\frac{\nu}{2}$ to being less than $\frac{\nu}{2}$ as T is varied because in order to do so there would have to be a value of T for which $\frac{\nu}{2}$ is a root but for all positive T its immediately true that $f(\frac{\nu}{2}) > 0$. With this analysis together we have that for $T > \frac{16\varepsilon}{27\nu}$ it is possible to uniquely compute the volume from the pressure and so there is only one phase of the fluid for such temperatures while for $T < \frac{16\varepsilon}{27\nu}$ there are two distinct real roots for $f(y)$ in the physical region and consequently two values of the volume for which the pressure loses local invertibility, thus making it possible for such temperatures to allow multiple phases (meaning some parts of the fluid to be in each branch of the inverse). Thus, the qualitative properties of the fluid change at this critical temperature. For the VdW fluid then the critical temperature is defined as:

$$T_c = \frac{16\varepsilon}{27\nu}. \quad (5.10.92)$$

By the factorization of $f(y)$ at this temperature, at the critical temperature the two physical volumes at which the pressure volume relation loses local invertibility actually coincide and define the critical volume:

$$\mathbb{V}_c = \frac{3}{2}\nu N. \quad (5.10.93)$$

At the critical volume and temperature the corresponding pressure is called the critical pressure:

$$p_c = \frac{NT_c}{\mathbb{V}_c - \frac{N\nu}{2}} - \frac{N^2\varepsilon}{\mathbb{V}_c^2} = \frac{4\varepsilon}{27\nu^2}. \quad (5.10.94)$$

Away from the critical values the VdW can be very nicely analyzed by defining the relative temperature $\mathfrak{t}$, relative volume $\mathfrak{v}$, and relative pressure $\mathfrak{p}$ by the ratio of the actual values to the critical values:

$$\mathfrak{t} = \frac{T}{T_c}, \quad \mathfrak{v} = \frac{\mathbb{V}}{\mathbb{V}_c}, \quad \mathfrak{p} = \frac{p}{p_c}. \quad (5.10.95)$$

In terms of the reduced values the VdW equation of state becomes:

$$\left(\mathfrak{p} + \frac{3}{\mathfrak{v}^2}\right)(3\mathfrak{v} - 1) = 8\mathfrak{t}. \quad (5.10.96)$$

Interestingly this reduced VdW equation no longer depends on the parameters ε or ν , which were the only constant parameters of the free energy. Therefore, this reduced form of the VdW equation is the same for all VdW fluids.

It is possible to explicitly compute all three complex branches of $\mathfrak{v}$ in terms of $\mathfrak{p}$ and $\mathfrak{t}$ using the cubic formula. However, this expression is so complicated as to be essentially useless outside of numerical applications. It may seem that below the critical temperature there will be a coexistence of three phases in the fluid. However, one of the three branches is unstable. For $\mathbb{V}_1$ near $\frac{\nu}{2}$ or very large the first term in equation (5.10.84) dominates the second and so p can be quickly seen to be decreasing for such $\mathbb{V}_1$. Because the same value of p is gotten at exactly three different $\mathbb{V}_1$, p must be decreasing at the lowest and highest such $\mathbb{V}_1$ and increasing at the middle one. Thus, at the middle solution uniquely the derivative of p with respect to $\mathbb{V}$ is positive. By equation (5.9.69):

$$p = -\frac{\partial E}{\partial \mathbb{V}} \implies \frac{\partial p}{\partial \mathbb{V}} = -\frac{\partial^2 E}{\partial \mathbb{V}^2}. \quad (5.10.97)$$

By equation (5.10.39) the second variation of the energy is necessarily positive which from above considering

a volume variation means that $\frac{\partial p}{\partial \mathbb{V}}$ is necessarily negative. Consequently, the middle solution where this is false is not allowed (the number of particles in the middle branch is always 0). Below the critical temperature then there is a coexistence of two phases, a phase with higher volume per particle $\mathbb{V}_{1g}$ called the gas phase and a phase with lower volume per particle $\mathbb{V}_{1l}$ called the liquid phase. These are the values of $\mathbb{V}_1$ satisfying equation (5.10.84) for a given p and T for which $\frac{\partial p}{\partial \mathbb{V}_1}$ is negative. This gives $\mathbb{V}_{1g}(p, T)$ and $\mathbb{V}_{1l}(p, T)$.

By the logic given in this section's discussion of phase transitions, along each of these two branches we can compute the volume per particle in terms of p and T and use this to compute the chemical potential on each branch in terms of p and T . Then, in the coexistence region the fraction of particles f_g and f_l in each of the two branches in terms of p and T are determined by the conditions that the total fraction add up to one and the total volume is given by extensivity:

$$f_g + f_l = 1, \quad N f_g \mathbb{V}_{1g} + N f_l \mathbb{V}_{1l} = \mathbb{V}. \quad (5.10.98)$$

By equation (5.10.51) coexistence can only occur when the chemical potentials coincide:

$$\mu_g(p, T) = \mu_l(p, T) \quad (5.10.99)$$

which defines a curve $p_{\text{co}}(T)$ so that at a fixed temperature there is only one pressure so that the two phases coexist (it is guaranteed that this can be inverted to find such a unique $p(T)$ owing to the concavity properties of the chemical potential). This $p_{\text{co}}(T)$ is called the coexistence curve. Differentiating the equality of the chemical potentials gives that along the coexistence curve:

$$\frac{\partial \mu_g}{\partial p} \frac{dp_{\text{co}}}{dT} + \frac{\partial \mu_g}{\partial T} = \frac{\partial \mu_l}{\partial p} \frac{dp_{\text{co}}}{dT} + \frac{\partial \mu_l}{\partial T}. \quad (5.10.100)$$

Using equations (5.9.41) and (5.9.42) and letting S_{1g} and S_{1l} be the entropy per particle in the gas and liquid phases respectively:

$$-\mathbb{V}_{1g} \frac{dp_{\text{co}}}{dT} + S_{1g} = -\mathbb{V}_{1l} \frac{dp_{\text{co}}}{dT} + S_{1l} \quad (5.10.101)$$

$$\implies \frac{dp_{\text{co}}}{dT} = \frac{S_{1l} - S_{1g}}{\mathbb{V}_{1l} - \mathbb{V}_{1g}} \quad (5.10.102)$$

which is known as the **Clausius–Clapeyron equation**. It gives a differential equation which defines the coexistence curve in terms of the entropies and volumes per particle of each of the phases. This differential equation can only be solved up to the critical temperature, beyond which there is only one phase any way. Off of the coexistence curve the system will be in precisely one phase.

By the matching of chemical potentials at a given temperature there is only one pressure at which the two phases can coexist. Below that coexistence pressure the system is at a lesser pressure and thus higher volume (owing to $\frac{\partial p}{\partial \mathbb{V}}$ being decreasing at $\mathbb{V} = N\mathbb{V}_g$) than at coexistence and thus must be purely in the gas phase. Above the coexistence pressure the system is at a higher pressure and thus lesser volume (owing to $\frac{\partial p}{\partial \mathbb{V}}$ being decreasing at $\mathbb{V} = N\mathbb{V}_l$) than at coexistence and thus must be purely in the liquid phase. At the coexistence pressure by varying the fractions f_l and f_g the gas can be at any volume between $N\mathbb{V}_l$ and $N\mathbb{V}_g$. One could from equation (5.10.84) plot p as a function of $\mathbb{V}$ at fixed T for a variety of T , called the plot of naive isotherms. The arguments given at the start of the paragraph indicate that the true isotherms of the full fluid system are to follow the naive isotherm up to the volume $N\mathbb{V}_g$, at which the pressure will hit the coexistence value. Then, to stay on a straight line at the coexistence value until reaching $N\mathbb{V}_l$ in the volume (because p is only determined by T between those two volumes by the coexistence curve). Finally, after the volume $N\mathbb{V}_l$ the true isotherm follows the naive isotherm.

There is a geometric consequence of the relationship between the true and naive isotherms that can be used to compute the coexistence curve. Let $N_g = N f_g$ and $N_l = N f_l$ be the numbers of particles in the gas and liquid phases respectively. Then, for all configurations the Gibbs energy of the system is given by:

$$G(p, T, N) = N_g \mu_g + N_l \mu_l. \quad (5.10.103)$$

Away from the coexistence curve either N_g or N_l is 0 and the other is N . At the value of the volume so that $\mathbb{V} = N\mathbb{V}_g$ we have $N_g = N$ and $N_l = 0$ while at the value of the volume so that $\mathbb{V} = N\mathbb{V}_l$ we have $N_l = N$ and $N_g = 0$. However, considering changes of N_g and N_l at fixed p and T gives (using that they must add up to N):

$$dG = \mu_g dN_g + \mu_l dN_l = \mu_g dN_g + \mu_l (-dN_g) = (\mu_g - \mu_l) dN_g = 0 \quad (5.10.104)$$

by using that the chemical potentials match. Therefore, the Gibbs energy at $\mathbb{V} = N\mathbb{V}_g(p, T)$ and $\mathbb{V} = N\mathbb{V}_l(p, T)$ coincide and no change occurs along the path. Expressed in terms of the free energy the Gibbs energy is

defined by (using equation (5.9.36)):

$$G = \mathcal{F} + p\mathbb{V}. \quad (5.10.105)$$

Comparing these at the two ends of the coexistence region then:

$$\mathcal{F}_g + p_{\text{co}}N\mathbb{V}_g = \mathcal{F}_l + p_{\text{co}}N\mathbb{V}_l \quad (5.10.106)$$

$$\implies p_{\text{co}}(N\mathbb{V}_l - N\mathbb{V}_g) = \mathcal{F}_g - \mathcal{F}_l. \quad (5.10.107)$$

The left hand side here is the area under the isotherm graph of p versus $\mathbb{V}$ between the end points of the coexistence region using the real isotherm. The right hand side only depends on the free energy at the end points of that region but because those free energies match the naive free energies from $\mathcal{F}_{\text{VdW}}$ in equation (5.10.79) we can rewrite them as:

$$\mathcal{F}_g - \mathcal{F}_l = \mathcal{F}_{\text{VdW}}(N, T, N\mathbb{V}_g) - \mathcal{F}_{\text{VdW}}(N, T, N\mathbb{V}_l) = \int_{N\mathbb{V}_l}^{N\mathbb{V}_g} \frac{\partial \mathcal{F}_{\text{VdW}}}{\partial \mathbb{V}} d\mathbb{V} \quad (5.10.108)$$

$$= - \int_{N\mathbb{V}_l}^{N\mathbb{V}_g} p_{\text{VdW}} d\mathbb{V} = \int_{N\mathbb{V}_g}^{N\mathbb{V}_l} p_{\text{VdW}} d\mathbb{V}. \quad (5.10.109)$$

This is precisely the area under the isotherm graph of p versus $\mathbb{V}$ between the end points of the coexistence region using the naive isotherm. Therefore, another way to determine the coexistence curve $p_{\text{co}}(T)$ is by the value of the pressure for which these two areas coincide. This is called the Maxwell construction. Thus, there are three equivalent ways of determining the coexistence curve: the matching of the chemical potentials, the solution to the Clausius–Clapeyron equation, and the Maxwell construction.

Unfortunately, even for the VdW fluid, which is about the simplest model with a phase transition, it is practically impossible to get insightful analytic expressions for $\mathbb{V}_{1g}, \mathbb{V}_{1l}, N_g, N_l, G$, or $p_{\text{co}}(T)$. Instead, numerical results are strongly favored.

5.10.3 Chemical Reactions and the Grand Canonical Ensemble

So far we have always studied systems with a fixed number of particles. However, statistical mechanics gives us a nice and direct way for studying a system with a variable number of particles, which is essentially for understanding chemical reactions. Suppose we have an $\mathcal{N}$ particle Hamiltonian $\mathcal{H}_{\mathcal{N}}$ of $\mathcal{N}$ identical particles. If we were to consider a distribution over $\mathcal{N}$ then by the logic of section 5.5 owing to $\mathcal{N}$ being an extensive conserved quantity we should introduce a Lagrange multiplier α and take the generalized Boltzmann distribution:

$$f_{\text{eq}}(Q_{\mathcal{N}}, P_{\mathcal{N}}, \mathcal{N}) = \frac{e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}}}{\mathcal{Z}} \quad (5.10.110)$$

where the so called “grand partition function” is defined as:

$$\mathcal{Z} = \int_{\mathbb{P}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} d\mathbb{P} \quad (5.10.111)$$

and the grand phase space $\mathbb{P}$ includes the phase space of a single particle, two particles, three particles, and so on for any number of particles. (The notation $Q_{\mathcal{N}}$ and $P_{\mathcal{N}}$ indicate a list of coordinates and momenta for n particles.) So, $\mathcal{N}$ in the grand partition function is a variable being summed over to represent a phase space for each particle number. Equivalently then the grand partition function can be written:

$$\mathcal{Z} = \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} d\mathbb{P}_{\mathcal{N}} \quad (5.10.112)$$

where $\mathbb{P}_{\mathcal{N}}$ is the $\mathcal{N}$ particle phase space. The distribution f_{eq} is called the grand canonical ensemble.

The Lagrange multiplier α controls the expected number of particles N . By explicit computation:

$$N = \mathbb{E}(\mathcal{N}) = \int \mathcal{N} f_{\text{eq}} d\mathbb{P} = \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} \frac{e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}}}{\mathcal{Z}} \mathcal{N} d\mathbb{P}_{\mathcal{N}} = -\frac{1}{\mathcal{Z}} \frac{\partial}{\partial \alpha} \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} d\mathbb{P}_{\mathcal{N}} = -\frac{\partial}{\partial \alpha} \ln \mathcal{Z}. \quad (5.10.113)$$

This is analogous to equation (5.5.23) but for the number of particles. Equation (5.5.23) is still true for the

energy:

$$E = \mathbb{E}(\mathcal{H}) = \int f \mathcal{H} d\mathbb{P} = \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} \frac{e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}}}{\mathcal{Z}} \mathcal{H}_{\mathcal{N}} d\mathbb{P}_{\mathcal{N}} = -\frac{1}{\mathcal{Z}} \frac{\partial}{\partial \beta} \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} d\mathbb{P}_{\mathcal{N}} = -\frac{\partial}{\partial \beta} \ln \mathcal{Z}. \quad (5.10.114)$$

The extensivity of E combined with the intensivity of $\beta = \frac{1}{T}$ guarantees then that $\ln \mathcal{Z}$ is extensive. The extensivity of $\ln \mathcal{Z}$ combined with the extensivity of N then guarantees that α is intensive so that equation (5.10.113) is true. A direct analog of equation (5.5.34) holds as well:

$$\delta N^2 = \mathbb{E}(\mathcal{N} - N)^2 = \mathbb{E} \mathcal{N}^2 - N^2 = \frac{1}{\mathcal{Z}} \int_{\mathbb{P}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} \mathcal{N}^2 d\mathbb{P} - N^2 \quad (5.10.115)$$

$$= \frac{1}{\mathcal{Z}} \left(\frac{\partial}{\partial \alpha} \right)^2 \mathcal{Z} - \frac{1}{\mathcal{Z}^2} \left(\frac{\partial \mathcal{Z}}{\partial \alpha} \right)^2 = \frac{\partial}{\partial \alpha} \left(\frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \alpha} \right) = -\frac{\partial N}{\partial \alpha}. \quad (5.10.116)$$

Consequently the relative fluctuation of the particle number is given by:

$$\frac{\delta N^2}{N^2} = -\frac{1}{N^2} \frac{\partial N}{\partial \alpha}. \quad (5.10.117)$$

Because α is intensive the right hand side scales inversely to the size of the system. Thus in the thermodynamic limit the relative variance of the particle number goes to 0 and it is as if the system has a definite number of particles $\mathcal{N} = N$. This is exactly analogous to the thermodynamic limit of the energy. We found before that the microcanonical ensemble which kept the energy exactly fixed and the canonical ensemble which only kept the expectation of the energy fixed exactly agree in the thermodynamic limit. In the very same way the canonical ensemble in which we keep the particle number fixed and the grand canonical ensemble in which we keep the expected particle number fixed exactly agree in the thermodynamic limit. The entropy of the grand canonical ensemble is easily:

$$S = - \int_{\mathbb{P}} f \ln f d\mathbb{P} = - \int_{\mathbb{P}} f \ln \left(\frac{e^{-\beta \mathcal{H} - \alpha \mathcal{N}}}{\mathcal{Z}} \right) d\mathbb{P} = \beta \int_{\mathbb{P}} f \mathcal{H} d\mathbb{P} + \alpha \int_{\mathbb{P}} f \mathcal{N} d\mathbb{P} + \ln \mathcal{Z} \int_{\mathbb{P}} f d\mathbb{P} \quad (5.10.118)$$

$$= \beta E + \alpha N + \ln \mathcal{Z}. \quad (5.10.119)$$

This gives the variation:

$$dS = E d\beta + \beta dE + N d\alpha + \alpha dN + \frac{\partial \ln \mathcal{Z}}{\partial \alpha} d\alpha + \frac{\partial \ln \mathcal{Z}}{\partial \beta} d\beta + \frac{\partial \ln \mathcal{Z}}{\partial x^a} dx^a + \frac{\partial \ln \mathcal{Z}}{\partial X^a} dX^a \quad (5.10.120)$$

where x, X are intensive and extensive quantities appearing in the Hamiltonian by the same notation as in equation (5.9.4). Solving for the variation of the energy and using what we have established about the derivatives of $\ln \mathcal{Z}$:

$$dE = T dS - T \alpha dN + \frac{\partial}{\partial x^a} (-T \ln \mathcal{Z}) dx^a + \frac{\partial}{\partial X^a} (-T \ln \mathcal{Z}) dX^a. \quad (5.10.121)$$

By using equation (5.9.33) we can identify the in fact α is related to the chemical potential μ :

$$\alpha = -\frac{\mu}{T}. \quad (5.10.122)$$

As well, we can see that the thermodynamic forces are:

$$f_a = \frac{\partial}{\partial X^a} (-T \ln \mathcal{Z}), \quad F_a = \frac{\partial}{\partial x^a} (-T \ln \mathcal{Z}). \quad (5.10.123)$$

Now that we have identified a familiar meaning to α we can also write the grand canonical ensemble as:

$$f_{\text{eq}}(Q_{\mathcal{N}}, P_{\mathcal{N}}, \mathcal{N}) = \frac{e^{-\beta(\mathcal{H}_{\mathcal{N}} - \mu \mathcal{N})}}{\mathcal{Z}}. \quad (5.10.124)$$

It is also nice to introduce the grand potential Φ defined by:

$$\Phi = -T \ln \mathcal{Z} \quad (5.10.125)$$

which looks quite like the free energy. By equation (5.10.119) Φ is related to the energy by:

$$\Phi(T, \mu, X, x) = E - TS - \mu N \quad (5.10.126)$$

and so can be seen as a Legendre transformation of the energy with respect to both the temperature/entropy and chemical potential/particle number. As well, we can see it is the free energy minus μN . The total differential of the grand potential using equations (5.10.113), (5.10.114), and (5.10.123) gives (or simply the

total differential of the energy):

$$d\Phi = -SdT - Nd\mu + f_a dX^a + F_a dx^a. \quad (5.10.127)$$

The grand canonical ensemble, grand partition function, and grand potential are convenient for studying systems with reversible chemical reactions which may change particle species. Suppose we have a list of K kinds of particles. Within each species of particle the particles are identical but the different species are distinct. Let Name_k be the name of particle species k . Further, suppose there is a type of chemical reaction that can happen in the system so that s_{01} particles of species 1, ..., s_{0K} particles of species K in this reaction turn into s_{f1} particles of species 1, ..., s_{fK} particles of species K or vice versa. This reaction is written as an equation as:

$$\sum_{k=1}^K s_{0k} \text{Name}_k \rightleftharpoons \sum_{k=1}^K s_{fk} \text{Name}_k. \quad (5.10.128)$$

The entropy variation of the system is given by:

$$dS = \sum_{k=1}^K \left(\frac{\partial S}{\partial E_k} dE_k + \frac{\partial S}{\partial N_k} dN_k + \frac{\partial S}{\partial X_k^a} dX_k^a \right) \quad (5.10.129)$$

$$= \sum_{k=1}^K \left(\frac{1}{T_k} dE_k - \frac{\mu_k}{T_k} dN_k - \frac{f_{ka}}{T_k} dX_k^a \right) \quad (5.10.130)$$

where we have assumed along the lines of equation (5.10.10) that we have written the underlying Hamiltonian so that all of its parameters X are extensive. The allowed variations for the energy and X^a are then that the totals are conserved:

$$dE = \sum_{k=1}^K dE_k = 0, \quad dX^a = \sum_{k=1}^K dX_k^a = 0. \quad (5.10.131)$$

Because all variations of E_k and X_k^a which satisfy these are possible and the variation of the entropy must be 0 in equilibrium, we find that like equation (5.10.15) all of the temperatures and intensive forces must match:

$$\frac{\partial S}{\partial E_1} = \dots = \frac{\partial S}{\partial E_K} = \frac{1}{T} \quad (5.10.132)$$

$$\frac{\partial S}{\partial X_1^a} = \dots = \frac{\partial S}{\partial X_K^a} = -\frac{f_a}{T}. \quad (5.10.133)$$

(To show this easily, add an energy conserving Lagrange multiplier and X^a conserving Lagrange multiplier for each a to the variation of the action and one will find that requiring vanishing variations means each of these derivatives are given by the value of the corresponding Lagrange multiplier and thus are equal.) Before we considered variations in which particles in system one could be directly exchanged with particles in system two while conserving the total. Now we have a different rule constraining the variations of the particle numbers. Let R be the number of reactions which have occurred. Then, by equation (5.10.128) the change in the number of particles in species k is related to the number of reactions by:

$$dN_k = (s_{fk} - s_{0k})dR. \quad (5.10.134)$$

This coefficient $s_{fk} - s_{0k}$ is called the stoichiometric coefficient for species k . Returning this to the variation of the entropy gives:

$$dS = -\frac{1}{T} \sum_{k=1}^K \mu_k (s_{fk} - s_{0k}) dR. \quad (5.10.135)$$

This must be true for any dR and so in equilibrium we have:

$$\boxed{\sum_{k=1}^K s_{0k} \mu_k = \sum_{k=1}^K s_{fk} \mu_k} \quad (5.10.136)$$

which gives the necessary condition for balancing the chemical potentials of the various particle species in equilibrium. This equation is very easy to remember because one simply takes the reaction equation (5.10.128) and replaces the names of each particle species with its chemical potential. Using the grand canonical ensemble we can compute the grand potential in terms of all of the chemical potentials of the various particle

species. The number of particles in each species N_k is then easily computed from the grand potential using equation (5.10.127) where we impose this balance condition in equilibrium.

It is quite nice to look in particular at the grand canonical ensemble of a system of noninteracting identical particles. Let $\mathcal{H}_1$ be the single particle Hamiltonian and Z_1 be the corresponding single particle partition function. Then:

$$\mathcal{Z} = \sum_{\mathcal{N}=0}^{\infty} \frac{1}{\mathcal{N}!} \int_{\mathbb{P}_{\mathcal{N}}^{\text{distinct}}} e^{-\beta \mathcal{H}_{\mathcal{N}} - \alpha \mathcal{N}} d\mathbb{P}_{\mathcal{N}}^{\text{distinct}} = \sum_{\mathcal{N}=0}^{\infty} \frac{e^{-\alpha \mathcal{N}}}{\mathcal{N}!} Z_1^{\mathcal{N}} = e^{Z_1 e^{-\alpha}} = e^{Z_1 e^{\frac{\mu}{T}}}. \quad (5.10.137)$$

An often useful quantity is the phase number density (or occupation number density, or phase space number distribution) $n(Q, P)$ which is the number density of the particles in the single particle phase space. Here (Q, P) are the coordinates of a single particle's phase space only. Then, $n(Q, P)$ is defined as:

$$n(Q, P) = \mathbb{E} \sum_{k=1}^N (2\pi\hbar)^d \delta(Q - Q_k) \delta(P - P_k). \quad (5.10.138)$$

Here d is the number of Q coordinates in the single particle phase space (so that phase space is $2d$ dimensional). These $2\pi\hbar$'s are included by convention to cancel the $2\pi\hbar$'s introduced by convention in the definition of the phase space measure in equation (5.2.4).

For noninteracting particles the quantities of interest can typically be written nicely as an integral of some function times n over just the single particle phase space. For example, the energy can be written:

$$E = \mathbb{E} \mathcal{H} = \mathbb{E} \left(\sum_{k=1}^N \mathcal{H}_1(Q_k, P_k) \right) = \int_{\mathbb{P}_1} \mathcal{H}_1(Q, P) \mathbb{E} \left(\sum_{k=1}^N \delta(Q - Q_k) \delta(P - P_k) \right) d^d Q d^d P \quad (5.10.139)$$

$$\implies E = \int_{\mathbb{P}_1} \mathcal{H}_1(Q, P) \frac{n(Q, P)}{(2\pi\hbar)^d} d^d Q d^d P \quad (5.10.140)$$

$$\implies E = \int_{\mathbb{P}_1} \mathcal{H}_1(Q, P) n(Q, P) d\mathbb{P}_1. \quad (5.10.141)$$

Similarly, the particle number can be written:

$$N = \mathbb{E} \mathcal{N} = \mathbb{E} \left(\sum_{k=1}^N 1 \right) = \int_{\mathbb{P}_1} \mathbb{E} \left(\sum_{k=1}^N \delta(Q - Q_k) \delta(P - P_k) \right) d^d Q d^d P = \int_{\mathbb{P}_1} \frac{n(Q, P)}{(2\pi\hbar)^d} d^d Q d^d P \quad (5.10.142)$$

$$\implies N = \int_{\mathbb{P}_1} n(Q, P) d\mathbb{P}_1. \quad (5.10.143)$$

In equilibrium the phase number density can be computed explicitly to give a very nice expression using the grand canonical ensemble. First, starting with the definition of n :

$$n(Q, P) = (2\pi\hbar)^d \sum_{\mathcal{N}=0}^{\infty} \int_{\mathbb{P}_{\mathcal{N}}} \frac{e^{-\beta(\mathcal{H}_{\mathcal{N}} - \mathcal{N}\mu)}}{\mathcal{Z}} \sum_{k=1}^{\mathcal{N}} \delta(Q - Q_k) \delta(P - P_k) d\mathbb{P}_{\mathcal{N}}. \quad (5.10.144)$$

Using the interchangeability of all of the particles, each term in the sum over k contributes the same amount and so we can rewrite that sum as N times the first term:

$$n(Q, P) = (2\pi\hbar)^d \sum_{\mathcal{N}=0}^{\infty} \int e^{-\beta(\mathcal{H}_1(Q_1, P_1) - \mu)} \frac{e^{-\beta \sum_{k=2}^{\mathcal{N}} \mathcal{H}_1(Q_k, P_k) + \beta(\mathcal{N}-1)\mu}}{\mathcal{Z}} \mathcal{N} \delta(Q - Q_1) \delta(P - P_1) \frac{1}{\mathcal{N}!} d\mathbb{P}_{\mathcal{N}}^{\text{distinct}} \quad (5.10.145)$$

$$= (2\pi\hbar)^d e^{-\beta(\mathcal{H}_1(Q, P) - \mu)} \sum_{\mathcal{N}=1}^{\infty} \frac{1}{(\mathcal{N}-1)!} \frac{e^{\beta(\mathcal{N}-1)\mu}}{\mathcal{Z}} \int e^{-\beta \sum_{k=2}^{\mathcal{N}} \mathcal{H}_1(Q_k, P_k)} \delta(Q - Q_1) \delta(P - P_1) d\mathbb{P}_{\mathcal{N}}^{\text{distinct}} \quad (5.10.146)$$

$$= (2\pi\hbar)^d e^{-\beta(\mathcal{H}_1(Q, P) - \mu)} \sum_{\mathcal{N}=1}^{\infty} \frac{1}{(\mathcal{N}-1)!} \frac{e^{\beta(\mathcal{N}-1)\mu}}{\mathcal{Z}} \frac{1}{(2\pi\hbar)^d} Z_1^{\mathcal{N}-1} \quad (5.10.147)$$

$$= e^{-\beta(\mathcal{H}_1(Q, P) - \mu)} \frac{1}{\mathcal{Z}} \mathcal{Z}. \quad (5.10.148)$$

Thus we have the Maxwell-Boltzmann (MB) phase number density:

$$n(Q, P) = e^{-\beta(\mathcal{H}_1(Q, P) - \mu)} \quad (5.10.149)$$

which is valid for any classical system of noninteracting identical particles. In fact, the entire thermodynamics of the system can be determined from this number density. Using equation (5.10.143) and the MB number density:

$$N = \int_{\mathbb{P}_1} e^{-\beta(\mathcal{H}_1 - \mu)} d\mathbb{P}_1 = e^{\frac{\mu}{T}} Z_1 \implies Z_1 = N e^{-\frac{\mu}{T}}. \quad (5.10.150)$$

Then, the grand potential is given by:

$$\Phi = -T \ln \mathcal{Z} = -T Z_1 e^{\frac{\mu}{T}} = -NT. \quad (5.10.151)$$

Hence, using equation (5.10.143) to determine $N(T, \mu, X, x)$ we can compute the grand potential $\Phi(T, \mu, X, x)$ in terms of all of the correct variables and from there use the fundamental thermodynamic relation in equation (5.10.127) to compute all of the thermodynamic properties of the system.

Exercises

Problem 5.45: Heat Capacity and the Adiabatic Ratio. The heat capacity $C(T)$ of a thermodynamic system in a process is defined as the amount of heat which must be supplied to the system per unit temperature change of the system. That is, $C(T)$ is given by:

$$dQ = C(T)dT.$$

In general, $C(T)$ depends on the process through which the heat is added. Later we will establish how to measure temperature. The heat transfer can be measured through energy changes of the of source of the heat. So, heat capacity is generally a directly experimentally measurable quantity. Consider an ideal gas of adiabatic ratio γ .

- (a) Show that if heat is added to the gas at constant volume the heat capacity is:

$$C_V = \frac{N}{\gamma - 1} = Nc.$$

Because this process is done at constant volume it is written C_V and in the above we introduced the symbol c for the per particle heat capacity at constant volume.

- (b) Show that if heat is added to the gas at constant pressure the heat capacity is:

$$C_p = \frac{N\gamma}{\gamma - 1}.$$

Thus show that the adiabatic ratio of the gas can be determined from the directly measurable C_V and C_p as:

$$\gamma = \frac{C_p}{C_V}.$$

Problem 5.46: Free Expansion of a Gas. Consider a nonrelativistic ideal gas with adiabatic ratio γ in a box of volume $\mathbb{V}_0$ initially in thermodynamic equilibrium. There is a larger container $\mathbb{V}_f$ surrounding the initial container. The initial container is removed and the gas is allowed to freely expand until it fills the larger container. It then reaches thermodynamic equilibrium in the full container. During the expansion you cannot assume quasistatic or quasidynamic evolution.

- (a) Show that during the expansion the change in energy of the gas, work done on the gas, and heat transfer to the gas are all 0.
 (b) Show that the change in temperature of the gas is 0 and that the change in entropy of the gas over the course of the expansion is:

$$\Delta S = N \ln \left(\frac{\mathbb{V}_f}{\mathbb{V}_0} \right)$$

- (c) Show that if we considered the possibility that the gas might spontaneously shrink into a volume $\mathbb{V}_1 < \mathbb{V}_0$ the second law of thermodynamics would preclude it from happening.

Problem 5.47: Gas Mixture Rules. Consider two ideal gases of per particle heat capacities at constant volumes c_1, c_2 , particle numbers N_1, N_2 , initially at temperatures T_1, T_2 in volumes $\mathbb{V}_1, \mathbb{V}_2$. Suppose these

gases are brought into contact and allowed to come to thermodynamic equilibrium together. Show that in thermodynamic equilibrium the mixture will reach volume $\mathbb{V}$, temperature T , and pressures p_1, p_2 satisfying:

$$\mathbb{V} = \mathbb{V}_1 + \mathbb{V}_2, \quad T = \frac{c_1 N_1 T_1 + c_2 N_2 T_2}{c_1 N_1 + c_2 N_2}, \quad \frac{p_1}{N_1} = \frac{p_2}{N_2} = \frac{T}{\mathbb{V}}$$

and show that thermodynamically the mixture can be treated as an ideal gas with particle number N , per particle heat capacity at constant volume c , and pressure p satisfying:

$$N = N_1 + N_2, \quad c = \frac{c_1 N_1 + c_2 N_2}{N_1 + N_2}, \quad p = p_1 + p_2.$$

The pressures p_1 and p_2 are then called the partial pressures of the constituent gases of the mixture.

Problem 5.48: ★ Heat Engines and the Carnot Cycle. A heat engine is a kind of device that uses a gas to perform mechanical work powered by heat. Consider a “hot reservoir”, meaning a system which is sufficiently large that its temperature can be treated as fixed when heat is drawn from or transferred to it and which is at a high temperature T_H and a “cold reservoir” which is the same thing but at a low temperature T_C . These idealized thermal reservoirs are able to transfer heat arbitrarily but not perform work. A heat engine operates in 4 stages which form a cycle. In stage I, the gas starts at an initial pressure and volume $(p_1, \mathbb{V}_1)$ and while in contact with the hot reservoir draws a heat $\mathcal{Q}_H$ out of that reservoir causing the gas to expand to a new pressure and volume $(p_2, \mathbb{V}_2)$. In stage II, the gas is disconnected from the hot reservoir and expands further to a new pressure and volume $(p_3, \mathbb{V}_3)$. In stage III, the gas is connected to the cold reservoir and compresses to $(p_4, \mathbb{V}_4)$ while expelling heat $\mathcal{Q}_C$ to that reservoir. Then, in stage IV, the gas is disconnected from the cold reservoir and compresses further until it returns to the original $(p_1, \mathbb{V}_1)$. We will assume that no heat is transferred between the gas and its environment in stages II or IV.

- (a) Explain that because the reservoirs are at fixed temperature, stages I and III are isothermal processes. Assume the gas is ideal with adiabatic ratio γ . Show that:

$$p_1 \mathbb{V}_1 = p_2 \mathbb{V}_2, \quad p_3 \mathbb{V}_3 = p_4 \mathbb{V}_4.$$

Explain that because the heat transfers in stages II and IV are 0 they are adiabatic processes. Show that:

$$p_2 \mathbb{V}_2^\gamma = p_3 \mathbb{V}_3^\gamma, \quad p_4 \mathbb{V}_4^\gamma = p_1 \mathbb{V}_1^\gamma.$$

- (b) Assume that at the end of each stage the gas is in thermodynamic equilibrium. Show that the changes in entropy of the reservoirs in stages I and III are:

$$\Delta S_H = -\frac{\mathcal{Q}_H}{T_H}, \quad \Delta S_C = \frac{\mathcal{Q}_C}{T_C}.$$

Further, show that the changes in entropy of the gas in each stage are:

$$\begin{aligned} \Delta S_I &= N \ln \left(\frac{\mathbb{V}_2}{\mathbb{V}_1} \right), & \Delta S_{II} &= N \ln \left(\frac{\mathbb{V}_3}{\mathbb{V}_2} \right) - \frac{N}{\gamma - 1} \ln \left(\frac{T_H}{T_C} \right), \\ \Delta S_{III} &= -N \ln \left(\frac{\mathbb{V}_3}{\mathbb{V}_4} \right), & \Delta S_{IV} &= N \ln \left(\frac{\mathbb{V}_1}{\mathbb{V}_4} \right) + \frac{N}{\gamma - 1} \ln \left(\frac{T_H}{T_C} \right). \end{aligned}$$

- (c) Show that the work done on the gas in each stage is given by:

$$W_I = -\mathcal{Q}_H, \quad W_{II} = -\frac{N}{\gamma - 1}(T_H - T_C), \quad W_{III} = \mathcal{Q}_C, \quad W_{IV} = \frac{N}{\gamma - 1}(T_H - T_C).$$

- (d) Show then that the efficiency η of the heat engine, defined as the amount of work done by the gas per cycle per unit heat that must be supplied to the gas for it to operate, is:

$$\eta = -\frac{W_I + W_{II} + W_{III} + W_{IV}}{\mathcal{Q}_H} = 1 - \frac{\mathcal{Q}_C}{\mathcal{Q}_H}.$$

- (e) Show using the second law of thermodynamics that the maximum such efficiency occurs when $\Delta S_H + \Delta S_C = 0$ and that this implies:

$$\eta_{\max} = 1 - \frac{T_C}{T_H}.$$

This is known as Carnot’s theorem and the operation cycle of the idealized optimal heat engine here described is called the Carnot cycle. Please note that the efficiency defined here is relevant when building a heat engine, which intends to use heat to power a gas to do mechanical work (such as move

a piston), but may be a completely irrelevant notion of efficiency for building another kind of device, such as a space heater.

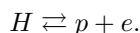
Problem 5.49: Heat Engines and Finite Reservoirs. Consider a Carnot heat engine with initial reservoir temperatures T_C and T_H . Assume now that in each cycle the reservoir temperatures can be treated as constant but that the reservoirs have finite constant heat capacities C_C and C_H . Suppose the heat engine operates for as long as possible. Show that it ceases operation when both of the reservoir temperatures reach the same value of:

$$T = \left(T_C^{C_C} T_H^{C_H} \right)^{\frac{1}{C_C + C_H}}$$

and that the total work done by the engine is:

$$W = C_H T_H + C_C T_C - (C_H + C_C) T.$$

Problem 5.50: Simple Model of Ionization. A hydrogen atom (mass m_H , charge neutral) is a bound system of a proton (mass m_p , charge q) and an electron (mass m_e , charge $-q$). It takes an energy ε to split the proton and the electron in a hydrogen atom apart. Or, an energy ε is released when a proton and electron bind together to form hydrogen. Thus, this system has the chemical reaction:



Let N_H, N_p, N_e be the numbers of each species, $N = N_H + N_p$ be the total number of protons in the system, $x = \frac{N_p}{N}$ be the ionization fraction (fraction of free protons), and Z_H, Z_p, Z_e be the individual one particle partition functions.

(a) Show using the grand canonical ensemble that in thermodynamic equilibrium:

$$\frac{N_p N_e}{N_H} = \frac{Z_p Z_e}{Z_H}.$$

(b) Assume that each of the particles are nonrelativistic so that their single particle Hamiltonians are:

$$\mathcal{H}_H = \frac{|\vec{p}_H|^2}{2m_H} - \varepsilon, \quad \mathcal{H}_p = \frac{|\vec{p}_p|^2}{2m_p}, \quad \mathcal{H}_e = \frac{|\vec{p}_e|^2}{2m_e}.$$

Suppose that the system is charge neutral. Show that the ionization fraction satisfies:

$$\frac{x^2}{1-x} \frac{N}{V} = \left(\frac{m_p m_e T}{2\pi \hbar^2 m_H} \right)^{\frac{3}{2}} e^{-\frac{\varepsilon}{T}}$$

Problem 5.51: Law of Mass Action. Consider a reversible chemical reaction as described in equation (5.10.128). The forward reaction is when the left hand side becomes the right hand side. The other direction is called the backward reaction.

(a) Let n_k be the number density of particle species k in the mixture of all the particles. Assume that each particle in each species has uniform spatial distribution and has position independent of the positions of the other particles. Assume that for a reaction to occur all of the necessary reactants must be sufficiently close to each other. Let R_f be the number of forward reactions which happen per unit time (the forward reaction rate). Show then that for some function $k_f(T)$:

$$R_f = k_f(T) n_1^{s_{01}} \dots n_K^{s_{0K}}.$$

Similarly, let R_b be the number of backward reactions which happen per unit time (the backward reaction rate). Show that for some function $k_b(T)$:

$$R_b = k_b(T) n_1^{s_{f1}} \dots n_K^{s_{fK}}.$$

(b) Assume that each of the species of particles can be treated as an ideal gas. Use that in thermodynamic equilibrium $R_f = R_b$ to show that k_f and k_b are related by:

$$\ln \left(\frac{k_f}{k_b} \right) = \ln A + \left(\sum_{j=1}^K \frac{s_{fj} - s_{0j}}{\gamma_j - 1} \right) \ln T$$

for a constant A independent of temperature. This is known as the law of mass action.

5.11 Linear Response Theory

To experimentally measure a system we have to interact with it in some way. When we interact with a system in thermodynamic equilibrium, it will be perturbed out of equilibrium by some amount. As such, it is important to the behavior of systems near equilibrium. Consider a thermodynamic system which has some macroscopic coordinates Q^a and is in equilibrium at temperature T with a thermal reservoir which holds it at that temperature as some external forces $F_b(t)$ are applied. In the absence of such external forces the expected value of Q^a is some constant $\bar{Q}^a$. This value is constant because the equilibrium distribution does not depend on time. In the presence of such external forces the expected value of Q^a will depend on time and the entire history of $F_b(t)$. So, $\mathbb{E}(Q^a)$ then will be a function of t and a functional of F_b . To consider just perturbations from equilibrium we consider a series in powers of F_b and only retain up to linear order so that for some function $G^{ab}(t, t')$:

$$\mathbb{E}(Q^a(t)) = \bar{Q}^a + \int_{-\infty}^{\infty} G^{ab}(t, t') F_b(t') dt' + \mathcal{O}(F^2). \quad (5.11.1)$$

Studying systems perturbed from equilibrium through this Green's function $G^{ab}(t, t')$ is called linear response theory. We can put some restrictions on the Green's function using time translation symmetry and the fact that $\mathbb{E}(Q^a)$ at time t should only depend on $F_b(t')$ for $t' \leq t$ (forces in the past make the present, not forces in the future). If we were to wait some amount of time τ to apply the forces $F_b(t)$ then by time translation symmetry we should arrive at the same $\mathbb{E}(Q^a)$ except also delayed by that same amount of time τ . Delaying the forces by τ is equivalent to using the forces $F_b(t - \tau)$. Delaying $\mathbb{E}(Q^a(t))$ is equivalent to considering $\mathbb{E}(Q^a(t - \tau))$. Then, time translation symmetry demands:

$$\bar{Q}^a + \int_{-\infty}^{\infty} G^{ab}(t, t') F_b(t' - \tau) dt' + \mathcal{O}(F^2) = \bar{Q}^a + \int_{-\infty}^{\infty} G^{ab}(t - \tau, t') F_b(t') dt' + \mathcal{O}(F^2) \quad (5.11.2)$$

$$\implies \int_{-\infty}^{\infty} G^{ab}(t + \tau, t' + \tau) F_b(t') dt' = \int_{-\infty}^{\infty} G^{ab}(t, t') F_b(t') dt'. \quad (5.11.3)$$

Because this must hold for all $F_b(t')$:

$$G^{ab}(t + \tau, t' + \tau) = G^{ab}(t, t'). \quad (5.11.4)$$

This must hold for all τ and so setting $\tau = -t'$:

$$G^{ab}(t, t') = G^{ab}(t - t', 0) = \chi^{ab}(t - t') \quad (5.11.5)$$

where we have defined the susceptibility tensor $\chi^{ab}(t)$. Then, time translation symmetry implies:

$$\mathbb{E}(Q^a(t)) = \bar{Q}^a + \int_{-\infty}^{\infty} \chi^{ab}(t - t') F_b(t') dt' + \mathcal{O}(F^2). \quad (5.11.6)$$

Due to causality, $\mathbb{E}(Q^a(t))$ cannot depend on $F_b(t')$ for $t' > t$ as those forces haven't happened yet:

$$\frac{\delta \mathbb{E}(Q^a(t))}{\delta F_b(t')} = \chi^{ab}(t - t') + \mathcal{O}(F) \stackrel{!}{=} 0 \quad \forall t' > t \quad (5.11.7)$$

$$\implies \chi^{ab}(t) = 0 \quad \forall t < 0. \quad (5.11.8)$$

So, $\chi^{ab}(t)$ is only non-zero for non-negative t . Consequently, we are free to write equation (5.11.6) as:

$$\boxed{\mathbb{E}(Q^a(t)) = \bar{Q}^a + \int_{-\infty}^t \chi^{ab}(t - t') F_b(t') dt' + \mathcal{O}(F^2).} \quad (5.11.9)$$

The susceptibility tensor characterizes our equilibrium system's lowest order response to perturbations. Conveniently, it can be computed directly from the equilibrium properties of the system using what is called the fluctuation-dissipation theorem. Consider a thermodynamic system in equilibrium to which we apply a constant force for all time before $t = 0$. That is, we take the forces to be:

$$F_b(t) = f_b \vartheta(-t). \quad (5.11.10)$$

It immediately follows that for $t > 0$:

$$\mathbb{E}(Q^a(t)) = \bar{Q}^a + f_b \int_t^{\infty} \chi^{ab}(t') dt' + \mathcal{O}(f^2). \quad (5.11.11)$$

Alternatively, we can simply compute this expectation from thermodynamics. If our free system is

described by some Hamiltonian $\mathcal{H}_0$ then in the presence of constant forces $\mathbf{f}_b$ the Hamiltonian is simply:

$$\mathcal{H} = \mathcal{H}_0 - \mathbf{f}_b Q^b \quad (5.11.12)$$

Then, in equilibrium the system will arrive at the Boltzmann distribution:

$$f(Q, P) = \frac{e^{-\beta \mathcal{H}(Q, P)}}{\int_{\mathbb{P}} e^{-\beta \mathcal{H}(Q', P')} d\mathbb{P}}. \quad (5.11.13)$$

Let $f_0(Q, P)$ be the equilibrium distribution of the system in the absence of external forces. Then:

$$f(Q, P) = \frac{e^{-\beta \mathcal{H}_0}(1 + \beta \mathbf{f}_b Q^b + \mathcal{O}(\mathbf{f}^2))}{\int_{\mathbb{P}} e^{-\beta \mathcal{H}_0}(1 + \beta \mathbf{f}_c Q'^c + \mathcal{O}(\mathbf{f}^2)) d\mathbb{P}} = f_0(Q, P)(1 + \beta \mathbf{f}_b(Q^b - \bar{Q}^b) + \mathcal{O}(\mathbf{f}^2)). \quad (5.11.14)$$

Letting $\mathbb{E}_0$ denote expectations taken with respect to the unperturbed distribution $f_0(Q, P)$:

$$\mathbb{E}(Q^a(t)) = \int_{\mathbb{P}} Q^a(t) f(0, Q(0), P(0)) d\mathbb{P}_0 = \int_{\mathbb{P}} Q^a(t) f_0(0, Q(0), P(0)) (1 + \beta \mathbf{f}_b(Q^b(0) - \bar{Q}^b) + \mathcal{O}(\mathbf{f}^2)) d\mathbb{P}_0 \quad (5.11.15)$$

$$= \bar{Q}^a + \beta \mathbf{f}_b \mathbb{E}_0(Q^a(t)(Q^b(0) - \bar{Q}^b)) + \mathcal{O}(\mathbf{f}^2) \quad (5.11.16)$$

$$= \bar{Q}^a + \beta \mathbf{f}_b \bar{Q}^a \mathbb{E}_0(Q^b(0) - \bar{Q}^b) + \beta \mathbf{f}_b \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)) + \mathcal{O}(\mathbf{f}^2) \quad (5.11.17)$$

$$= \bar{Q}^a + \beta \mathbf{f}_b \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)) + \mathcal{O}(\mathbf{f}^2). \quad (5.11.18)$$

Comparing this with (5.11.11), we have:

$$\bar{Q}^a + \mathbf{f}_b \int_t^\infty \chi^{ab}(t') dt' + \mathcal{O}(\mathbf{f}^2) = \bar{Q}^a + \beta \mathbf{f}_b \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)) + \mathcal{O}(\mathbf{f}^2) \quad (5.11.19)$$

$$\implies \int_t^\infty \chi^{ab}(t') dt' = \beta \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)). \quad (5.11.20)$$

Differentiating both sides with respect to t then yields the fluctuation dissipation theorem:

$$\boxed{\chi^{ab}(t) = -\beta \frac{d}{dt} \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b))}. \quad (5.11.21)$$

Hence, the susceptibility tensor can be computed direction from this time dependent correlation of the coordinates in equilibrium.

Another consequence of time translational symmetry is that the covariance of the coordinates at different times in the equilibrium distribution can only depend on the time difference between them. This is because said correlation must be preserved under an overall shift of the time coordinates:

$$\mathbb{E}_0((Q^a(t + \tau) - \bar{Q}^a)(Q^b(t' + \tau) - \bar{Q}^b)) = \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(t') - \bar{Q}^b)). \quad (5.11.22)$$

From this:

$$\chi^{ab}(t) = -\beta \frac{d}{dt} \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)) = -\beta \frac{d}{dt} \mathbb{E}_0((Q^a(t + \tau) - \bar{Q}^a)(Q^b(\tau) - \bar{Q}^b)) \quad (5.11.23)$$

$$\implies \chi^{ab}(t - \tau) = -\beta \frac{d}{dt} \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(\tau) - \bar{Q}^b)) = -\beta \mathbb{E}_0(\dot{Q}^a(t)(Q^b(\tau) - \bar{Q}^b)) \quad (5.11.24)$$

$$\implies -\frac{d}{dt} \chi^{ab}(t - \tau) = \frac{d}{d\tau} \chi^{ab}(t - \tau) = -\beta \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(\tau)) \quad (5.11.25)$$

$$\implies \boxed{\dot{\chi}^{ab}(t) = \beta \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0))}. \quad (5.11.26)$$

Hence, the time derivative of the susceptibility is proportional to the time dependent correlation of the coordinate velocities.

It is also interesting to look at the expectation of the coordinate velocities in the presence of an external force. From the definition of the susceptibility:

$$\mathbb{E} \dot{Q}^a(t) = \frac{d}{dt} \mathbb{E} Q^a(t) = \frac{d}{dt} \left(\bar{Q}^a + \int_{-\infty}^\infty \chi^{ab}(t - t') \mathbf{F}_b(t') dt' + \mathcal{O}(\mathbf{F}^2) \right) = \int_{-\infty}^t \dot{\chi}^{ab}(t - t') \mathbf{F}_b(t') dt' + \mathcal{O}(\mathbf{F}^2). \quad (5.11.27)$$

Now suppose we have a system in equilibrium to which we turn on a constant force at $t = 0$ so that

$F_b(t) = f_b \vartheta(t)$. Then:

$$\mathbb{E}\dot{Q}^a(t) = \int_{-\infty}^t \dot{\chi}^{ab}(t-t') F_b(t') dt' + \mathcal{O}(F^2) = \int_{-\infty}^t \dot{\chi}^{ab}(t-t') f_b \vartheta(t') dt' + \mathcal{O}(f^2) = f_b \int_0^t \dot{\chi}^{ab}(t') dt' + \mathcal{O}(f^2). \quad (5.11.28)$$

Using equation (5.11.26), in the very long run the coordinate velocity equilibrates to the value:

$$\lim_{t \rightarrow \infty} \mathbb{E}\dot{Q}^a(t) = \beta f_b \int_0^\infty \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) dt + \mathcal{O}(F^2). \quad (5.11.29)$$

So, if we apply a force f_b to a system for so long that it reaches a steady state then the coordinates will develop the velocity given by equation (5.11.29). Alternatively, if the force varies only very slowly with time so that the velocity approximately reaches its steady state then in that approximation we can take the velocity to be:

$$\mathbb{E}\dot{Q}^a(t) \approx \beta F_b(t) \int_0^\infty \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) dt + \mathcal{O}(F^2). \quad (5.11.30)$$

This is known as the Green-Kubo equation. The matrix of coefficients here is called the transport matrix:

$$\gamma^{ab} \stackrel{\text{def}}{=} \int_0^\infty \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) dt. \quad (5.11.31)$$

This expectation is generically a function of temperature and so the transport matrix is as well. Then, in the Green-Kubo approximation a slowly varying force produces an average velocity proportional to it by:

$$\boxed{\mathbb{E}\dot{Q}^a(t) \approx \beta \gamma^{ab} F_b(t)}. \quad (5.11.32)$$

Suppose now we have applied this force $F_b(t)$ to the system and that that system has reached equilibrium in the presence of that force. If such an equilibrium exists then once it has reached said equilibrium $\mathbb{E}\dot{Q}^a(t)$ must be 0 (as it has come to a steady state). So, in equilibrium there must be an equal and opposite contribution to the velocity to cancel the Green-Kubo effect. This effect, called the dissipation response, arises due to microscopic forces between the variables but has a net effect on the macroscopic variables due to their interaction. Then, in that equilibrium:

$$\mathbb{E}\dot{Q}^a(t) = \mathbb{E}\dot{Q}^a(t) \Big|_{\text{Green-Kubo}} + \mathbb{E}\dot{Q}^a(t) \Big|_{\text{Dissipation}} \stackrel{!}{=} 0 \quad (5.11.33)$$

$$\implies \mathbb{E}\dot{Q}^a(t) \Big|_{\text{Dissipation}} \approx -\beta \gamma^{ab} F_b(t). \quad (5.11.34)$$

So, the equilibrium balance between applied force and dissipation means that there is an effective dissipative force $F_{b;\text{Dissipation}}$ given by:

$$\boxed{\mathbb{E}\dot{Q}^a(t) \approx -\beta \gamma^{ab} F_{b;\text{Dissipation}}(t)}. \quad (5.11.35)$$

Thus, the Green-Kubo equation predicts that if a system is perturbed from equilibrium so that it acquires a non-zero velocity, a linear restoring force proportional to that velocity will develop and return that system toward equilibrium. This allows the Green-Kubo equation to also predict the way in which a system near equilibrium approaches that equilibrium.

If the system at hand has time reversal symmetry then the expectations in the time reversed theory of time reversal even quantities must match those of the original theory. Because velocities are time reversal odd, the product of two velocities is time reversal even. Consequently:

$$\mathbb{E}_0(\dot{Q}_{\mathcal{T}}^a(t) \dot{Q}_{\mathcal{T}}^b(0)) = \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) \quad (5.11.36)$$

where the subscript $\mathcal{T}$ indicates time reversal. Explicitly applying the time reversal transformation we have:

$$\mathbb{E}_0((- \dot{Q}^a(-t))(- \dot{Q}^b(-0))) = \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) \implies \mathbb{E}_0(\dot{Q}^a(-t) \dot{Q}^b(0)) = \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)). \quad (5.11.37)$$

Applying time translation symmetry we can shift both arguments in the left-hand side by t giving:

$$\mathbb{E}_0(\dot{Q}^a(0) \dot{Q}^b(t)) = \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)). \quad (5.11.38)$$

which just says that $\mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0))$ is symmetric under swapping a and b . Because this is the integrand of the matrix of transport coefficients, we have that if a system has time reversal symmetry then its transport coefficient matrix is a symmetric matrix:

$$\gamma^{ba} = \int_0^\infty \mathbb{E}_0(\dot{Q}^a(0) \dot{Q}^b(t)) dt = \int_0^\infty \mathbb{E}_0(\dot{Q}^a(t) \dot{Q}^b(0)) dt = \gamma^{ab}. \quad (5.11.39)$$

This is known as the Onsager Reciprocal Relation.

Theorem 5.10: Fluctuation-Dissipation Theorem

When a system with time translational symmetry in thermodynamic equilibrium experiences external forces $F_a(t)$, the expected value of the coordinates $Q^a(t)$ will drift away from their equilibrium values $\bar{Q}^a$ by:

$$\mathbb{E}Q^a(t) = \bar{Q}^a + \int_{-\infty}^t \chi^{ab}(t-t')F_b(t')dt' + \mathcal{O}(F^2) \quad (5.11.40)$$

where the susceptibility tensor $\chi^{ab}(t)$ is given by the fluctuation-dissipation theorem:

$$\chi^{ab} = -\beta \frac{d}{dt} \mathbb{E}_0((Q^a(t) - \bar{Q}^a)(Q^b(0) - \bar{Q}^b)) \quad (5.11.41)$$

where $\beta = \frac{1}{T}$ is the usual thermodynamic beta and $\mathbb{E}_0$ represents the expectation value taken with respect to the equilibrium distribution without any external forces applied. The time derivative of the susceptibility tensor is given by:

$$\dot{\chi}^{ab} = \beta \mathbb{E}_0(\dot{Q}^a(t)\dot{Q}^b(0)). \quad (5.11.42)$$

If the applied external forces vary very slowly, the system asymptotically develops the velocity:

$$\mathbb{E}\dot{Q}^a \approx \beta \gamma^{ab} F_b + \mathcal{O}(F^2) \quad (5.11.43)$$

where γ^{ab} , the transport matrix, is given by:

$$\gamma^{ab} = \int_0^\infty \mathbb{E}_0(\dot{Q}^a(t)\dot{Q}^b(0))dt = T \lim_{t \rightarrow \infty} (\chi^{ab}(t) - \chi^{ab}(0)). \quad (5.11.44)$$

This is known as the Green-Kubo relation. When the system in the absence of external forces has time reversal symmetry, the susceptibility tensor and transport matrix are both symmetric in exchanging their indices:

$$\gamma^{ba} = \gamma^{ab}, \quad \chi^{ab}(t) = \chi^{ba}(t). \quad (5.11.45)$$

This is known as the Onsager reciprocal relation.

We have actually essentially derived the fluctuation-dissipation theorem and corresponding Green-Kubo relation before for a current carrying wire and the result was Ohm's law. It is useful to see this more formally and doing so will actually teach us how to measure temperature using circuits. Suppose we have N charges (with uniform number density n), each of mass m and charge q , in a wire of cross section $\mathbb{A}$ and length ℓ . These charges absent any applied field are free except for that they occasionally scatter off of much heavier ions in the wire. We assume that each particle experiences an average time τ , called the relaxation time, between collisions and that after a collision the direction of a particle's velocity is uniformly distributed. Let $\vec{x}_i(t)$ be the position of particle i at time t . The transport matrix is then defined as:

$$\hat{\gamma}_{ij} = \int_0^\infty \mathbb{E}_0(\dot{\vec{x}}_i(t)\dot{\vec{x}}_j(0))dt. \quad (5.11.46)$$

Then, because of the isotropy of the distribution and the fact that the different particles are independent of each other:

$$\mathbb{E}_0(\dot{\vec{x}}_i(t)\dot{\vec{x}}_j(0)) = \frac{1}{3}\delta_{ij}\mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0)). \quad (5.11.47)$$

The factor of $\frac{1}{3}$ is fixed by tracing over both sides. If in the time between 0 and t particle i does not experience a collision, then its velocity at time t is the same as its velocity at time 0. If it does experience a collision then its velocity at time t is completely uncorrelated with its velocity at time 0 (as it is set by the direction it scatters off the target in the matter, which can be anything uniformly). Because at each time particle may or may not scatter and it does so independently through time, the distribution of its scattering time is exponential, by the logic of problem 5.11. Recall that τ is the average time between scattering events. Let $S_i(t)$ be the event that particle i scatters between the times 0 and t . Then:

$$\begin{aligned} \mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0) | S_i(t)) &= 0, \\ \mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0) | \text{not } S_i(t)) &= \mathbb{E}_0(|\dot{\vec{x}}_i(0)|^2), \end{aligned}$$

$$\text{Prob}(S_i(t)) = 1 - e^{-\frac{t}{\tau}}. \quad (5.11.48)$$

Consequently, we have:

$$\mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0)) = \mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0)|S_i(t))\text{Prob}(S_i(t)) + \mathbb{E}_0(\dot{\vec{x}}_i(t) \cdot \dot{\vec{x}}_i(0)|\text{not } S_i(t))(1 - \text{Prob}(S_i(t))) \quad (5.11.49)$$

$$= e^{-\frac{t}{\tau}} \mathbb{E}_0(|\dot{\vec{x}}_i(0)|^2). \quad (5.11.50)$$

In thermodynamic equilibrium we can compute $\mathbb{E}_0(|\dot{\vec{x}}_i(0)|^2)$ quite easily using the canonical ensemble:

$$\mathbb{E}_0(|\dot{\vec{x}}_i(0)|^2) = \frac{\int \frac{|\vec{p}|^2}{m^2} e^{-\frac{|\vec{p}|^2}{2mT}} d^3\vec{p}}{\int e^{-\frac{|\vec{p}|^2}{2mT}} d^3\vec{p}} = \frac{3T}{m} \quad (5.11.51)$$

$$\implies \mathbb{E}_0(\dot{\vec{x}}_i(t) \dot{\vec{x}}_j(0)) = \frac{T}{m} \delta_{ij} \mathbb{1} e^{-\frac{t}{\tau}}. \quad (5.11.52)$$

Consequently the transport matrix is:

$$\hat{\gamma}_{ij} = \int_0^\infty \frac{T}{m} \delta_{ij} \mathbb{1} e^{-\frac{t}{\tau}} dt = \frac{\tau T}{m} \delta_{ij} \mathbb{1}. \quad (5.11.53)$$

Under an external force $\vec{F}_i$ then on particle i , that particle develops the velocity (by the fluctuation-dissipation theorem):

$$\mathbb{E} \dot{\vec{x}}_i = \frac{1}{T} \hat{\gamma}_{ij} \vec{F}^j + \mathcal{O}(F^2) = \frac{\tau}{m} \vec{F}_i + \mathcal{O}(F^2). \quad (5.11.54)$$

When that external force is due to an electric field $\vec{E}$ we have $\vec{F} = q\vec{E}$:

$$\mathbb{E} \dot{\vec{x}}_i = \frac{q\tau}{m} \vec{E}_i + \mathcal{O}(E^2) \quad (5.11.55)$$

and so the induced current density in the charges is:

$$\vec{J} = \sum_{i=1}^N qn \mathbb{E} \dot{\vec{x}}_i = \frac{q^2 n \tau}{m} \vec{E} + \mathcal{O}(E^2). \quad (5.11.56)$$

This is precisely Ohm's law as derived in problem 3.62 with the very same expression for the conductivity:

$$\sigma = \frac{q^2 n \tau}{m}. \quad (5.11.57)$$

The expectation in equation (5.11.52) can be expressed in a more symmetric form by using the time-translational symmetry of the underlying distribution:

$$\mathbb{E}_0(\dot{\vec{x}}_i(t) \dot{\vec{x}}_j(t')) = \frac{T}{m} \delta_{ij} \mathbb{1} e^{-\frac{|t-t'|}{\tau}}. \quad (5.11.58)$$

We also know from problem 3.62 that the voltage V across this resisting wire (resistor) is related to the current I across it by the macroscopic version of Ohm's law:

$$V = IR \quad (5.11.59)$$

and that the resistance R is given by:

$$R = \frac{\ell}{\sigma \mathbb{A}}. \quad (5.11.60)$$

Further we know from problem 3.65 that the instantaneous power dissipated through the resistor is:

$$\mathcal{P}_{\text{inst}} = IV. \quad (5.11.61)$$

In thermodynamic equilibrium, even without any applied fields, the charges in the wire will move around and thus generate currents. Microscopically they will then induce local electric fields and thus voltages and lead to some power dissipation. This noisy fluctuating current, voltage, and power is called **Johnson noise**. The total energy dissipated by the circuit is given by:

$$E = \int_{-\infty}^{\infty} \mathcal{P}_{\text{inst}} dt = \int_{-\infty}^{\infty} I(t) V(t) dt = R \int_{-\infty}^{\infty} I^2(t) dt. \quad (5.11.62)$$

Let $\tilde{I}(\omega)$ indicate the usual Fourier-transform of $I(t)$. Then (by the results of problem 2.28):

$$E = R \int_{-\infty}^{\infty} I^2(t) dt = R \int_{-\infty}^{\infty} |\tilde{I}(\omega)|^2 d\omega. \quad (5.11.63)$$

Let us consider the energy dissipated by our resistor between a time t_0 and a time $t_0 + \Lambda$, where Λ here is the duration of time we measure the dissipation (called the listening time). We can model this by simply considering a current which is 0 before t_0 and 0 after $t_0 + \Lambda$. Then:

$$\tilde{I}(\omega) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{2\pi}} I(t) dt = \int_{t_0}^{t_0+\Lambda} \frac{e^{i\omega t}}{\sqrt{2\pi}} I(t) dt. \quad (5.11.64)$$

The time-averaged power dissipated $\mathcal{P}$ by the resistor is then given by the total energy dissipated divided by the observation time. To perform full time averaging we will take the limit that the listening time is large:

$$\mathcal{P} = \lim_{\Lambda \rightarrow \infty} \frac{E}{\Lambda} = \lim_{\Lambda \rightarrow \infty} \frac{R}{\Lambda} \int_{-\infty}^{\infty} |\tilde{I}(\omega)|^2 d\omega. \quad (5.11.65)$$

Because $I(t)$ is a real-valued function, $\tilde{I}(-\omega) = \tilde{I}^*(\omega)$ and so we can express the integral positive and negative frequencies as simply an integral over positive frequencies:

$$\mathcal{P} = \lim_{\Lambda \rightarrow \infty} \frac{2R}{\Lambda} \int_0^{\infty} |\tilde{I}(\omega)|^2 d\omega. \quad (5.11.66)$$

This motivates defining the power spectral density (psd) $S(\omega)$ as the function which when integrated over positive frequencies gives the time-averaged power dissipation:

$$S(\omega) = \lim_{\Lambda \rightarrow \infty} \frac{2R}{\Lambda} |\tilde{I}(\omega)|^2 \implies \mathcal{P} = \int_0^{\infty} S(\omega) d\omega. \quad (5.11.67)$$

Let the z -direction be the axial direction of the wire. The total current through the wire at time t is given in terms of the individual particle velocities by:

$$I(t) = \sum_{i=1}^N \frac{q}{\ell} \dot{z}_i. \quad (5.11.68)$$

Because we are working the thermodynamic limit, the quantity $|\tilde{I}(\omega)|^2$ can be replaced by its expectation in the canonical ensemble (by the logic of problem 5.31):

$$|\tilde{I}(\omega)|^2 = \mathbb{E}_0(|\tilde{I}(\omega)|^2) = \mathbb{E}_0(\tilde{I}^*(\omega)\tilde{I}(\omega)) = \int_{t_0}^{t_0+\Lambda} \int_{t_0}^{t_0+\Lambda} e^{i\omega(t-t')} \mathbb{E}_0(I(t)I(t')) \frac{dt dt'}{2\pi}. \quad (5.11.69)$$

Using equation (5.11.58):

$$\mathbb{E}_0(I(t)I(t')) = \mathbb{E}_0\left(\sum_{i=1}^N \frac{q}{\ell} \dot{z}_i(t) \sum_{j=1}^N \frac{q}{\ell} \dot{z}_j(t')\right) = \frac{q^2}{\ell^2} \sum_{i=1}^N \sum_{j=1}^N \mathbb{E}_0(\dot{z}_i(t) \dot{z}_j(t')) \quad (5.11.70)$$

$$= \frac{q^2}{\ell^2} \sum_{i=1}^N \sum_{j=1}^N \frac{T}{m} \delta_{ij} e^{-\frac{|t-t'|}{\tau}} = \frac{q^2 NT}{m\ell^2} e^{-\frac{|t-t'|}{\tau}}. \quad (5.11.71)$$

After performing integration then we have:

$$|\tilde{I}(\omega)|^2 = \frac{q^2 NT}{\pi m\ell^2} \text{Re} \left(\frac{e^{-(\frac{1}{\tau} - i\omega)\Lambda} - 1}{(\frac{1}{\tau} - i\omega)^2} + \frac{\Lambda}{\frac{1}{\tau} - i\omega} \right). \quad (5.11.72)$$

This results in a power spectral density:

$$S(\omega) = \frac{2}{\pi} \frac{T}{1 + \omega^2 \tau^2} \quad (5.11.73)$$

$$\implies \mathcal{P} = \int_0^{\infty} S(\omega) d\omega = \frac{T}{\tau}. \quad (5.11.74)$$

Thus, a resistor in thermal equilibrium will actually radiate electromagnetic thermal energy at this rate (generally this rate is very small and counterbalanced easily by heat transfer from the environment so that T stays steady).

Now suppose we are capable of measuring time dependent voltages across R . We will assume that we are only capable of measuring voltages with a finite time resolutions and so are only sensitive to voltages at angular frequencies between ω_l and ω_h . That is, if $V(t)$ is the actual voltage across R and $\tilde{V}(\omega)$ is its Fourier transform, the voltage we measure $V_m(t)$ will have its Fourier-transform match the Fourier-transform of the

full signal on the interval (ω_l, ω_h) and will be 0 outside of this interval:

$$\tilde{V}_m(\omega) = \begin{cases} \tilde{V}(\omega), & \omega_l < |\omega| < \omega_h \\ 0, & \text{otherwise} \end{cases}. \quad (5.11.75)$$

Then, the time averaged value of measured square of the voltage is:

$$\mathbb{T}(V_m^2) = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_{-\infty}^{\infty} V_m^2(t) dt = \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int_{-\infty}^{\infty} |\tilde{V}_m(\omega)|^2 d\omega \quad (5.11.76)$$

$$= \lim_{\Lambda \rightarrow \infty} \frac{2}{\Lambda} \int_{\omega_l}^{\omega_h} R^2 |\tilde{I}(\omega)|^2 d\omega = R \int_{\omega_l}^{\omega_h} S(\omega) d\omega \quad (5.11.77)$$

$$= \frac{2RT}{\pi} \int_{\omega_l}^{\omega_h} \frac{d\omega}{1 + \omega^2 \tau^2}. \quad (5.11.78)$$

For typical conductors, the relaxation time is extremely small (10^{-12} seconds or shorter for metals at room temperature) and so let us consider frequencies much smaller than $\frac{1}{\tau}$ and let $\Delta f = 2\pi(\omega_h - \omega_l)$ be the “bandwidth” of our measuring device in terms of ordinary frequency (instead of angular frequency). In the small τ limit we see that:

$$\boxed{\mathbb{T}(V_m^2) = 4RT\Delta f}. \quad (5.11.79)$$

This result is known as **Nyquist’s Theorem**. We see that it relates the time averaged square of voltage across a resistor in a given frequency range to that range, the resistance, and the temperature of the resistor. Because in chapters 2 and 3 we established how to measure times, resistances, and voltages, everything in this equation we know how to measure except the temperature. Finally then, by measuring everything in this equation we can indirectly measure the temperature of the resistor and thus can use a resistor as a thermometer. (When our resistor is in thermal equilibrium with another system, the temperature of the resistor will give a measurement of the temperature of that other system.) Typically this thermal noise is very small and needs to be amplified by an amplification circuit to be large enough to be registered by measurement equipment. The amplification circuit will also have its own noise, but as Richard Myers pointed out to me, if the resistor is attached to two amplifiers of the same gain in parallel then in the limit of long listening time the cross correlation of the outputs of the two amplifier channels will cancel each of their noises (assuming they are uncorrelated, which is reasonable if they are separate devices with different power sources) leaving only the thermal noise of the resistor behind.

Exercises

Problem 5.52: ★ Measuring numbers of particles. Explain how now that we are capable of using a resistor as a thermometer and a piston to measure pressure (as in problem 5.44), we can use the ideal gas law to measure the number of particles in a gas. In any macroscopic amount of gas this number will be enormous. Historically, Avogadro’s number N_A was defined by the number of carbon atoms in 12 grams of carbon-12. Now N_A is defined by $N_A = 6.02214076 \times 10^{23}$ which for all practical purposes satisfies the same definition. In g grams of gas made of an element with a total of A protons and neutrons per atom, there will be very nearly $\frac{gN_A}{A}$ atoms⁷

⁷The very large value of $\frac{gN_A}{A}$ for everyday situations is why the Boltzmann constant has such a small numerical value in SI units. Atmospheric pressure on earth in SI units is of order $10^5 \frac{\text{kg}}{\text{m}^2 \text{s}^2}$. A 1 liter = 10^{-3}m^3 volume bottle of air then has pV of order 100 Joules. Such a bottle of air will have about $.05N_A$ molecules in it, resulting in a temperature from the ideal gas law $pV = NT$ of about 4×10^{-21} Joules. Because in such ordinary situations we desire the temperature to be a more human friendly number, like 300, we introduce a conversion factor of about $\frac{4}{3} \times 10^{-23}$ to invent the unit of Kelvin. The argument obviously doesn’t fix the precise value of k_B , which is instead fixed by matching to historical unit systems, but it does explain that the vague order of magnitude of k_B is fixed by the sociological desire for human relevant numbers to be close to 1 and the number of atoms in a human relevant amount of substance.

5.12 The Ultraviolet Catastrophe

So far in our examples and homework questions we have only considered the statistical mechanics of systems with a finite dimensional phase space. If we were to consider the statistical mechanics of a system of moving electrically charged particles though we should in principle also consider the electromagnetic fields in the Hamiltonian and thus need to deal with an infinite dimensional phase space. Familiarly, the Lagrangian for the electromagnetic fields in general is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\frac{1}{2} |\nabla \phi + \dot{\vec{A}}|^2 - \frac{1}{2} |\nabla \times \vec{A}|^2 + \vec{J} \cdot \vec{A} - \rho \phi \right) d\mathbb{S}. \quad (5.12.1)$$

Throughout this section we will use Lorentz natural units $\epsilon_0 = c = 1$.

Let us consider electromagnetism in a cube of side length ℓ and so volume $\mathbb{V} = \ell^3$ which has conducting walls and no sources of charge or current inside (we take $\rho = 0$, $\vec{J} = 0$). Due to the conducting boundary conditions, the force on any charge in the walls in any direction tangent to the walls must be 0. Consequently, the components of the electric field parallel to the wall must vanish and the component of the magnetic field normal to the wall must vanish. To do statistical mechanics, we need the Hamiltonian and to integrate over the phase space. In order to have a well-defined Hamiltonian and phase space with no additional constraints, we need to select a gauge for the potentials. Let us choose our gauge to be Hamiltonian gauge so that $\phi(t, \vec{x}) = 0$. Then:

$$\vec{E} = -\dot{\vec{A}}. \quad (5.12.2)$$

So, the electric field boundary conditions become:

$$\dot{A}_x(t, x, 0, z) = -E_x(t, x, 0, z) = 0 \implies A_x(t, x, 0, z) = A_x(0, x, 0, z) \quad (5.12.3)$$

$$\dot{A}_x(t, x, \ell, z) = -E_x(t, x, \ell, z) = 0 \implies A_x(t, x, \ell, z) = A_x(0, x, \ell, z) \quad (5.12.4)$$

$$\dot{A}_x(t, x, y, 0) = -E_x(t, x, y, 0) = 0 \implies A_x(t, x, y, 0) = A_x(0, x, y, 0) \quad (5.12.5)$$

$$\dot{A}_x(t, x, y, \ell) = -E_x(t, x, y, \ell) = 0 \implies A_x(t, x, y, \ell) = A_x(0, x, y, \ell) \quad (5.12.6)$$

and cyclically so taking $x \rightarrow y \rightarrow z \rightarrow x$. The magnetic field boundary conditions are:

$$B_x(t, 0, y, z) = B_x(t, \ell, y, z) = B_y(t, x, 0, z) = B_y(t, x, \ell, z) = B_z(t, x, y, 0) = B_z(t, x, y, \ell) = 0. \quad (5.12.7)$$

In terms of the vector potential:

$$B_z(t, x, y, 0) = \frac{\partial A_y}{\partial x}(0, x, y, 0) - \frac{\partial A_x}{\partial y}(0, x, y, 0) = 0, \quad (5.12.8)$$

$$B_z(t, x, y, \ell) = \frac{\partial A_y}{\partial x}(0, x, y, \ell) - \frac{\partial A_x}{\partial y}(0, x, y, \ell) = 0 \quad (5.12.9)$$

and again cyclically so for $x \rightarrow y \rightarrow z \rightarrow x$. Here we have used that the vector potential evaluated at the points appearing here are time independent due to the electric field boundary conditions. Define the function:

$$F_{z0}(x, y) = C_{z0} + \int_0^y A_y(0, 0, y', 0) dy' + \int_0^x A_x(0, x', y, 0) dx' \quad (5.12.10)$$

where C_{z0} is an arbitrary constant. This function then satisfies:

$$\frac{\partial F_{z0}}{\partial x} = A_x(0, x, y, 0) \quad (5.12.11)$$

$$\frac{\partial F_{z0}}{\partial y} = A_y(0, 0, y, 0) + \int_0^x \frac{\partial A_x}{\partial y}(0, x', y, 0) dx' = A_y(0, 0, y, 0) + \int_0^x \frac{\partial A_y}{\partial x}(0, x', y, 0) dx' = A_y(0, x, y, 0). \quad (5.12.12)$$

Thus, on the wall at $z = 0$:

$$A_x(t, x, y, 0) = \frac{\partial F_{z0}}{\partial x}(x, y), \quad A_y(t, x, y, 0) = \frac{\partial F_{z0}}{\partial y}(x, y). \quad (5.12.13)$$

We can use the boundary conditions at $z = \ell$ to construct a function $F_{z\ell}(x, y)$ by the same procedure so that:

$$A_x(t, x, y, \ell) = \frac{\partial F_{z\ell}}{\partial x}(x, y), \quad A_y(t, x, y, \ell) = \frac{\partial F_{z\ell}}{\partial y}(x, y). \quad (5.12.14)$$

And, cyclically doing the same thing for the other four walls we can also write the tangential components of the vector potentials as gradients along those walls as well.

Because we are considering a charge free region we have that the divergence of $\vec{E}$ should be zero by Gauss' law. In Hamiltonian gauge, Gauss' law becomes:

$$\nabla \cdot \vec{E} = -\nabla \cdot \dot{\vec{A}} = -\frac{\partial}{\partial t} \nabla \cdot \vec{A} = 0 \implies \nabla \cdot \vec{A} = f(\vec{x}) \quad (5.12.15)$$

for some time independent function $f(\vec{x})$. We can make a gauge transformation preserving $\phi = 0$ by using a gauge function $\chi(\vec{x})$ which is time independent. Then, the vector potential and its divergence change as:

$$\vec{A}' = \vec{A} + \nabla \chi \implies \nabla \cdot \vec{A}' = \nabla \cdot \vec{A} + \nabla^2 \chi = f + \nabla^2 \chi. \quad (5.12.16)$$

Let us choose $\chi(\vec{x})$ by solving the Poisson equation:

$$\nabla^2 \chi = -f. \quad (5.12.17)$$

Then, the gauge transformed vector potential is divergence free. Hence, in a charge free region it is always possible to go to a gauge in which $\phi = 0$ and the vector potential is divergence free. However, even after setting $\phi = 0$ and $\nabla \cdot \vec{A} = 0$ we still have some gauge freedom left. In order to preserve $\phi = 0$, any further gauge transformation function χ we use must not depend on t . In order to preserve $\nabla \cdot \vec{A} = 0$, any further gauge transformation function we use must have vanishing Laplacian: $\nabla^2 \chi = 0$ according to equation (5.12.16). Let us look at what happens to the boundary conditions of the vector potential when we apply a gauge transformation with vanishing Laplacian. Then:

$$A'_x(t, x, y, 0) = A_x(t, x, y, 0) + \frac{\partial \chi}{\partial x}(x, y, 0) = \frac{\partial F_{z0}}{\partial x}(x, y) + \frac{\partial \chi}{\partial x}(x, y, 0) \quad (5.12.18)$$

$$A'_y(t, x, y, 0) = A_y(t, x, y, 0) + \frac{\partial \chi}{\partial y}(x, y, 0) = \frac{\partial F_{z0}}{\partial y}(x, y) + \frac{\partial \chi}{\partial y}(x, y, 0). \quad (5.12.19)$$

Hence, such a gauge transformation effectively replaces the function $F_{z0}(x, y)$ with:

$$F'_{z0}(x, y) = F_{z0}(x, y) + \chi(x, y, 0) \quad (5.12.20)$$

and similarly so for the other five walls. Now suppose we select χ to be the solution to the Laplace equation $\nabla^2 \chi = 0$ with the inhomogeneous Dirichlet boundary conditions that on each of the six walls it is given by the negative of the corresponding F . The Laplace equation with inhomogeneous Dirichlet boundary conditions has solutions (given by the Green's function solution with the Dirichlet Green's function as in equation (3.4.25)) and so such a χ is guaranteed to exist. Then, after performing this gauge transformation we have now fixed:

$$\phi = 0, \quad \nabla \cdot \vec{A} = 0 \quad (5.12.21)$$

$$A_x(t, x, y, 0) = A_x(t, x, y, \ell) = A_y(t, x, y, 0) = A_y(t, x, y, \ell) = 0 \quad (5.12.22)$$

$$A_y(t, 0, y, z) = A_y(t, \ell, y, z) = A_z(t, 0, y, z) = A_z(t, \ell, y, z) = 0 \quad (5.12.23)$$

$$A_z(t, x, 0, z) = A_z(t, x, \ell, z) = A_x(t, x, 0, z) = A_x(t, x, \ell, z) = 0. \quad (5.12.24)$$

5.12.1 An aside on Fourier Series

To deal with these boundary conditions and that we are working with fields on a finite volume, it will be nice to introduce Fourier series. Recall the fundamental Fourier integral:

$$\int_{-\infty}^{\infty} e^{ikx} dx = \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} e^{-\varepsilon|x|+ikx} dx = \lim_{\varepsilon \rightarrow 0} \frac{2\varepsilon}{\varepsilon^2 + k^2} = 2\pi\delta(k). \quad (5.12.25)$$

Fourier series rest on computing the fundamental Fourier series:

$$\sum_{n=-\infty}^{\infty} e^{in\theta} = ? \quad (5.12.26)$$

In order to evaluate this series we use the same ε damping definition as we did with the fundamental Fourier integral and break the sum into two pieces (of positive and negative n ; don't double count the $n = 0$ term!):

$$\sum_{n=-\infty}^{\infty} e^{in\theta} = \lim_{\varepsilon \rightarrow 0^+} \sum_{n=-\infty}^{\infty} e^{-\varepsilon|n|+in\theta} = \lim_{\varepsilon \rightarrow 0^+} \left(\sum_{n=0}^{\infty} e^{-(\varepsilon-i\theta)n} + \sum_{n=0}^{\infty} e^{-(\varepsilon+i\theta)n} - 1 \right). \quad (5.12.27)$$

Now using the geometric series:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad (5.12.28)$$

valid for $|x| < 1$, we have:

$$\sum_{n=-\infty}^{\infty} e^{in\theta} = \lim_{\varepsilon \rightarrow 0^+} \left(\frac{1}{1 - e^{-\varepsilon} e^{-i\theta}} + \frac{1}{1 - e^{-\varepsilon} e^{i\theta}} - 1 \right) = \lim_{\varepsilon \rightarrow 0^+} \frac{1 - e^{-2\varepsilon}}{1 - 2e^{-\varepsilon} \cos \theta + e^{-2\varepsilon}} \quad (5.12.29)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \frac{(1 - e^{-\varepsilon})(1 + e^{-\varepsilon})}{(1 - e^{-\varepsilon})^2 + 2e^{-\varepsilon}(1 - \cos \theta)} = \lim_{\varepsilon \rightarrow 0^+} \frac{\sinh\left(\frac{\varepsilon}{2}\right) \cosh\left(\frac{\varepsilon}{2}\right)}{\sinh^2\left(\frac{\varepsilon}{2}\right) + \sin^2\left(\frac{\theta}{2}\right)}. \quad (5.12.30)$$

Now define the new limit variable $\eta = \sinh\left(\frac{\varepsilon}{2}\right)$ and use the limit in equation (5.12.25):

$$\sum_{n=-\infty}^{\infty} e^{in\theta} = \lim_{\eta \rightarrow 0^+} \frac{\eta \sqrt{1 + \eta^2}}{\eta^2 + \sin^2\left(\frac{\theta}{2}\right)} = \pi \delta\left(\sin \frac{\theta}{2}\right). \quad (5.12.31)$$

Finally using the change of variables formula for the Dirac delta:

$$\sum_{n=-\infty}^{\infty} e^{in\theta} = \pi \delta\left(\sin \frac{\theta}{2}\right) = \pi \sum_{n=-\infty}^{\infty} \frac{\delta(\theta - 2\pi n)}{\left|\frac{\partial}{\partial \varphi} \sin \frac{\varphi}{2}\right|_{\varphi=2\pi n}} = 2\pi \sum_{n=-\infty}^{\infty} \delta(\theta - 2\pi n). \quad (5.12.32)$$

If we only consider θ in the range $(-\pi, \pi]$ then we have the fundamental Fourier series:

$$\boxed{\sum_{n=-\infty}^{\infty} e^{in\theta} = 2\pi \delta(\theta).} \quad (5.12.33)$$

Now suppose we have a 2π periodic function $\phi(\theta)$. Then:

$$\phi(\theta) = \int_{-\infty}^{\infty} \phi(\varphi) \delta(\theta - \varphi) d\varphi = \sum_{n=-\infty}^{\infty} \int_{-\pi+2\pi n}^{\pi+2\pi n} \phi(\varphi) \delta(\theta - \varphi) d\varphi = \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} \phi(\varphi + 2\pi n) \delta(\theta - \varphi - 2\pi n) d\varphi \quad (5.12.34)$$

$$= \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} \phi(\varphi) \delta(\theta - \varphi - 2\pi n) d\varphi = \int_{-\pi}^{\pi} \phi(\varphi) \sum_{n=-\infty}^{\infty} \delta(\theta - \varphi - 2\pi n) d\varphi. \quad (5.12.35)$$

Using our fundamental Fourier series:

$$\phi(\theta) = \int_{-\pi}^{\pi} \phi(\varphi) \sum_{n=-\infty}^{\infty} \frac{e^{in(\theta-\varphi)}}{2\pi} d\varphi = \sum_{n=-\infty}^{\infty} \frac{e^{in\theta}}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \phi(\varphi) \frac{e^{-in\varphi}}{\sqrt{2\pi}} d\varphi. \quad (5.12.36)$$

Hence an arbitrary 2π periodic function $\phi(\theta)$ can be written as a series in terms of complex exponentials as:

$$\phi(\theta) = \sum_{n=-\infty}^{\infty} \frac{e^{in\theta}}{\sqrt{2\pi}} \phi_n \quad (5.12.37)$$

where the series coefficients are given by:

$$\phi_n = \int_{-\pi}^{\pi} \frac{e^{-in\theta}}{\sqrt{2\pi}} \phi(\theta) d\theta. \quad (5.12.38)$$

This series representation is called a Fourier series.

We can generalize the Fourier series from applying to 2π periodic functions to applying to 2ℓ periodic functions where ℓ is an arbitrary real number. Suppose $\phi(x)$ is a 2ℓ periodic function. Then, let $\theta = \frac{\pi x}{\ell}$ and $\phi'(\theta) = \phi(x)$. As a function of θ , $\phi'(\theta)$ is 2π periodic automatically. So, it has the representation:

$$\phi'(\theta) = \sum_{n=-\infty}^{\infty} \frac{e^{in\theta}}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \phi'(\varphi) \frac{e^{-in\varphi}}{\sqrt{2\pi}} d\varphi \quad (5.12.39)$$

$$\Rightarrow \phi(x) = \phi'\left(\frac{\pi x}{\ell}\right) = \sum_{n=-\infty}^{\infty} \frac{e^{\frac{i\pi n x}{\ell}}}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \phi\left(\frac{\ell \varphi}{\pi}\right) \frac{e^{-in\varphi}}{\sqrt{2\pi}} d\varphi = \sum_{n=-\infty}^{\infty} \frac{e^{\frac{i\pi n x}{\ell}}}{\sqrt{2\ell}} \int_{-\ell}^{\ell} \phi(y) \frac{e^{-\frac{i\pi n y}{\ell}}}{\sqrt{2\ell}} dy. \quad (5.12.40)$$

Hence, any 2ℓ periodic function can be expressed as a Fourier series with Fourier coefficients as:

$$\phi(x) = \sum_{n=-\infty}^{\infty} \frac{e^{\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n, \quad \phi_n = \int_{-\ell}^{\ell} \phi(y) \frac{e^{-\frac{i\pi ny}{\ell}}}{\sqrt{2\ell}} dy. \quad (5.12.41)$$

We can generalize this even further to consider any function on an interval. Suppose we are considering a function $\phi(x)$ on the interval $(-\ell, \ell)$. Then, from that function we could define a 2ℓ periodic function by copying $\phi(x)$ and translating it by 2ℓ up and down the real line. Then, this 2ℓ periodic function has the above Fourier series and coincides with the original $\phi(x)$ on the interval $(-\ell, \ell)$. So, any function on such an interval can be represented by the Fourier series we have given. In this perspective, we can view these complex exponentials as a basis for the vector space of integrable functions on the interval $(-\ell, \ell)$.

We often consider real valued functions. For such functions the ϕ_n are not purely independent. Taking the complex conjugate of the Fourier coefficients:

$$\phi_n^* = \int_{-\ell}^{\ell} \phi(y) \frac{e^{\frac{i\pi ny}{\ell}}}{\sqrt{2\ell}} dy = \phi_{-n} \quad (5.12.42)$$

$$\Rightarrow \phi(x) = \sum_{n=-\infty}^{\infty} \frac{e^{\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n = \frac{\phi_0}{\sqrt{2\ell}} + \sum_{n=1}^{\infty} \frac{e^{\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n + \sum_{n=-\infty}^{-1} \frac{e^{\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n \quad (5.12.43)$$

$$\Rightarrow \phi(x) = \frac{\phi_0}{\sqrt{2\ell}} + \sum_{n=1}^{\infty} \left(\frac{e^{\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n + \frac{e^{-\frac{i\pi nx}{\ell}}}{\sqrt{2\ell}} \phi_n^* \right) = \phi(x) = \frac{\phi_0}{\sqrt{2\ell}} + \sum_{n=1}^{\infty} \sqrt{\frac{2}{\ell}} \operatorname{Re} \left(e^{\frac{i\pi nx}{\ell}} \phi_n \right). \quad (5.12.44)$$

Define then the coefficients:

$$A_0 = \int_{-\ell}^{\ell} \phi(y) \frac{dy}{\sqrt{2\ell}}, \quad A_n = \int_{-\ell}^{\ell} \phi(y) \cos\left(\frac{n\pi y}{\ell}\right) \frac{dy}{\sqrt{2\ell}}, \quad B_n = \int_{-\ell}^{\ell} \phi(y) \sin\left(\frac{n\pi y}{\ell}\right) \frac{dy}{\sqrt{2\ell}}. \quad (5.12.45)$$

$$\Rightarrow \phi_0 = A_0, \quad \phi_n = \int_{-\ell}^{\ell} \phi(y) \left(\cos\left(\frac{n\pi y}{\ell}\right) - i \sin\left(\frac{n\pi y}{\ell}\right) \right) \frac{dy}{\sqrt{2\ell}} = A_n - iB_n \quad (5.12.46)$$

$$\Rightarrow \operatorname{Re} \left(e^{\frac{i\pi nx}{\ell}} \phi_n \right) = \operatorname{Re} \left(\left(\cos\left(\frac{n\pi x}{\ell}\right) + i \sin\left(\frac{n\pi x}{\ell}\right) \right) (A_n - iB_n) \right) = A_n \cos\left(\frac{n\pi x}{\ell}\right) + B_n \sin\left(\frac{n\pi x}{\ell}\right). \quad (5.12.47)$$

With these definitions, we have:

$$\phi(x) = \frac{A_0}{\sqrt{2\ell}} + \sum_{n=1}^{\infty} \left(A_n \sqrt{\frac{2}{\ell}} \cos\left(\frac{n\pi x}{\ell}\right) + B_n \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi x}{\ell}\right) \right). \quad (5.12.48)$$

Here the A_n and B_n coefficients are completely independent and by definition are automatically real.

5.12.2 Electromagnetism in a Conducting Box

Now let us return to our problem in electromagnetism. We are considering the fields on the ranges $0 \leq x \leq \ell$, $0 \leq y \leq \ell$, $0 \leq z \leq \ell$. We could consider a Fourier series in each variable on these ranges but it turns out to be more convenient to consider a Fourier series for each variable on the ranges $-\ell \leq x \leq \ell$, $-\ell \leq y \leq \ell$, $-\ell \leq z \leq \ell$. Consider the x component of the vector potential. Then, at field t, x, z it is a function of y which we are considering for $-\ell \leq y \leq \ell$. So, we can write the x component of the vector potential as a series of the form:

$$A_x(t, x, y, z) = \frac{A_0(t, x, z)}{\sqrt{2\ell}} + \sum_{n=1}^{\infty} \left(A_n(t, x, z) \sqrt{\frac{2}{\ell}} \cos\left(\frac{n\pi y}{\ell}\right) + B_n(t, x, z) \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi y}{\ell}\right) \right). \quad (5.12.49)$$

We only need the vector potential for $0 \leq y \leq \ell$ and so we will only apply this series on that interval. Because of this, we can define how the vector potential behaves for $-\ell \leq y < 0$ arbitrarily (as we will never evaluate it in that region). Due to the conducting walls, we need the x component to vanish for $y = 0$ and $y = \ell$. We can make this happen automatically by defining the x component of the vector potential for negative y to be the negative of its value for positive y . That is, we define the x component of the vector potential in the opposite region to be so that it is an odd function of y :

$$A_x(t, x, -y, z) = -A_x(t, x, y, z). \quad (5.12.50)$$

This allows us to simplify the series coefficients by using the properties of even and odd functions on symmetric

intervals:

$$A_0(t, x, z) = \int_{-\ell}^{\ell} A_x(t, x, y, z) \frac{dy}{\sqrt{2\ell}} = 0, \quad A_n(t, x, z) = \int_{-\ell}^{\ell} A_x(t, x, y, z) \cos\left(\frac{n\pi y}{\ell}\right) \frac{dy}{\sqrt{2\ell}} = 0 \quad (5.12.51)$$

$$B_n(t, x, z) = \int_{-\ell}^{\ell} A_x(t, x, y, z) \sin\left(\frac{n\pi y}{\ell}\right) \frac{dy}{\sqrt{2\ell}} = \int_0^{\ell} A_x(t, x, y, z) \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi y}{\ell}\right) dy. \quad (5.12.52)$$

Thus the resulting x component is:

$$A_x(t, x, y, z) = \sum_{n_y=1}^{\infty} B_{n_y}(t, x, z) \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_y \pi y}{\ell}\right). \quad (5.12.53)$$

The coefficients $B_n(t, x, z)$ are then functions of z for which we can perform the same argument. They must have a Fourier series representation:

$$B_{n_y}(t, x, z) = \frac{C_{n_y 0}(t, x)}{\sqrt{2\ell}} + \sum_{n_z=1}^{\infty} \left(C_{n_y n_z}(t, x) \sqrt{\frac{2}{\ell}} \cos\left(\frac{n_z \pi z}{\ell}\right) + D_{n_y n_z}(t, x) \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_z \pi z}{\ell}\right) \right) \quad (5.12.54)$$

The series coefficients are then given by:

$$C_{n_y 0}(t, x) = \int_{-\ell}^{\ell} B_{n_y}(t, x, z) \frac{dz}{\sqrt{2\ell}} = \int_0^{\ell} \int_{-\ell}^{\ell} A_x(t, x, y, z) \frac{1}{\ell} \sin\left(\frac{n_y \pi y}{\ell}\right) dy dz \quad (5.12.55)$$

$$C_{n_y n_z}(t, x) = \int_{-\ell}^{\ell} B_{n_y}(t, x, z) \cos\left(\frac{n_z \pi z}{\ell}\right) \frac{dz}{\sqrt{2\ell}} = \int_0^{\ell} \int_{-\ell}^{\ell} A_x(t, x, y, z) \frac{1}{\ell} \sin\left(\frac{n_y \pi y}{\ell}\right) \cos\left(\frac{n_z \pi z}{\ell}\right) dy dz \quad (5.12.56)$$

$$D_{n_y n_z}(t, x) = \int_{-\ell}^{\ell} B_{n_y}(t, x, z) \sin\left(\frac{n_z \pi z}{\ell}\right) \frac{dz}{\sqrt{2\ell}} = \int_0^{\ell} \int_{-\ell}^{\ell} A_x(t, x, y, z) \frac{1}{\ell} \sin\left(\frac{n_y \pi y}{\ell}\right) \sin\left(\frac{n_z \pi z}{\ell}\right) dy dz. \quad (5.12.57)$$

Just as with the y behavior, we can define the x component of the vector potential for negative z to be anything and so we again define the vector potential to be an odd function of z . Then:

$$A_x(t, x, y, -z) = -A_x(t, x, y, z) \quad (5.12.58)$$

$$\implies C_{n_y 0}(t, x) = 0, \quad C_{n_y n_z}(t, x) = 0, \quad D_{n_y n_z}(t, x) = \int_0^{\ell} \int_0^{\ell} A_x(t, x, y, z) \frac{2}{\ell} \sin\left(\frac{n_y \pi y}{\ell}\right) \sin\left(\frac{n_z \pi z}{\ell}\right) dy dz. \quad (5.12.59)$$

So, the x component of the vector potential is given by:

$$A_x(t, x, y, z) = \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} D_{n_y n_z}(t, x) \frac{2}{\ell} \sin\left(\frac{n_y \pi y}{\ell}\right) \sin\left(\frac{n_z \pi z}{\ell}\right). \quad (5.12.60)$$

This now automatically satisfies the conducting wall boundary conditions on the walls of the cube at $y = 0$, $y = \ell$, $z = 0$, or $z = \ell$. There is no such requirement that $A_x(t, x, y, z)$ vanish for $x = 0$ or $x = \ell$. The coefficients $D_{n_y n_z}(t, x)$ can also be written as a Fourier series on $-\ell \leq x \leq \ell$:

$$D_{n_y n_z}(t, x) = \frac{A_{x0n_y n_z}(t)}{\sqrt{2\ell}} + \sum_{n_x=1}^{\infty} \left(A_{xn_x n_y n_z}(t) \sqrt{\frac{2}{\ell}} \cos\left(\frac{n_x \pi x}{\ell}\right) + B_{xn_x n_y n_z}(t) \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_x \pi x}{\ell}\right) \right). \quad (5.12.61)$$

So, the x component of the vector potential is generally given by:

$$A_x = \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{A_{x0n_y n_z}(t)}{2} + \sum_{n_x=1}^{\infty} \left(A_{xn_x n_y n_z}(t) \cos\left(\frac{n_x \pi x}{\ell}\right) + B_{xn_x n_y n_z}(t) \sin\left(\frac{n_x \pi x}{\ell}\right) \right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_y \pi y}{\ell}\right) \sin\left(\frac{n_z \pi z}{\ell}\right) \quad (5.12.62)$$

where $\vec{n} = (n_x, n_y, n_z)$. Because the cube and the boundary conditions have symmetry under the interchange $x \rightarrow y \rightarrow z \rightarrow x$ we have that the y and z components of the vector potential can be written as:

$$A_y = \sum_{n_z=1}^{\infty} \sum_{n_x=1}^{\infty} \left(\frac{A_{yn_x 0n_z}(t)}{2} + \sum_{n_y=1}^{\infty} \left(A_{yn_y n_x n_z}(t) \cos\left(\frac{n_y \pi y}{\ell}\right) + B_{yn_y n_x n_z}(t) \sin\left(\frac{n_y \pi y}{\ell}\right) \right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_z \pi z}{\ell}\right) \sin\left(\frac{n_x \pi x}{\ell}\right) \quad (5.12.63)$$

$$A_z = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{A_{zn_x n_y 0}(t)}{2} + \sum_{n_z=1}^{\infty} \left(A_{zn\vec{n}}(t) \cos\left(\frac{n_z \pi z}{\ell}\right) + B_{zn\vec{n}}(t) \sin\left(\frac{n_z \pi z}{\ell}\right) \right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_x \pi x}{\ell}\right) \sin\left(\frac{n_y \pi y}{\ell}\right). \quad (5.12.64)$$

These expressions for the vector potential satisfy all the conducting wall boundary conditions. Additionally, we need $\nabla \cdot \vec{A} = 0$ to satisfy our gauge conditions/Gauss' law. For convenience, define the shorthand:

$$\begin{aligned} c_x &= \sqrt{\frac{2}{\ell}} \cos\left(\frac{n_x \pi x}{\ell}\right), & c_y &= \sqrt{\frac{2}{\ell}} \cos\left(\frac{n_y \pi y}{\ell}\right), & c_z &= \sqrt{\frac{2}{\ell}} \cos\left(\frac{n_z \pi z}{\ell}\right), \\ s_x &= \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_x \pi x}{\ell}\right), & s_y &= \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_y \pi y}{\ell}\right), & s_z &= \sqrt{\frac{2}{\ell}} \sin\left(\frac{n_z \pi z}{\ell}\right). \end{aligned} \quad (5.12.65)$$

Then, the divergence of $\vec{A}$ is:

$$\nabla \cdot \vec{A} = \frac{\pi}{\ell} \sum_{n_a=1}^{\infty, \infty, \infty} \left(-(n_x A_{x\vec{n}} + n_y A_{y\vec{n}} + n_z A_{z\vec{n}}) s_x s_y s_z + n_x B_{x\vec{n}} c_x s_y s_z + n_y B_{y\vec{n}} s_x c_y s_z + n_z B_{z\vec{n}} s_x s_y c_z \right) \stackrel{!}{=} 0. \quad (5.12.66)$$

Because the various sines and cosines are linearly independent of each other as functions, we must have that these different combinations of sine and cosine vanish individually:

$$n_x A_{x\vec{n}} + n_y A_{y\vec{n}} + n_z A_{z\vec{n}} = n_x B_{x\vec{n}} = n_y B_{y\vec{n}} = n_z B_{z\vec{n}} = 0. \quad (5.12.67)$$

So, all of the B coefficients must vanish and the vector $\vec{A}_{\vec{n}}(t) = (A_{x\vec{n}}, A_{y\vec{n}}, A_{z\vec{n}})$ must satisfy:

$$\vec{n} \cdot \vec{A}_{\vec{n}}(t) = 0. \quad (5.12.68)$$

Then, all of our boundary and gauge conditions together imply the vector potential is given by:

$$A_x(t, \vec{x}) = \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{A_{x0n_y n_z}(t)}{2} + \sum_{n_x=1}^{\infty} A_{x\vec{n}}(t) \cos\left(\frac{n_x \pi x}{\ell}\right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_y \pi y}{\ell}\right) \sin\left(\frac{n_z \pi z}{\ell}\right) \quad (5.12.69)$$

$$A_y(t, \vec{x}) = \sum_{n_z=1}^{\infty} \sum_{n_x=1}^{\infty} \left(\frac{A_{yn_x 0n_z}(t)}{2} + \sum_{n_y=1}^{\infty} A_{y\vec{n}}(t) \cos\left(\frac{n_y \pi y}{\ell}\right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_z \pi z}{\ell}\right) \sin\left(\frac{n_x \pi x}{\ell}\right) \quad (5.12.70)$$

$$A_z(t, \vec{x}) = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{A_{zn_x n_y 0}(t)}{2} + \sum_{n_z=1}^{\infty} A_{z\vec{n}}(t) \cos\left(\frac{n_z \pi z}{\ell}\right) \right) \left(\frac{2}{\ell} \right)^{\frac{3}{2}} \sin\left(\frac{n_x \pi x}{\ell}\right) \sin\left(\frac{n_y \pi y}{\ell}\right) \quad (5.12.71)$$

where the components of $\vec{A}_{\vec{n}}(t)$ must satisfy equation (5.12.68).

Now that we have a fully general expression for the vector potential with all of our gauge conditions, Gauss' law, and boundary conditions applied we see that all of those constraints manifest as holonomic constraints that the vector potential is of the given form with $\phi = 0$. Because, we have a holonomic expression for the vector potential, we can insert it directly into the Lagrangian. For this, let us first rewrite the magnetic field term using integration by parts and that our vector potential is divergence free:

$$\int_{\mathbb{S}} |\nabla \times \vec{A}|^2 d^3 \vec{x} = \int_{\mathbb{S}} \nabla \times \vec{A} \cdot \nabla \times \vec{A} d^3 \vec{x} = \int_{\mathbb{S}} \vec{A} \cdot \nabla \times \nabla \times \vec{A} d^3 \vec{x} \quad (5.12.72)$$

$$= \int_{\mathbb{S}} \vec{A} \cdot (\nabla \nabla \cdot \vec{A} - \nabla^2 \vec{A}) d^3 \vec{x} = - \int_{\mathbb{S}} \vec{A} \cdot \nabla^2 \vec{A} d^3 \vec{x}. \quad (5.12.73)$$

So, we can equivalently write our Lagrangian as:

$$\mathcal{L} = \int_{\mathbb{V}} \left(\frac{1}{2} |\dot{\vec{A}}|^2 + \frac{1}{2} \vec{A} \cdot \nabla^2 \vec{A} \right). \quad (5.12.74)$$

In order to go further some particular integrals are useful. For integer $n \neq 0$:

$$\int_{-\ell}^{\ell} e^{\frac{in\pi x}{\ell}} dx = \frac{\ell}{in\pi} ((-1)^n - (-1)^n) = 0. \quad (5.12.75)$$

For $n = 0$:

$$\int_{-\ell}^{\ell} e^{\frac{in\pi x}{\ell}} dx = \int_{-\ell}^{\ell} dx = 2\ell. \quad (5.12.76)$$

Therefore:

$$\int_{-\ell}^{\ell} e^{\frac{i(n-m)\pi x}{\ell}} dx = 2\ell\delta_{nm}. \quad (5.12.77)$$

Breaking this into real and imaginary parts and using the evenness and oddness properties of cosine and sine we have:

$$\begin{aligned} \int_0^{\ell} \cos\left(\frac{n\pi x}{\ell}\right) \cos\left(\frac{m\pi x}{\ell}\right) dx &= \int_0^{\ell} \sin\left(\frac{n\pi x}{\ell}\right) \sin\left(\frac{m\pi x}{\ell}\right) dx = \frac{\ell}{2}\delta_{nm} \\ \int_0^{\ell} \sin\left(\frac{n\pi x}{\ell}\right) \cos\left(\frac{m\pi x}{\ell}\right) dx &= 0. \end{aligned} \quad (5.12.78)$$

With these integrals, we can directly insert our series expression into the Lagrangian and complete all integrations. Doing so and simplifying we arrive at:

$$\begin{aligned} \mathcal{L} &= \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} |\dot{\vec{A}}_{\vec{n}}|^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} |\vec{A}_{\vec{n}}|^2 \right) + \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} \dot{A}_{x0n_y n_z}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{x0n_y n_z}^2 \right) \\ &+ \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} \dot{A}_{yn_x 0n_z}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{yn_x 0n_z}^2 \right) + \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{1}{2} \dot{A}_{zn_x n_y 0}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{zn_x n_y 0}^2 \right) \end{aligned} \quad (5.12.79)$$

where $\vec{A}_{\vec{n}} = (A_{x\vec{n}}(t), A_{y\vec{n}}(t), A_{z\vec{n}}(t))$. This still hasn't fully implemented the constraints as we haven't fully imposed that $\vec{n} \cdot \vec{A}_{\vec{n}} = 0$. We can use the theory of circular polarizations developed in problem 4.40 to identify vectors $\vec{\xi}_{\vec{n}j}$ so that:

$$i\vec{n} \times \vec{\xi}_{\vec{n}j} = j|\vec{n}|\vec{\xi}_{\vec{n}j} \quad (5.12.80)$$

with $j \in \{-1, 0, 1\}$. The $j = 0$ vector is simply proportional to $\vec{n}$. For $j = \pm 1$, $\vec{\xi}_{\vec{n}j}$ is automatically orthogonal to $\vec{n}$ by taking the inner product of the above equation with $\vec{n}$. As well, these three vectors we see diagonalize the matrix $i\vec{n} \times$ which is self-adjoint and so define a basis (which is orthogonal and can be normalized to be orthonormal, which do by definition). Then, for some coefficients $A_{\vec{n}j}(t)$ we can write:

$$\vec{A}_{\vec{n}}(t) = \sum_{j=-1}^j A_{\vec{n}j}(t) \vec{\xi}_{\vec{n}j} = A_{\vec{n}-1}(t) \vec{\xi}_{\vec{n}-1} + A_{\vec{n}0}(t) \vec{\xi}_{\vec{n}0} + A_{\vec{n}1}(t) \vec{\xi}_{\vec{n}1}. \quad (5.12.81)$$

Then, $\vec{n} \cdot \vec{A}_{\vec{n}}$ selects out the coefficient $A_{\vec{n}0}$. The requirement that $\vec{n} \cdot \vec{A}_{\vec{n}} = 0$ then implies that $A_{\vec{n}0} = 0$. Consequently, after constraint:

$$\vec{A}_{\vec{n}}(t) = A_{\vec{n}-1}(t) \vec{\xi}_{\vec{n}-1} + A_{\vec{n}1}(t) \vec{\xi}_{\vec{n}1} \quad (5.12.82)$$

and using orthonormality:

$$|\vec{A}_{\vec{n}}|^2 = A_{\vec{n}-1}^2 + A_{\vec{n}1}^2. \quad (5.12.83)$$

Then, the Lagrangian with all constraints included is:

$$\begin{aligned} \mathcal{L} &= \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} \dot{A}_{\vec{n}-1}^2 + \frac{1}{2} \dot{A}_{\vec{n}1}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} (A_{\vec{n}-1}^2 + A_{\vec{n}1}^2) \right) + \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} \dot{A}_{x0n_y n_z}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{x0n_y n_z}^2 \right) \\ &+ \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{1}{2} \dot{A}_{yn_x 0n_z}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{yn_x 0n_z}^2 \right) + \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{1}{2} \dot{A}_{zn_x n_y 0}^2 - \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{zn_x n_y 0}^2 \right) \end{aligned} \quad (5.12.84)$$

If we compute the conjugate momenta:

$$\begin{aligned} P_{\vec{n}\pm 1} &= \frac{\partial \mathcal{L}}{\partial \dot{A}_{\vec{n}\pm 1}} = \dot{A}_{\vec{n}\pm 1}, & P_{x0n_y n_z} &= \frac{\partial \mathcal{L}}{\partial \dot{A}_{x0n_y n_z}} = \dot{A}_{x0n_y n_z}, \\ P_{yn_x 0n_z} &= \frac{\partial \mathcal{L}}{\partial \dot{A}_{yn_x 0n_z}} = \dot{A}_{yn_x 0n_z}, & P_{zn_x n_y 0} &= \frac{\partial \mathcal{L}}{\partial \dot{A}_{zn_x n_y 0}} = \dot{A}_{zn_x n_y 0} \end{aligned} \quad (5.12.85)$$

then we can complete the Legendre transformation to arrive at the Hamiltonian:

$$\mathcal{H} = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{P_{\vec{n}-1}^2}{2} + \frac{P_{\vec{n}1}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} (A_{\vec{n}-1}^2 + A_{\vec{n}1}^2) \right) + \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{P_{x0n_y n_z}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{x0n_y n_z}^2 \right)$$

$$+ \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{P_{y n_x 0 n_z}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{y n_x 0 n_z}^2 \right) + \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{P_{z n_x n_y 0}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} A_{z n_x n_y 0}^2 \right). \quad (5.12.86)$$

This is simply a series (of an infinite number) of non-interacting harmonic oscillators. Each of these oscillators has angular frequency given by:

$$\omega_{\vec{n}} = \frac{\pi |\vec{n}|}{\ell}. \quad (5.12.87)$$

Due to the multiplicativity of the partition function (equation (5.5.37)), $\ln Z$ is extensive and then automatically the Helmholtz free energy is as well. Because electromagnetism consists of this series of non-interacting harmonic oscillators the free energy for electromagnetism is simply given by the sum over the free energies for each oscillator:

$$\mathcal{F} = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} (\mathcal{F}_{\vec{n}+1} + \mathcal{F}_{\vec{n}-1}) + \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_{x 0 n_y n_z} + \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_{y n_x 0 n_z} + \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \mathcal{F}_{z n_x n_y 0}. \quad (5.12.88)$$

Because we are doing thermodynamics, we would like to take the thermodynamic limit and thus need to scale all extensive variables together while keeping the intensive quantities fixed. So, we want to compute the limit of $\mathcal{F}/\mathbb{V}$ as $\mathbb{V} = \ell^3 \rightarrow \infty$ to get the free energy in the thermodynamic limit. The frequency of each oscillator implicitly depends on ℓ but because the frequency of an oscillator is intensive we will need to keep it fixed. That is, we will scale $\vec{n}$ with ℓ so that ω is fixed. For this, it is useful to define the wavevector $\vec{k}$:

$$\vec{k} = \frac{\pi \vec{n}}{\ell} \implies \omega = |\vec{k}|. \quad (5.12.89)$$

Then, because each component of $\vec{n}$ increments by 1 between each term in the sum, $\Delta n_x = \Delta n_y = \Delta n_z = 1$. The corresponding increment in the components of $\vec{k}$ is:

$$\Delta^3 \vec{k} = \Delta k_x \Delta k_y \Delta k_z = \frac{\pi \Delta n_x}{\ell} \frac{\pi \Delta n_y}{\ell} \frac{\pi \Delta n_z}{\ell} = \frac{\pi^3}{\mathbb{V}} \quad (5.12.90)$$

$$\implies \frac{1}{\mathbb{V}} = \frac{\Delta^3 \vec{k}}{\pi^3}. \quad (5.12.91)$$

So, we have:

$$\begin{aligned} \frac{\mathcal{F}}{\mathbb{V}} &= \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} (\mathcal{F}_{\vec{n}+1} + \mathcal{F}_{\vec{n}-1}) \Delta^3 \vec{k} + \frac{1}{\pi^3} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_{x 0 n_y n_z} \Delta^3 \vec{k} \\ &+ \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_{y n_x 0 n_z} \Delta^3 \vec{k} + \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \mathcal{F}_{z n_x n_y 0} \Delta^3 \vec{k}. \end{aligned} \quad (5.12.92)$$

Let $\mathcal{F}_1(T, \omega)$ be the free energy of a single harmonic oscillator of angular frequency ω at temperature T . Then:

$$\begin{aligned} \frac{\mathcal{F}}{\mathbb{V}} &= \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} 2\mathcal{F}_1(T, |\vec{k}|) \Delta^3 \vec{k} + \frac{1}{\pi^3} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_1(T, |\vec{k}|) \Delta^3 \vec{k} \\ &+ \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \mathcal{F}_1(T, |\vec{k}|) \Delta^3 \vec{k} + \frac{1}{\pi^3} \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \mathcal{F}_1(T, |\vec{k}|) \Delta^3 \vec{k}. \end{aligned} \quad (5.12.93)$$

In the limit $\mathbb{V} \rightarrow \infty$ these sums then become Riemann sums and thus turn into integrals over $\vec{k}$. So, in the thermodynamic limit we have:

$$\begin{aligned} \frac{\mathcal{F}}{\mathbb{V}} &= \frac{2}{\pi^3} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3 \vec{k} + \frac{1}{\pi^3} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3 \vec{k} \\ &+ \frac{1}{\pi^3} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3 \vec{k} + \frac{1}{\pi^3} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3 \vec{k}. \end{aligned} \quad (5.12.94)$$

We can see that the modes which had a single component of $\vec{n}$ as equal to 0 have a contribution which limits to 0 in the thermodynamic limit. So:

$$\mathcal{F} = \frac{2\mathbb{V}}{\pi^3} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3 \vec{k}. \quad (5.12.95)$$

Because the integrand is an even function of each component of $\vec{k}$, we can extend the integral to over all $\vec{k}$ by using the properties of even functions:

$$\mathcal{F} = \frac{2\mathbb{V}}{\pi^3} \frac{1}{8} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{F}_1(T, |\vec{k}|) d^3\vec{k}. \quad (5.12.96)$$

Then, using spherical coordinates and that $\omega = |\vec{k}|$:

$$\mathcal{F} = \frac{\mathbb{V}}{4\pi^3} \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} \mathcal{F}_1(T, \omega) \omega^2 \sin \theta d\varphi d\theta d\omega \quad (5.12.97)$$

$$= \frac{\mathbb{V}}{\pi^2} \int_0^{\infty} \mathcal{F}_1(T, \omega) \omega^2 d\omega. \quad (5.12.98)$$

Thus, all we need is the free energy of a single harmonic oscillator to get the free energy of electromagnetism.

For a single harmonic oscillator we found before that the partition function is given by equation (5.5.25):

$$Z_1 = \frac{1}{\hbar\omega\beta} \implies \mathcal{F}_1(T, \omega) = -T \ln Z_1 = T \ln \left(\frac{\hbar\omega}{T} \right). \quad (5.12.99)$$

Then, the free energy is given by:

$$\mathcal{F} = \frac{\mathbb{V}}{\pi^2} \int_0^{\infty} T \ln \left(\frac{\hbar\omega}{T} \right) \omega^2 d\omega. \quad (5.12.100)$$

This integral has quite the problem! As $\omega \rightarrow \infty$, the integrand diverges and so the integral does as well. Thus, it seems the free energy of electromagnetism is ill-defined. Perhaps there is some way we can find around this. Because this has trouble for large frequencies, let us consider it up to some cutoff frequency Ω and see if there is any way to get some physical prediction which drops the Ω dependence. Sometimes it happens that a quantity in a theory may naively diverge or become 0 but the observable predictions computed from that quantity remain finite in the limit of interest. Up to this cutoff frequency:

$$\mathcal{F}_{\Omega} = \frac{\mathbb{V}}{\pi^2} \int_0^{\Omega} T \ln \left(\frac{\hbar\omega}{T} \right) \omega^2 d\omega \stackrel{\omega = \frac{T}{\hbar}x}{=} \frac{\mathbb{V}T^4}{\pi^2\hbar^3} \int_0^{\frac{\hbar\Omega}{T}} x^2 \ln x dx = \frac{\mathbb{V}T^4}{\pi^2\hbar^3} \left(\frac{\hbar^3\Omega^3}{3T^3} \ln \frac{\hbar\Omega}{T} - \frac{\hbar^3\Omega^3}{9T^3} \right) \quad (5.12.101)$$

$$= \frac{\mathbb{V}T\Omega^3}{9\pi^2} \left(3 \ln \frac{\hbar\Omega}{T} - 1 \right). \quad (5.12.102)$$

We can see explicitly that this diverges in the limit $\Omega \rightarrow \infty$. Experiments don't directly measure $\mathcal{F}$ for a system. Instead they measure the way that system responds to probes, such as its heat capacity. A system's temperature can be measured, a known amount of energy can be transferred to that system, and then its final temperature measured. This allows one to measure its heat capacity defined as the necessary amount of heat that must be transferred to a system per unit change of temperature. So, the heat capacity at fixed volume of our system is given by:

$$C_V = \frac{dQ}{dT} = \frac{dE - dW}{dT} = \frac{dE}{dT} \quad (5.12.103)$$

where $dW = -pdV = 0$ because the volume (the only macroscopic variable in the Hamiltonian) does not change and the T derivative is taken at fixed $\mathbb{V}$. We can compute the energy by the Legendre transformation:

$$S = -\frac{\partial \mathcal{F}}{\partial T} = \frac{\mathbb{V}\Omega^3}{3\pi^2} - \frac{\mathbb{V}\Omega^3}{9\pi^2} \left(3 \ln \frac{\hbar\Omega}{T} - 1 \right) \quad (5.12.104)$$

$$\implies E = \mathcal{F} + TS = \frac{\mathbb{V}\Omega^3 T}{3\pi^2}. \quad (5.12.105)$$

Then, the heat capacity is:

$$C_V = \frac{dE}{dT} = \frac{\mathbb{V}\Omega^3}{3\pi^2}. \quad (5.12.106)$$

So, the heat capacity also diverges as $\Omega \rightarrow \infty$ and appears to be temperature independent. This would suggest that it would take an infinite amount of energy to raise the temperature of any conducting volume by any amount and that an infinite amount of energy is released by the cooling of a conducting volume. This is of course completely experimentally incorrect. Experimentally the heat capacity should be finite. As well, it is observed to be temperature dependent. So, somehow and for some reason applying thermodynamics to classical electromagnetism is just completely wrong. This fundamental disagreement between the application of thermodynamics to electromagnetism and experiment fact is known as the ultraviolet catastrophe. The

catastrophe is called “ultraviolet” because the diverging result comes from the high frequency behavior of the integral in (5.12.100).

This glitch that the free energy, energy, and heat capacity diverge at any finite temperature is not specific to electromagnetism. It happens for any classical field theory when put into statistical mechanics. It is easy enough to see why this is the case. Any stable theory near equilibrium is approximately some number of harmonic oscillators by theorem 1.14. Any field theory though has an infinite number of degrees of freedom and so in this limit becomes an infinite number of harmonic oscillators. Each harmonic oscillator has a heat capacity of 1 and so any field theory in the weak field limit will have infinite heat capacity. There are just too many oscillators! There is no way to resolve this in classical mechanics. One could think that perhaps statistical mechanics just isn’t valid for field theories. But, it is certainly true that conducting objects have a measurable temperature. It is further true that sufficiently hot objects radiate measurable amounts of light and so there must be some theory which describes electromagnetism with thermodynamics. Because classical field theory and classical statistical mechanics are incapable of solving this issue, there must be some better theory which reduces to these two as effective theories under appropriate circumstances yet can harmonize the two of them for electromagnetism (and other field theories). That better theory will be the subject of Part II.

5.12.3 Black Body Radiation

We can get another perspective on what is going on with the relationship between electromagnetism and statistical mechanics by now allowing our conducting box to radiate energy. Everything was looking pretty reasonable with our previous analysis before we actually supplied a formula for $\mathcal{F}_1(T, \omega)$, so let us hold off on doing so for now. If our conducting box is very large ($\mathbb{V} \rightarrow \infty$) we saw that it develops a continuous spectrum (ω becomes continuous). Imagine we have a very large conducting box with a small hole in it so that electromagnetic waves may exit through the hole. By the result of problem 4.38, the time averaged Poynting vector (or energy density) of the entire radiation is simply given by summing over the time averaged Poynting vector (or energy density) of each wave of different frequency. As well, by the rest of the same problem, the magnitude of each plane wave’s time averaged Poynting vector is simply given by the time averaged energy density of that wave. So, the total time averaged power radiated through the hole per unit area of the hole is:

$$\frac{d\mathcal{P}}{d\mathbb{A}} = \mathbb{T}(\vec{S}_{\text{total}}) \cdot \vec{n} = \mathbb{T}(\mathcal{E}_{\text{total}}) \cos \theta \quad (5.12.107)$$

where $\vec{n}$ is the vector pointing toward the point at which the radiation is to be detected far away and θ is the angle between the Poynting vector and $\vec{n}$. The total free energy of our system is given by (5.12.98). From there we can compute the total energy using the Legendre transform:

$$\mathbb{E} = \mathcal{F} - T \frac{\partial \mathcal{F}}{\partial T} = \frac{\mathbb{V}}{\pi^2} \int_0^\infty \left(\mathcal{F}_1 - T \frac{\partial \mathcal{F}_1}{\partial T} \right) \omega^2 d\omega = \frac{\mathbb{V}}{\pi^2} \int_0^\infty \mathbb{E}_1(T, \omega) \omega^2 d\omega \quad (5.12.108)$$

where $\mathbb{E}_1(T, \omega)$ is the energy of a single oscillator of frequency ω at temperature T . Then, the total time averaged energy density is given by:

$$\mathbb{T}(\mathcal{E}_{\text{total}}) = \frac{\mathbb{E}}{\mathbb{V}} = \frac{1}{\pi^2} \int_0^\infty \mathbb{E}_1(T, \omega) \omega^2 d\omega. \quad (5.12.109)$$

With this the power radiated per unit area of the hole becomes:

$$\frac{d\mathcal{P}}{d\mathbb{A}} = \frac{\cos \theta}{\pi^2} \int_0^\infty \mathbb{E}_1(T, \omega) \omega^2 d\omega. \quad (5.12.110)$$

Now consider that the entire surface of the box is allowed to radiate (an object which radiates and absorbs energy but does not reflect it is called a black-body, so this is often called black-body radiation). Then, the spectral radiance $R(T, \omega)$, which is the radiated power per unit surface area of the radiating body per unit solid angle of outgoing radiation per unit frequency is by definition the function which satisfies:

$$\frac{d\mathcal{P}}{d\mathbb{A}} = \int_\Omega \int_0^\infty R(T, \omega, \theta, \varphi) \cos \theta d\omega d\Omega. \quad (5.12.111)$$

Comparing this to (5.12.110) gives that the spectral radiance of electromagnetic radiation from a body at temperature T is:

$$R(T, \omega) = \frac{\omega^2}{4\pi^3} \mathbb{E}_1(T, \omega). \quad (5.12.112)$$

We have suppressed that in principle the spectral radiance of a general object is allowed to be anisotropic

(and so R may depend on θ and φ) because for our black body in thermodynamic equilibrium R is isotropic. Because $R(T, \omega)$ is directly observable (we have detectors that detect incident electromagnetic energy and can be tuned to be sensitive to specific frequencies) and because we know how to measure temperatures, we can use this formula to measure $E_1(T, \omega)$ empirically.

5.12.4 Planck's Law

Because the integrand in equation (5.12.100) is perfectly okay for small ω one might expect that for small ω E_1 measured this way should agree with our established understanding of a harmonic oscillator that $E_1 = T$. Empirically, this is actually true. So, for small frequencies:

$$E_1 \approx T \implies R(T, \omega) \approx \frac{\omega^2 T}{4\pi^3}. \quad (5.12.113)$$

However, these do not hold for sufficiently large frequencies. They can't due to the divergence of the equation (5.12.100) integrand for large frequencies. Instead, $R(T, \omega)$ for large frequencies can be fit to a functional form by matching against experimental data. Historically, doing so against simple experimental forms found that for large frequencies $R(T, \omega)$ is approximately given by:

$$R(T, \omega) \approx \frac{\hbar \omega^3}{4\pi^3} e^{-\frac{\hbar \omega}{T}} \implies E_1 \approx \hbar \omega e^{-\frac{\hbar \omega}{T}} \quad (5.12.114)$$

for some positive constant $\hbar$ (known as Planck's constant) which is fit to data. At this time in our development we will treat this as an empirical formula; we won't fully figure out the theory that explains it until chapter 9.

We are now going to be very speculative and guess at what is going on. The arguments here will be suggestive, not deductive and we make them for the purpose of trying to lead us in the correct direction. The small ω condition can be written (using the relationship between temperature, energy, and entropy) as:

$$\frac{\partial S_1}{\partial E_1} = \frac{1}{T} \approx \frac{1}{E_1} \quad (5.12.115)$$

$$\implies \frac{\partial^2 S_1}{\partial E_1^2} \approx -\frac{1}{E_1^2}. \quad (5.12.116)$$

The large ω condition can be written as:

$$\frac{\partial S_1}{\partial E_1} = \frac{1}{T} \approx -\frac{1}{\hbar \omega} \ln \left(\frac{E_1}{\hbar \omega} \right) \quad (5.12.117)$$

$$\implies \frac{\partial^2 S_1}{\partial E_1^2} \approx -\frac{1}{\hbar \omega E_1}. \quad (5.12.118)$$

We can make (5.12.116) valid for small ω and (5.12.118) valid for large ω by the single guessed formula:

$$\frac{\partial^2 S_1}{\partial E_1^2} = -\frac{1}{E_1(E_1 + \hbar \omega)}. \quad (5.12.119)$$

This is certainly not the only way to make both approximations valid in their respective regimes, it is just a simple guess. We can integrate this guess once with respect to E_1 to get that for some constant C :

$$\frac{\partial S_1}{\partial E_1} = \frac{1}{T} = C + \frac{1}{\hbar \omega} \ln \left(1 + \frac{\hbar \omega}{E_1} \right). \quad (5.12.120)$$

For small ω this must reproduce (5.12.117) and that requirement fixes $C = 0$. Then, both the large ω and small ω behavior of this formula correctly matches out previous approximate expressions. We can invert this to find that E_1 is given by:

$$E_1 = \frac{\hbar \omega}{e^{\frac{\hbar \omega}{T}} - 1}. \quad (5.12.121)$$

The resulting spectral radiance this produces is:

$$R(T, \omega) = \frac{\hbar \omega^3}{4\pi^3} \frac{1}{e^{\frac{\hbar \omega}{T}} - 1}. \quad (5.12.122)$$

This result is known as Planck's law and is in extremely good correspondence with experiment across frequencies we are capable of measuring.

Using our expression for E_1 we can infer the partition function Z_1 of a single oscillator with this model

by:

$$-\frac{\partial}{\partial \beta} \ln Z_1 = E_1 = \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \quad (5.12.123)$$

$$\implies Z_1 = \frac{A}{1 - e^{-\beta \hbar \omega}} \quad (5.12.124)$$

for some constant A . The small ω expansion of this gives:

$$Z_1 \approx \frac{AT}{\hbar \omega}. \quad (5.12.125)$$

Previously we found in (5.5.25) that the partition function for a single oscillator is $\frac{T}{\hbar \omega}$ where the $\hbar$ appearing there is the arbitrary positive constant with units of the action that is put in the phase space measure for the purposes of making it unitless. If we choose that arbitrary factor to match the $\hbar$ that appears here in our guessed formula (this is allowed because the one in the phase space measure is truly arbitrary) then to match our classical oscillator formula at low frequencies we must have $A = 1$. With this we now have:

$$\mathcal{F}_1 = -T \ln Z_1 = T \ln \left(1 - e^{-\frac{\hbar \omega}{T}} \right). \quad (5.12.126)$$

Returning this integrand to (5.12.98):

$$\mathcal{F} = \frac{\mathbb{V}}{\pi^2} \int_0^\infty T \omega^2 \ln \left(1 - e^{-\frac{\hbar \omega}{T}} \right) d\omega. \quad (5.12.127)$$

Make the integration change of variables $x = \frac{\hbar \omega}{T}$. Then:

$$\mathcal{F} = \frac{\mathbb{V} T^4}{\pi^2 \hbar^3} \int_0^\infty x^2 \ln(1 - e^{-x}) dx. \quad (5.12.128)$$

The remaining integral is able to be analytically evaluated:

$$\int_0^\infty x^2 \ln(1 - e^{-x}) dx = -\frac{\pi^4}{45}. \quad (5.12.129)$$

Thus we arrive at the free energy:

$$\mathcal{F} = -\frac{\pi^2 \mathbb{V} T^4}{45 \hbar^3} \quad (5.12.130)$$

and the expected energy:

$$E = \mathcal{F} - T \frac{\partial \mathcal{F}}{\partial T} = \frac{\pi^2 \mathbb{V} T^4}{15 \hbar^3}. \quad (5.12.131)$$

This then produces that the heat capacity for a black body should be:

$$C_V = \frac{dE}{dT} = \frac{4\pi^2 \mathbb{V} T^3}{15 \hbar^3} \quad (5.12.132)$$

which is also in very good agreement with experiment. So, there is something nontrivial working about our weird guessed formula.

We can also compute the total electromagnetic power radiated away by the black body. Radiation only escapes the black body if the radiation at the surface is directed out of the body and so only half of the solid angle sphere contributes. Then, the total power radiated is:

$$\mathcal{P} = \int_{\mathbb{A}} \int_{\Omega} \int_0^\infty R(T, \omega) \cos \theta d\omega d\Omega d\mathbb{A} \quad (5.12.133)$$

$$= \int_{\mathbb{A}} d\mathbb{A} \int_0^{2\pi} d\varphi \int_0^{\frac{\pi}{2}} \sin \theta \cos \theta d\theta \int_0^\infty \frac{\hbar \omega^3}{4\pi^3} \frac{1}{e^{\frac{\hbar \omega}{T}} - 1} d\omega \quad (5.12.134)$$

$$= \mathbb{A}(2\pi) \frac{1}{2} \frac{T^4}{4\pi^3 \hbar^3} \int_0^\infty \frac{x^3 dx}{e^x - 1} \quad (5.12.135)$$

using the same integral change of variables as before. Again this integral can be analytically calculated (and is actually related to our previous integral by integration by parts):

$$\int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}. \quad (5.12.136)$$

Therefore we arrive at the total radiated power:

$$\mathcal{P} = \frac{\pi^2 \mathbb{A} T^4}{60 \hbar^3}. \quad (5.12.137)$$

This is known as the Stefan-Boltzmann law and it is again in very good agreement with experiment.

We have derived several formulas which are in good agreement with experiment from our weird guess (5.12.119). But, we don't know how to actually produce that equation on theoretical grounds. Equivalently, we have (at this point) no idea how to derive (5.12.121) or (5.12.126) from some microscopic theory. By using a different internal energy per oscillator than the standard result, we are essentially saying that electromagnetism must not be just pure classical harmonic oscillators at high frequencies. But what is it? We can learn a little bit about the correct microscopic theory but studying what the thermodynamics we have found here imply. We know that the partition function Z is related to the density of states $g(E)$ by the Laplace transform by the result of problem 5.29:

$$Z(\beta) = \int_{-\infty}^{\infty} e^{-\beta E} g(E) dE \quad (5.12.138)$$

which is known to be invertible (Lerch's theorem). For a classical harmonic oscillator the density of states can be easily calculated to be:

$$g(E) = \frac{1}{\hbar \omega} \vartheta(E). \quad (5.12.139)$$

And through the Laplace transform this produces the correct classical partition function in equation (5.5.25). Alternatively, the partition function we found in (5.12.124) can be written as:

$$Z_1 = \frac{1}{1 - e^{-\beta \hbar \omega}} = \sum_{n=0}^{\infty} e^{-n\beta \hbar \omega} = \int_{-\infty}^{\infty} e^{-\beta E} \left(\sum_{n=0}^{\infty} \delta(E - n\hbar \omega) \right) dE. \quad (5.12.140)$$

Therefore, the density of states implied by (5.12.124) is:

$$g(E) = \sum_{n=0}^{\infty} \delta(E - n\hbar \omega). \quad (5.12.141)$$

So somehow whatever microscopic theory corrects the high frequency behavior of electromagnetism it apparently seems to have a density of states which is given by this discrete systematic placement of Dirac deltas. Max Planck originally discovered this and inferred that sufficiently microscopically light is actually made of wave packets (called photons, which had previously been suggested by Einstein) with energy proportional to their frequency ω and proportionality constant $\hbar$. Then, the interpretation of this formula is that for a given frequency ω there will be some number of wave packets n and the total energy of such a collection would then be $n\hbar\omega$. Because any number of wave packets is possible the density of states has a spike for each n . There was some hint of all of this back in problem 4.50 but the analysis there gives no indication that the different wave packets should have the same value of $\hbar$. The ultimate resolution to why microscopically electromagnetism behaves like a collection of wavepackets of energy $\hbar\omega$ each will have to wait for chapter 9.

Exercises

Problem 5.53: Parseval's Theorem for Fourier Series. Consider two (possibly complex) functions $f(x)$ and $g(x)$ on the interval $(-\ell, \ell)$. Using the fundamental Fourier series, show that the Fourier series for $f(x)$ and $g(x)$ satisfy:

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \int_{-\ell}^{\ell} f^*(x) g(x) dx.$$

Problem 5.54: Some Common Thermodynamic Integrals. Often in thermodynamics, as we found in this section, we face integrals of the types:

$$I(\alpha) = \int_0^{\infty} x^{\alpha} \ln(1 - e^{-x}) dx, \quad J(\alpha) = \int_0^{\infty} \frac{x^{\alpha}}{e^x - 1} dx$$

where $\alpha > 0$. Often but not always we find that in applications α is an integer.

(a) Show using integration by parts that:

$$J(\alpha) = -\alpha I(\alpha - 1).$$

(b) Show that in $I(\alpha)$ we can safely series expand the natural logarithm as:

$$\ln(1 - e^{-x}) = - \sum_{n=1}^{\infty} \frac{e^{-nx}}{n}$$

and that the series commutes with the integral so that:

$$I(\alpha) = - \sum_{n=1}^{\infty} \frac{1}{n} \int_0^{\infty} x^{\alpha} e^{-nx} dx.$$

(c) Recall the definition of the Gamma function $\Gamma(x)$ and define the Riemann Zeta function $\zeta(x)$:

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt, \quad \zeta(x) = \sum_{n=1}^{\infty} \frac{1}{n^x}.$$

Show that:

$$I(\alpha) = -\Gamma(\alpha+1)\zeta(\alpha+2), \quad J(\alpha) = \Gamma(\alpha+1)\zeta(\alpha+1).$$

(d) Consider the function $f(x) = x$ on the interval $(-\pi, \pi)$. Show that the Fourier coefficients f_n are:

$$f_0 = 0, \quad f_n = i\sqrt{2\pi} \frac{(-1)^n}{n} \quad (n \neq 0).$$

Show using Parseval's theorem for Fourier series with $g(x) = f(x)$ that:

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

Use this to show that:

$$I(0) = -\frac{\pi^2}{6}, \quad J(1) = \frac{\pi^2}{6}.$$

(e) Consider the function $f(x) = x^2$ on the interval $(-\pi, \pi)$. Show that the Fourier coefficients f_n are:

$$f_0 = \frac{\pi^2}{3}\sqrt{2\pi}, \quad f_n = \frac{2}{n^2}\sqrt{2\pi}(-1)^n \quad (n \neq 0).$$

Show using Parseval's theorem for Fourier series with $g(x) = f(x)$ that:

$$\zeta(4) = \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90}.$$

Use this to show that:

$$I(2) = -\frac{\pi^4}{45}, \quad J(3) = \frac{\pi^4}{15}$$

thus providing the values to the relevant integrals for electromagnetism.

5.13 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 5.1: Characteristic function of a probability distribution** introduces the characteristic function and demonstrates its useful properties for calculations.
- **Problem 5.6: The Gamma function and Sterling's Theorem** introduces the Gamma function $\Gamma(x)$ which will be repeatedly useful for us.
- **Problem 5.24: Borel-Kolmogorov Paradox or how I learned to start living and stop dividing by 0** demonstrates that one needs to be very careful when attempting to define conditional probability when conditioning on a continuous random variable.
- **Problem 5.28: Equipartition Theorem** establishes a useful shortcut formula for computing the expected energy of a quadratic Hamiltonian.
- **Problem 5.31: Thermodynamic Limit of Extensive Quantities** establishes that in the thermodynamic limit the relative fluctuations of extensive quantities vanish and so the quantities develop effectively precise values.
- **Problem 5.38: No Classical Magnetization** establishes that no classical system of charges can explain the observed macroscopic properties of matter.
- **Problem 5.39: Heating up a table** gives a simple example of how to compute some of the basic effects of friction.
- **Problem 5.42: Lorentz Invariance of the Phase Space Density** demonstrates that the phase space density of a relativistic free particle is Lorentz invariant. The result persists if the particle is subject to interactions which have symmetry under Lorentz transformations.
- **Problem 5.43: Relativistic Ideal Gas** demonstrates that the analysis of the ideal gas can be extended to relativistic particles, identifies that temperature is Lorentz invariant, defines the Lorentz invariant momentum space measure, and shows how to express the equilibrium momentum distribution for relativistic particles in a Lorentz invariant way.
- **Problem 5.48: Heat Engines and the Carnot Cycle** demonstrates what limits the laws of thermodynamics place on the possible operation of a heat engine.
- **Problem 5.52: Measuring numbers of particles** explains how using the established method of measuring temperature one can measure the number of particles in an ideal gas.

In this chapter we developed the theory of statistical mechanics and thermodynamics of classical systems. This theory allows us to describe the long term and very slow behavior of very large systems composed of many weakly interacting degrees of freedom. In doing so we introduced several new interesting experimental quantities, including the temperature, entropy, and thermodynamic potentials. The theory of statistical mechanics is essential for connecting our highly overly idealized models of a single or just a few particles and no other degrees of freedom from the first several chapters to realistic experiments which involve overwhelmingly many degrees of freedom, most of which the experiment will be insensitive to measuring.

In section 5.1, we introduced the mathematical theory of probability, which is the formalism for how to appropriately make calculation in a system with incomplete information. In section 5.2, we derived the Liouville equation to describe the evolution of the probability density function of our phase space variables in time. The Liouville equation acts as the equation of motion of statistical mechanics. In section 5.3, we introduced the concepts of macroscopic variables and microscopic variables and used them to define the concepts of useful work and heat as well as derive the first law of thermodynamics. In section 5.4, we discussed the assumptions under which it is reasonable to use the microcanonical ensemble distribution to describe a system. In section 5.5, we discussed the assumptions under which it is reasonable to use the canonical ensemble distribution to describe a system. In section 5.6, we formally introduced the notion of information in probability and discussed its usefulness in statistical mechanics. In section 5.7, we used the notion of entropy from information theory to derive the second law of thermodynamics and give a coordinate independent characterization of thermodynamic equilibrium. In section 5.8, we introduced the quasidynamic approximation in which some macroscopic degrees of freedom of a system evolve so slowly that its microscopic degrees of freedom can always be assumed to be in thermodynamic equilibrium and found the appropriate equations of motion for those macroscopic variables. In section 5.9, we introduced the quasistatic approximation which is the quasidynamic approximation combined with the approximation that the macroscopic variables evolve so slowly that we can always instantaneously approximate their velocities to 0. In doing so, we were able to introduce and understand the chemical potential, thermodynamic potentials, and equations of state of a thermodynamic

system. In section 5.10, we defined various types of thermodynamic processes and studied the concavity properties of the energy, entropy, and chemical potential necessary for stability. In section 5.11, we studied the behavior of a system initially in equilibrium when it is subjected to a weak force to bring it weakly out of equilibrium. This provided us with direct methods of measuring temperature. In section 5.12, we found that there is no way for a classical field theory to reach thermodynamic equilibrium, in contradiction with the experimental fact that hot metal glows.

The very real incompatibility of classical field theory and statistical mechanics is a fundamental theoretical issue which will be essential to Part II. We found that the apparently correct theory seems to correspond to a microscopic theory in which electromagnetism consists of wave packets each carrying energy proportional to their frequency. Point particles have divergent interactions and classical fields aren't compatible with statistical mechanics. Knowing both of these approaches are flawed, what else could we try? This perspective is summarized in figure 5.2.

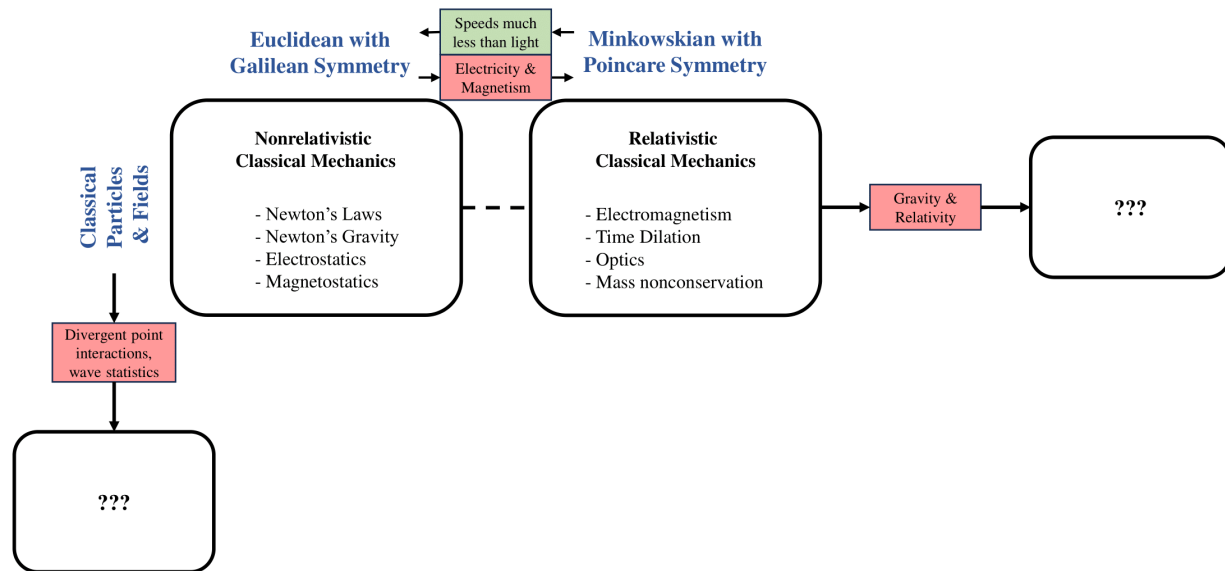


Figure 5.2: Our perspective on physics as of the end of this chapter. We have yet to work out a relativistically consistent theory of gravity which allows for mass nonconservation. We have found that point particles have divergent interactions once relativity is accounted for and that classical fields have divergent thermodynamic properties once statistical mechanics is accounted for. There is a fundamental tension between classical field theory and statistical mechanics.

This chapter is by no means a complete treatment of essential topics in the mathematical theories probability or statistics or in Classical Statistical Mechanics. For completeness sake, refer to [7], [4], [20], [53], [19], [123] for further discussions of probability and statistics and [61], [57], [118], [106], [116] for further discussions and insight into statistical mechanics.

Chapter 6

Continuum Mechanics

*Tide goes in, tide goes out.
Never a miscommunication.
You can't explain that.*
– Bill O'Reilly [85]

Take anything in the universe, throw a bunch of it in a box, and turn up the heat. Then it doesn't matter what you started with, the motion of this substance will be governed by the equations of fluid dynamics.

– David Tong [119]

In chapters 2, 3, and 4 we analyzed systems of a few particles. In chapter 5 we developed statistical mechanics so that we could analyze much larger systems. Here we come to one of the many applications of statistical mechanics, the dynamics of matter on everyday scales. We actually touched on this in chapter 2 when we discussed rigid bodies. Now though we will study matter which is not rigid, such as elastic solids or fluids. Throughout this chapter we will be working in the approximation that the systems we are looking at consist of many smaller moving elements (particles) but that our experimental resolution is such that we will only be sensitive to averages over volumes which contain many such particles. This way, even though the underlying particles could be enumerated discretely and studied through a many many particle Lagrangian along the lines we would get from chapters 2-4, we will average over enough such particles that we arrive at a smoothened out continuous field theory. The study of such macroscopic smoothened out theories is known as **Continuum Mechanics**. This may seem abstract but it is common in daily life. A glass of water consists of very many water molecules, yet you are unlikely to be asked how many water you would like. The water molecules could be counted individually but instead for all practical purposes of daily life water is continuous because the relevant experiments we perform in daily life are not sensitive on small enough length scales to resolve the discreteness of water molecules. Because continuum mechanics is built on this averaging over a discrete theory, it is not valid at all length scales. It is only valid on scales large enough that the replacement of individual molecular behavior with locally averaged behavior is an acceptable approximation within the given experimental resolution.

6.1 Degrees of Freedom in Continuum Mechanics

Because in continuum mechanics we will seek to describe a material consisting of N discrete particles by smoothened out average continuous functions, we will be using classical field theory. A macroscopically continuous material occupies some region of space which we could specify by a continuous set of points. As that material evolves, each of those points may move around (in for example a fluid, each fluid droplet may go anywhere). These moving points are not literal particles as remember we assume we are locally averaging over many particles. Instead these moving points are called matter elements (conceptually they are like droplets). We can define then some initial positions for each matter element $\vec{x}_0$ and then at a later time t

the matter element which was at $\vec{x}_0$ will be at some other location $\vec{z}(t, \vec{x}_0)$. If we knew this $\vec{z}$, called the position field, everywhere and for all times it would precisely specify the motion of the entire material. Thus, in continuum mechanics knowing $\vec{z}(t, \vec{x}_0)$ amounts to knowing “everything” (at least, everything we care about). This $\vec{z}(t, \vec{x}_0)$ can also be called the **streamlines** of the system.

If $\vec{z}(t, \vec{x}_0)$ is to correspond meaningfully to the representative position of a matter element in the material, its conjugate variable should be the linear momentum $\vec{p}(t, \vec{x}_0)$ carried by that matter element as that linear momentum generates translations of the matter element. The conjugate momentum should of course have some expression in terms of $\vec{z}$ and $\dot{\vec{z}}$ by a Legendre transformation. Then, that conjugate momentum will have some equation of motion which will in turn specify the evolution of $\vec{z}$. The microscopic system has many variables which are not present within $\vec{z}(t, \vec{x}_0)$. Conceptually, $\vec{z}$ will be the “averaged” motion (in a sense we will rigorously define). Essentially, this average will be locally taken over many particles and each of those particles will generally not individually follow the average and so those deviations or fluctuations from average are not captured by $\vec{z}(t, \vec{x}_0)$. (Think of $\vec{z}(t, \vec{x}_0)$ as the representative position of a “center” of a moving water droplet consisting of a large number of water molecules.) Consequently, in order to find equations of motion for $\vec{z}$ we will have to locally have some distribution for these microscopic variables and integrate them out as done in the quasidynamic approximation in section 5.8. The cost of doing this is we will need an equation of motion for the entropy from this averaging (which by the results of section 5.8 will be given by the evolution of the energy). However, because we are doing this averaging locally, there will be an entropy $S(t, \vec{x}_0)$ associated to each matter element. Thus, in continuum mechanics the full set of independent variables which appear in the equations of motion can be taken to be $\vec{z}(t, \vec{x}_0)$, $\vec{p}(t, \vec{x}_0)$ and $S(t, \vec{x}_0)$.

The variables $(\vec{z}(t, \vec{x}_0), \vec{p}(t, \vec{x}_0), S(t, \vec{x}_0))$ are called **Lagrangian coordinates** and using them is called the Active Picture or convective picture. These coordinates essentially track individual matter elements as they move around, labeled by some label which for now we have taken to be their initial position. We could also view continuum mechanics through a Passive Picture in which instead of tracking individual matter elements in time we look at a fixed position $\vec{x}$ in space and look at the flow of the matter past that point. When we take a time derivative in the active picture, it is taken at fixed initial condition $\vec{x}_0$ and written $\frac{d}{dt}$. This is called a convective derivative. When we take a time derivative in the passive picture, it is taken at fixed location $\vec{x}$ and written $\frac{\partial}{\partial t}$. So, for a function $g(t, \vec{x})$ its convective and partial time derivatives are related by:

$$\frac{dg}{dt} = \frac{d}{dt}g(t, \vec{z}(t, \vec{x}_0)) = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial \vec{x}} \bigg|_{\vec{x}=\vec{z}(t, \vec{x}_0)} \cdot \frac{d\vec{z}}{dt}(t, \vec{x}_0) \quad (6.1.1)$$

$$\implies \frac{dg}{dt} = \frac{\partial g}{\partial t} + \frac{d\vec{z}}{dt}(t, \vec{x}_0) \cdot \nabla g(t, \vec{x}). \quad (6.1.2)$$

Here it is useful to introduce the velocity field $\vec{v}(t, \vec{x})$ by the velocity of matter elements which are at the position $\vec{x}$ at the time t . Then, by definition:

$$\vec{v}(t, \vec{z}(t, \vec{x}_0)) = \frac{d\vec{z}}{dt}(t, \vec{x}_0). \quad (6.1.3)$$

This equation alternatively can be thought of as an equation of motion for $\vec{z}$ if $\vec{v}$ is given:

$$\boxed{\frac{d\vec{z}}{dt} = \vec{v}(t, \vec{z})}. \quad (6.1.4)$$

Thus, specifying the velocity field gives a dynamical system which we can solve to find $\vec{z}$ in terms of initial conditions $\vec{x}_0$. Consequently, knowing the velocity field $\vec{v}(t, \vec{x})$ implicitly defines $\vec{z}(t, \vec{x}_0)$. With the velocity field the convective derivative can be rewritten:

$$\boxed{\frac{dg}{dt} = \frac{\partial g}{\partial t} + \vec{v}(t, \vec{x}) \cdot \nabla g(t, \vec{x})}. \quad (6.1.5)$$

It is useful to define $n(t, \vec{x})$, the number density of particles at the location $\vec{x}$ and the time t . Let $n_0(\vec{x}_0)$ be the initial number density. The number of particles in an initial region $\mathbb{M}_0$ at $t = 0$ will be the same as the number of particles in a later region $\mathbb{M}(t)$ given by evolving that initial region forward under the equations of motion:

$$\int_{\mathbb{M}_0} n_0(\vec{x}_0) d^3 \vec{x}_0 = \int_{\mathbb{M}(t)} n(t, \vec{x}) d^3 \vec{x}. \quad (6.1.6)$$

This is true simply because we assume the particles flow around and are not created or destroyed. Then,

because the matter element at $\vec{x}_0$ at time $t = 0$ will be found at $\vec{z}(t, \vec{x}_0)$ at the time t by the definition of $\vec{z}$, we can rewrite this second integral as:

$$\int_{\mathbb{M}(t)} n(t, \vec{x}) d^3 \vec{x} = \int_{\mathbb{M}_0} n(t, \vec{z}(t, \vec{x}_0)) \det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) d^3 \vec{x}_0 \quad (6.1.7)$$

$$\implies \int_{\mathbb{M}_0} \left(n_0(\vec{x}_0) - n(t, \vec{z}(t, \vec{x}_0)) \det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) \right) d^3 \vec{x}_0 = 0. \quad (6.1.8)$$

Because this is true for all integration regions, the integrand must be 0:

$$n_0(\vec{x}_0) - n(t, \vec{z}(t, \vec{x}_0)) \det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) = 0 \quad (6.1.9)$$

$$\implies \boxed{n(t, \vec{z}(t, \vec{x}_0)) = \frac{n_0(\vec{x}_0)}{\det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right)}}. \quad (6.1.10)$$

This looks identical to equation (5.2.11) and in fact we will follow the same steps to simplify it. Differentiating this in time and using equations (5.2.36) and (6.1.4) gives:

$$\frac{dn}{dt} = - \frac{n_0}{\left(\det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) \right)^2} \frac{d}{dt} \det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) = - \frac{n_0}{\left(\det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) \right)^2} \det \left(\frac{\partial \vec{z}}{\partial \vec{x}_0} \right) \nabla \cdot \vec{v} = -n \nabla \cdot \vec{v}. \quad (6.1.11)$$

Then, with equation (6.1.5):

$$\frac{dn}{dt} = \frac{\partial n}{\partial t} + \vec{v} \cdot \nabla n = -n \nabla \cdot \vec{v} \implies \boxed{\frac{\partial n}{\partial t} + \nabla \cdot (n \vec{v}) = 0}. \quad (6.1.12)$$

Hence, the number density satisfies a continuity equation with current density $n \vec{v}$. Specifying the velocity field and an initial number density then allows one to compute $n(t, \vec{x})$.

Instead of using the matter element momentum $\vec{p}(t, \vec{x}_0)$ we can define the linear momentum density $\vec{\varphi}(t, \vec{x})$ by the momentum of each element at a particular location times the number density of particles at that location:

$$\boxed{\vec{\varphi}(t, \vec{z}(t, \vec{x}_0)) = n(t, \vec{z}(t, \vec{x}_0)) \vec{p}(t, \vec{x}_0)}. \quad (6.1.13)$$

Because $\vec{p}$ should have an expression in terms of $\vec{z}$ and $\dot{\vec{z}}$, the momentum density will have some expression in terms of $\vec{x}, \vec{v}$ and this factor of n . Then, knowing an equation of motion for $\vec{p}$ is equivalent to knowing an equation of motion for the momentum density $\vec{\varphi}$. Similarly, instead of using the matter element entropy $S(t, \vec{x}_0)$ we can define the entropy field $s(t, \vec{x})$ by:

$$\boxed{s(t, \vec{z}(t, \vec{x}_0)) = S(t, \vec{x}_0)}. \quad (6.1.14)$$

This $s(t, \vec{x})$ is not the entropy density (as that would involve another factor of the number density analogously to the definition of the momentum density). Instead, this $s(t, \vec{x})$ is the entropy per particle for particles at $\vec{x}$ at time t . By equation (5.8.41), the time evolution of the entropy is implicitly determined by the time evolution of the energy. The energy per particle could be multiplied by the number density to give the energy density just like we did with the momentum density. Thus, the evolution of the energy density will tell us the evolution of the entropy.

In place of the position field $\vec{z}(t, \vec{x}_0)$, in the passive picture we simply use $\vec{v}(t, \vec{x})$ (it may seem like we lose access to the initial conditions but they can be recovered from integrating the streamlines and using that by definition $\vec{z}(0, \vec{x}_0) = \vec{x}_0$). Introducing the number density (which does not have independent evolution as it just satisfies the continuity equation), we can use the momentum density $\vec{\varphi}$ in place of the element momentum $\vec{p}$. Then, the $\vec{p}$ equation of motion is equivalent to an equation of motion for the momentum density. There will be some expression for $\vec{\varphi}$ in terms of $n, \vec{z}$, and $\vec{v}$ using the Legendre transform so this effectively gives the equation of motion for $\vec{v}$. As well, the equation of motion for the element entropy can be exchanged for an equation of motion for the entropy field or the energy density. So, in the passive picture we use the **Eulerian coordinates** given by $n(t, \vec{x}), \vec{v}(t, \vec{x}), s(t, \vec{x})$. This set of coordinates contains exactly the same information found in the Lagrangian coordinates, just represented differently.

Exercises

Problem 6.1: Active/Passive Conversion. Suppose that a continuous material is moving in 1 dimension

and that its streamlines have been solved to be:

$$z(t, x_0) = \frac{1}{2}gt^2 + \omega tx_0 + x_0$$

for constants ω and g . As well, assume that the initial number density of the material is:

$$n_0(x_0) = \frac{N}{\ell\sqrt{\pi}}e^{-\frac{x_0^2}{\ell^2}}$$

for constants N and ℓ . Show that the velocity field and number density of the system in passive coordinates are:

$$v(t, x) = \frac{\omega x + gt + \frac{1}{2}\omega gt^2}{1 + \omega t}, \quad n(t, x) = \frac{N}{\ell\sqrt{\pi}(1 + \omega t)}e^{-\frac{1}{\ell^2}\left(\frac{x - \frac{1}{2}gt^2}{1 + \omega t}\right)^2}.$$

Verify by explicit calculation that n satisfies the continuity equation with v as its velocity field and that $v(t, x)$ satisfies the equation of motion:

$$\frac{\partial v(t, x)}{\partial t} + v(t, x)\frac{\partial v(t, x)}{\partial x} = g.$$

6.2 Nonrelativistic Transport Equations

We will look at two different approaches for finding continuum mechanical equations of motion. There is kinetic theory, in which one works directly with the underlying microscopic equations of motion and averages them explicitly to derive equations of motion for the average quantities and there is continuum effective theory, in which one works directly with the averaged quantities and derives their possible equations of motion from transformation properties and symmetry considerations. Continuum effective theory is nice in that it provides simpler derivations of the equations of motion than kinetic theory, but has the disadvantage that some unknown quantities will appear in the equations of motion which then have to be modeled by an appropriate constitutive relation. Kinetic theory is nice because it can be used to derive constitutive relations, at least for some systems, but generally proves to be quite difficult. We will begin here with continuum effective theory and discuss kinetic theory in the next section.

We know from our reasoning in section 6.1 that the appropriate variables for continuum mechanics can be considered as $\vec{z}(t, \vec{x}_0), \vec{p}(t, \vec{x}_0), S(t, \vec{x}_0)$ or as $n(t, \vec{x}), \vec{v}(t, \vec{x}), s(t, \vec{x})$. Let us assume there is some underlying theory responsible for the dynamics of matter and its interactions with electromagnetism (or some other forces). Of course we will assume that theory has time and space translational symmetries, rotational symmetry, and is local. Because we are working in the nonrelativistic regime we will assume this theory has Galilean boost symmetry as well. It is often nicer to work with the mass density $\rho(t, \vec{x}) = mn(t, \vec{x})$ where m is the mass per particle rather than the number density $n(t, \vec{x})$. Due to the continuity equation for $n(t, \vec{x})$, the mass density also satisfies the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0. \quad (6.2.1)$$

Due to space translational symmetry, in the absence of interactions the total free linear momentum of any blob of matter is conserved as that blob evolves and because the theory is local it is locally conserved. In the presence of interactions the free linear momentum of that blob is no longer conserved as there may now be momentum transfer from the blob to neighboring blobs through local surface interactions and also momentum transfer to the blob due to external forces (such as electromagnetism). Let $\mathbb{M}(t)$ be the region in space occupied by a particular blob of matter at time t . Then, locality combined with space translational symmetry imply that the free linear momentum density satisfies an equation of the form:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{\varphi}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{f}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \hat{\sigma}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.2.2)$$

for some tensor $\hat{\sigma}$ which represents the surface forces per unit area between blobs and vector $\vec{f}$ which represents the external force density on the blob.

Due to time translational symmetry, in the absence of interactions the total free energy (free in the sense of energy of the free system, not free energy in the sense of thermodynamics) of any blob of matter is conserved as that blob evolves and because the theory is local it is locally conserved. In the presence of interactions the free energy of that blob is no longer conserved as there may now be energy transfer from the blob to neighboring blobs through local surface interactions and also energy transfer to the blob due to work done on the blob by external forces. Then, locality combined with time translational symmetry imply that the free energy density $\mathcal{E}$ satisfies an equation of the form:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \mathcal{E}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \mathcal{P}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \vec{\mathcal{I}}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.2.3)$$

for some vector $\vec{\mathcal{I}}$ which represents the surface energy transfer per unit area and scalar $\mathcal{P}$ which represents the external power density to the blob.

Due to rotational symmetry, in the absence of interactions the total free angular momentum of any blob of matter is conserved as that blob evolves and because the theory is local it is locally conserved. In the presence of interactions the free angular momentum of that blob is no longer conserved as there may now be angular momentum transfer from the blob to neighboring blobs through local surface interactions and also angular momentum transfer to the blob due to torque on the blob by external forces. Then, locality combined with rotational symmetry imply that the free angular momentum density $\vec{j}$ satisfies an equation of the form:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{j}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{\tau}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \hat{M}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.2.4)$$

for some tensor $\hat{M}$ which represents the surface angular momentum transfer per unit area and vector $\vec{\tau}$ which

represents the external torque density on the blob.

Due to Galilean boost symmetry, in the absence of interactions the total free dynamic mass moment of any blob of matter is conserved as that blob evolves and because the theory is local it is locally conserved. In the presence of interactions the free dynamic mass moment of that blob is no longer conserved as there may now be moment transfer from the blob to neighboring blobs through local surface interactions and also moment transfer to the blob due to external forces. Then, locality combined with Galilean boost symmetry imply that the free dynamic mass moment density $\vec{g}$ satisfies an equation of the form:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{g}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{B}(t, \vec{x}) d\mathbb{S} + \int_{\partial\mathbb{M}(t)} \hat{N}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.2.5)$$

for some tensor $\hat{N}$ which represents the surface dynamic mass moment transfer per unit area and vector $\vec{B}$ which represents the external moment transfer force density on the blob.

We now have four instances of needing the total time derivative of a volume integral over the blob. This derivative will contain two contributions: one term from partial differentiating the integrand and one term from differentiating the region of the blob itself. Consider variation of the integral of a quantity (use $\mathcal{E}$ for example) over the blob:

$$\delta \int_{\mathbb{M}(t)} \mathcal{E} d\mathbb{S} = \int_{\mathbb{M}} \delta \mathcal{E} d\mathbb{S} + \int_{\delta\mathbb{M}} \mathcal{E} d\mathbb{S}. \quad (6.2.6)$$

The variation $\delta\mathbb{M}$ of the region can be expressed as a surface integral combined with the variation of the coordinates at the boundary of the region. This is because the region $\mathbb{M}$ only changes in the variation by changing the boundary and the enclosing shell of that change locally has thickness $\delta\vec{x} \cdot d\vec{\mathbb{A}}$. Thus:

$$\int_{\delta\mathbb{M}} \mathcal{E} d\mathbb{S} = \int_{\partial\mathbb{M}} \mathcal{E} \delta\vec{x} \cdot d\vec{\mathbb{A}}. \quad (6.2.7)$$

Because the blob evolves locally with the velocity $\vec{v}(t, \vec{x})$, for a time derivative then it immediately follows that:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \mathcal{E} d\mathbb{S} = \int_{\mathbb{M}} \frac{\partial \mathcal{E}}{\partial t} d\mathbb{S} + \int_{\partial\mathbb{M}} \mathcal{E} \vec{v} \cdot d\vec{\mathbb{A}} = \int_{\mathbb{M}} \left(\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) \right) d\mathbb{S}. \quad (6.2.8)$$

Returning this to equation (6.2.3) gives that:

$$\int_{\mathbb{M}} \left(\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) \right) d\mathbb{S} = \int_{\mathbb{M}} \mathcal{P} d\mathbb{S} + \int_{\partial\mathbb{M}} \vec{\mathcal{I}} \cdot d\vec{\mathbb{A}} = \int_{\mathbb{M}} (\mathcal{P} + \nabla \cdot \vec{\mathcal{I}}) d\mathbb{S}. \quad (6.2.9)$$

Because this holds for all choices of matter blob $\mathbb{M}$ it follows that:

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) = \mathcal{P} + \nabla \cdot \vec{\mathcal{I}}. \quad (6.2.10)$$

The corresponding analyses for equations (6.2.2), (6.2.4), and (6.2.5) give:

$$\frac{\partial \wp^a}{\partial t} + \partial_b (\wp^a v^b) = f^a + \partial_b \sigma^{ab} \quad (6.2.11)$$

$$\frac{\partial j^a}{\partial t} + \partial_b (j^a v^b) = \tau^a + \partial_b M^{ab} \quad (6.2.12)$$

$$\frac{\partial g^a}{\partial t} + \partial_b (g^a v^b) = B^a + \partial_b N^{ab} \quad (6.2.13)$$

Let us analyze these equations of motion starting with the last one. The free dynamic mass moment carried by a point mass m is $\vec{G} = t\vec{p} - m\vec{x}$. Because the dynamic mass moment is a linear function of the momentum, the locally averaged dynamic mass moment density will simply be:

$$\vec{g} = t\vec{\wp} - \rho\vec{x}. \quad (6.2.14)$$

The time derivative of $\vec{G}$ for a mass under an external force $\vec{F}$ is $t\vec{\dot{F}}$ (because $p - m\dot{x} = 0$ for the free momentum of a nonrelativistic mass). This is also a linear function of the force and power and so behaves well under the local averaging to give that $\vec{B}$ (which is the external force density corresponding to $\vec{g}$) and $\hat{N}$ (which is the external force surface density corresponding to $\vec{g}$) are:

$$\vec{B} = t\vec{f}, \quad \hat{N} = t\hat{\sigma}. \quad (6.2.15)$$

Returning these to equation (6.2.13) and expanding out derivatives gives:

$$\wp^a - \rho v^a + t \left(\frac{\partial \wp^a}{\partial t} + \partial_b (\wp^a v^b) - f^a - \partial_b \sigma^{ab} \right) - x^a \left(\frac{\partial \rho}{\partial t} + \partial_b (\rho v^b) \right) = 0 \quad (6.2.16)$$

Using equations (6.2.1) and (6.2.11) we have:

$$\wp^a = \rho v^a. \quad (6.2.17)$$

Therefore, the local momentum density has a simple relationship with the mass density and local average velocity and this is the only independent condition implied by Galilean boost symmetry.

Next let us study the angular momentum equation. The free orbital angular momentum carried by a mass m moving at velocity $\vec{x}$ is $\vec{x} \times \vec{p} = m\vec{x} \times \vec{v}$ in the Galilean theory. So, the free orbital angular momentum density carried by a mass density ρ moving at velocity $\vec{v}$ is $\vec{x} \times \vec{\wp} = \rho\vec{x} \times \vec{v}$. In principle the matter may also carry spin angular momentum density $\vec{s}$ and so:

$$\vec{j} = \rho\vec{x} \times \vec{v} + \vec{s}. \quad (6.2.18)$$

Suppose that the matter flows locally with both a finite mass density and finite angular velocity. The free angular momentum carried by a moving point mass is $\vec{S} = m r^2 \vec{\omega}$ where r is the distance of the point particle from the axis of rotation. Therefore, in the continuum limit if we consider a finite mass density, then m scales as $\rho \Delta x^3$ where Δx is the discretization scale and r scales as Δx . This gives a spin contribution of $\vec{S} = \rho \vec{\omega} \Delta x^5$ up to a possible numerical coefficient. The spin density then scales as $\vec{s} = \rho \vec{\omega} \Delta x^2$. In the continuum limit $\Delta x \rightarrow 0$ then matter which flows with well defined velocity, finite density, and finite angular velocity contributes no independent spin angular momentum density and we can simply take:

$$\vec{j} = \rho\vec{x} \times \vec{v}. \quad (6.2.19)$$

The torque on a particle is simply $\vec{x} \times \vec{F}$ where $\vec{F}$ is the force acting on the body. Therefore, the differential torque on a body element is $\vec{x} \times d\vec{F}$ and so we have:

$$\vec{\tau} = \vec{x} \times \vec{f}, \quad \hat{M} \cdot d\vec{\mathbb{A}} = \vec{x} \times (\hat{\sigma} \cdot d\vec{\mathbb{A}}). \quad (6.2.20)$$

In components:

$$j^a = \rho \epsilon^a_{bc} x^b v^c, \quad \tau^a = \epsilon^a_{bc} x^b f^c, \quad M^{ab} = \epsilon^a_{cd} x^c \sigma^{db}. \quad (6.2.21)$$

Returning these to equation (6.2.12) using (6.2.17):

$$\epsilon^a_{bc} x^b \left(\frac{\partial}{\partial t} (\rho v^c) + \partial_d (\rho v^c v^d) \right) = \epsilon^a_{bc} x^b f^c + \partial_d (\epsilon^a_{bc} x^b \sigma^{cd}). \quad (6.2.22)$$

Now using equation (6.2.11):

$$\epsilon^a_{bc} x^b f^c + \epsilon^a_{bc} x^b \partial_d \sigma^{cd} = \epsilon^a_{bc} x^b f^c + \epsilon^a_{bc} x^b \partial_d \sigma^{cd} + \epsilon^a_{dc} \sigma^{cd} \quad (6.2.23)$$

$$\implies \epsilon^a_{cd} \sigma^{cd} = 0. \quad (6.2.24)$$

Contracting with ϵ_{abe} and simplifying gives that:

$$\sigma^{ab} = \sigma^{ba}. \quad (6.2.25)$$

Hence, matter which flows with a well-defined local velocity, finite mass density, and finite angular velocity necessarily has a symmetric stress tensor due to the continuity law of angular momentum. As well, this is the only consequence of rotational symmetry.

Having accounted for the dynamical consequences of rotational symmetry and Galilean boost symmetry, the only two remaining independent equations of motion are (6.2.10) and (6.2.11). To understand these it is helpful to analyze the Galilean boost properties of each term appearing in them. The volume element $d\mathbb{S}$ is invariant under Galilean boost and so quantities and their densities have the same Galilean boost properties. By equations (3.3.76) we know how the differential operators transform under Galilean boosts:

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t} - \vec{u} \cdot \nabla, \quad \nabla' = \nabla \quad (6.2.26)$$

for boost velocity $\vec{u}$. We know that mass density and force density are Galilean boost invariant and that $\vec{v}$ should shift by $\vec{u}$. Due to Galilean boost symmetry equations (6.2.10) and (6.2.11) must be invariant under Galilean boosts. Applying this to the momentum equation:

$$\frac{\partial}{\partial t'} (\rho' v'^a) + \partial'_b (\rho' v'^a v'^b) = f'^a + \partial'_b \sigma'^{ab} \quad (6.2.27)$$

$$\implies \left(\frac{\partial}{\partial t} - \vec{u} \cdot \nabla \right) (\rho(\vec{v} + \vec{u})) + \partial_b (\rho(v^a + u^a)(v^b + u^b)) = f^a + \partial_b \sigma'^{ab} \quad (6.2.28)$$

$$\implies \frac{\partial}{\partial t} (\rho v^a) + \partial_b (\rho v^a v^b) = f^a + \partial_b \sigma'^{ab} \quad (6.2.29)$$

after using the continuity equation for ρ . Thus the original momentum equation is satisfied if we take the stress tensor to be Galilean boost invariant:

$$\sigma'^{ab} = \sigma^{ab}. \quad (6.2.30)$$

We can perform the same analysis for the energy equation. Energy density is not Galilean boost invariant. Let $\mathfrak{u}$ be the energy density per unit mass of the matter in the instantaneous rest frame. We found in section 2.1 that for a Galilean particle the energy is $\frac{1}{2}m|\vec{x}'|^2 + U(t, \vec{x})$ and so under a shift of the velocity by $\vec{u}$ the energy shifts by $m\vec{v} \cdot \vec{u} + \frac{1}{2}m|\vec{u}|^2$. Consequently the energy density transforms as:

$$\mathcal{E}' = \mathcal{E} + \rho \vec{v} \cdot \vec{u} + \frac{1}{2} \rho |\vec{u}|^2. \quad (6.2.31)$$

It immediately follows that:

$$\mathcal{E}' - \frac{1}{2} \rho' |\vec{v}'|^2 = \mathcal{E} - \frac{1}{2} \rho |\vec{v}|^2 \quad (6.2.32)$$

and that this combination equals $\rho \mathfrak{u}$ in the rest frame (this equation trivially equals $\rho \mathfrak{u}$ when $\vec{v} = 0$ and this equation itself states that this combination is independent of $\vec{v}$ and thus it equals $\mathfrak{u}$ for all $\vec{v}$). So, we have:

$$\mathcal{E} = \frac{1}{2} \rho |\vec{v}|^2 + \rho \mathfrak{u}. \quad (6.2.33)$$

Now let us use this to compute the Galilean boost properties of equation (6.2.10):

$$\frac{\partial \mathcal{E}'}{\partial t} + \nabla' \cdot (\mathcal{E}' \vec{v}') = \mathcal{P}' + \nabla' \cdot \vec{\mathcal{I}}' \quad (6.2.34)$$

$$\implies \left(\frac{\partial}{\partial t} - \vec{u} \cdot \nabla \right) \left(\mathcal{E} + \rho \vec{v} \cdot \vec{u} + \frac{1}{2} \rho |\vec{u}|^2 \right) + \nabla \cdot \left(\left(\mathcal{E} + \rho \vec{v} \cdot \vec{u} + \frac{1}{2} \rho |\vec{u}|^2 \right) (\vec{v} + \vec{u}) \right) = \mathcal{P}' + \nabla \cdot \vec{\mathcal{I}}' \quad (6.2.35)$$

$$\implies \frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) + \vec{u} \cdot \left(\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) \right) = \mathcal{P} + \nabla \cdot \vec{\mathcal{I}}. \quad (6.2.36)$$

Using equation (6.2.11):

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) = \mathcal{P}' - \vec{u} \cdot \vec{f} + \nabla \cdot (\vec{\mathcal{I}}' - \hat{\sigma} \cdot \vec{u}). \quad (6.2.37)$$

By comparing with equation (6.2.10) we can see that $\mathcal{P}$ and $\vec{\mathcal{I}}$ transform under a Galilean boost as:

$$\mathcal{P}' = \mathcal{P} + \vec{u} \cdot \vec{f}, \quad \vec{\mathcal{I}}' = \vec{\mathcal{I}} + \hat{\sigma} \cdot \vec{u}. \quad (6.2.38)$$

Now define Φ as the value of $\mathcal{P}$ in the local instantaneous rest frame of the matter. It immediately follows that:

$$\mathcal{P} = \Phi + \vec{v} \cdot \vec{f} \quad (6.2.39)$$

as well it is automatic that Φ is invariant under Galilean boosts. Similarly define $\vec{q}$ as the value of $-\vec{\mathcal{I}}$ in the local instantaneous rest frame of the matter. It similarly follows that:

$$\vec{\mathcal{I}} = -\vec{q} + \hat{\sigma} \cdot \vec{v} \quad (6.2.40)$$

and that $\vec{q}$ is invariant under Galilean boosts.

Simplifying our results, we have the equations of motion:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (6.2.41)$$

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v} - \hat{\sigma}) = \vec{f} \quad (6.2.42)$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\vec{v}|^2 + \rho \mathfrak{u} \right) + \nabla \cdot \left(\frac{1}{2} \rho |\vec{v}|^2 \vec{v} + \rho \mathfrak{u} \vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q} \right) = \vec{v} \cdot \vec{f} + \Phi \quad (6.2.43)$$

together with the additional information that $\hat{\sigma}$ equals its own transpose and that $\hat{\sigma}$, $\mathfrak{u}$, $\vec{q}$, $\vec{f}$, Φ are invariant under Galilean boosts. These are known as the nonrelativistic transport equations and they give the equations of motion for nonrelativistic continuum mechanics. All that remains is to identify specific expressions for the

listed quantities for particular cases of different types of matter. The specific expressions for $\hat{\sigma}$, $\mathbf{u}$, $\vec{q}$, $\vec{f}$, and Φ are called constitutive relations and they are sensitive to the specific matter being studied. Once they are supplied, these form a complete set of equations of motion that determine the behavior of the matter.

While the particular forms of $\hat{\sigma}$, $\mathbf{u}$, $\vec{q}$, $\vec{f}$, Φ are dependent on the matter under consideration, their interpretations as quantities in the theory are the same regardless of their particular expressions. We have already identified that $\hat{\sigma}$ is the stress tensor for the blob as it represents the force per unit area on the surface of the blob. We also identified that $\vec{f}$ is the external force density on the blob. $\rho\mathbf{u}$ by definition is energy density of the matter in its local instantaneous rest frame. Therefore, viewing the matter which is locally averaged over as a system with many internal degrees of freedom (the positions of all the various particles averaged over), $\rho\mathbf{u}$ is the thermodynamic internal energy density in that rest frame. $\vec{q}$ enters the energy equation as a contribution to the energy current density whose divergence is taken and it is the only contribution that survives in the instantaneous rest frame. Therefore, $\vec{q}$ represents energy current density due to the microscopic averaged over variables (because it is invariant under the boosts of the macroscopic velocity field $\vec{v}(t, \vec{x})$). So, $\vec{q}$ is the heat current density. Finally, Φ is the contribution from the power density which is independent of the velocity field. Therefore, it is the heat transfer density to the body.

Theorem 6.1: Nonrelativistic Kinetic Theory

Nonrelativistic continuum matter is described by the transport equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (6.2.44)$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v} - \hat{\sigma}) = \vec{f} \quad (6.2.45)$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\vec{v}|^2 + \rho \mathbf{u} \right) + \nabla \cdot \left(\frac{1}{2} \rho |\vec{v}|^2 \vec{v} + \rho \mathbf{u} \vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q} \right) = \vec{v} \cdot \vec{f} + \Phi \quad (6.2.46)$$

where $\rho(t, \vec{x})$ is the mass density of the matter, $\vec{v}(t, \vec{x})$ is its local average velocity field, $\hat{\sigma}(t, \vec{x})$ is the symmetric stress tensor of the matter, $\vec{f}(t, \vec{x})$ is the force density acting on the matter, $\mathbf{u}(t, \vec{x})$ is the internal energy per unit mass of the matter, $\vec{q}(t, \vec{x})$ is the heat current density in the matter, and $\Phi(t, \vec{x})$ is the heat transfer density to the body. The linear momentum density of the matter is $\vec{\varrho} = \rho \vec{v}$ and the energy density of the matter is $\mathcal{E} = \frac{1}{2} \rho |\vec{v}|^2 + \rho \mathbf{u}$.

Exercises

Problem 6.2: Simplified Transfer Equations. Using the transport equations, expand out the derivatives and simplify to show that they can equivalently be written as:

$$\frac{d\rho}{dt} + \rho \nabla \cdot \vec{v} = 0, \quad \rho \frac{d\vec{v}}{dt} = \nabla \cdot \hat{\sigma} + \vec{f}, \quad \rho \frac{d\mathbf{u}}{dt} = \sigma^{ab} \partial_a v_b - \nabla \cdot \vec{q} + \Phi.$$

6.3 Nonrelativistic Kinetic Theory

The most direct approach to continuum mechanics is to study the underlying many particle theory and try to perform the averaging at the level of the equations of motion. This is known as kinetic theory. The goal here is to derive an effective theory of the Eulerian or Lagrangian coordinates directly from the microscopic theory, and so this is a top-down effective theory. It is very much the messy way of doing things. For this section, suspend the implicit summation of indices.

Let us suppose we have N nonrelativistic particles with positions $\vec{x}_1(t), \dots, \vec{x}_N(t)$ with all of the same microscopic properties, such as their masses m and charges q . These particles may have some internal degrees of freedom $\mathbf{q}, \mathbf{p}$ each. For example, a molecule may have some spin degrees of freedom to rotate about its center of mass or some vibrational degrees of freedom to expand and contract. In any case, we will assume these internal degrees of freedom have been defined so that they are unchanged by translations, boosts, or rotations of the overall system. Each particle then will contribute $\frac{|\vec{p}_k|^2}{2m} + h(\mathbf{q}_k, \mathbf{p}_k)$ to the free Hamiltonian where $h(\mathbf{q}, \mathbf{p})$ is whatever the free Hamiltonian happens to be for the particle internal degrees of freedom. h cannot depend on the positions or momenta of the particles due to translational symmetry and Galilean boost symmetry. Of course, there may be interparticle interactions in the material so that the total Hamiltonian differs from the sum of free Hamiltonians. All of the interactions we studied before with Galilean symmetry (meaning electrostatics and Newtonian gravity) in chapter 2 gave that the interparticle interactions is be pairwise (meaning there are only interactions between two particles, no three particle or higher particle interactions) and that they add a term to the Hamiltonian which only depends on $|\vec{x}_k - \vec{x}_l|$ for the two particles, not on their momenta (to establish this see problem 3.69). Then, we take the full Hamiltonian for the system of particles to be:

$$\mathcal{H} = \sum_{k=1}^N \left(\frac{|\vec{p}_k|^2}{2m} + h(\mathbf{q}_k, \mathbf{p}_k) \right) + \sum_{k=1}^{N-1} \sum_{l=k+1}^N U(|\vec{x}_k - \vec{x}_l|, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l) \quad (6.3.1)$$

where U is some function called the two particle potential that characterizes the interparticle interactions. This Hamiltonian is the very same form as equation (3.4.87), with the additional possibility of internal structure and non-point-particles. There may also be external forces from outside the system on each particle. So, the equations of motion for a single particle give:

$$\dot{\vec{x}}_k = \frac{\partial \mathcal{H}}{\partial \vec{p}_k} = \frac{\vec{p}_k}{m}, \quad \dot{\mathbf{p}}_k = -\frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} + \vec{F}_k = \vec{F}_k - \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} \quad (6.3.2)$$

$$\implies m\ddot{\vec{x}}_k = \vec{F}_k - \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} \quad (6.3.3)$$

where we have introduced the shorthand $U_{kl} = U(|\vec{x}_k - \vec{x}_l|, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l)$. And, for the internal degrees of freedom:

$$\dot{\mathbf{q}}_k = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} = \frac{\partial h_k}{\partial \mathbf{p}_k} + \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \mathbf{p}_k}, \quad \dot{\mathbf{p}}_k = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}_k} + \mathbf{f}_k = \mathbf{f}_k - \frac{\partial h_k}{\partial \mathbf{q}_k} - \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \quad (6.3.4)$$

where we have introduced the shorthand $h_k = h(\mathbf{q}_k, \mathbf{p}_k)$. $\vec{F}_k$ represents the external force on the translational degrees of freedom of each particle and $\mathbf{f}_k$ represents the external force on the internal degrees of freedom of each particle.

6.3.1 Particle Transfer

When describing the mass density or charge density of a point particle we represent that density through the Dirac delta centered at the position of that particle $\delta(\vec{x} - \vec{x}_k(t))$. However, because the Dirac delta is quite mathematically problematic, it will be both important and useful to instead describe the density of our particles by some **profile function** $R_0(r)$ so that the number density of a single particle is given by $R_0(|\vec{x} - \vec{x}_k(t)|)$. By virtue of depending on the difference $\vec{x} - \vec{x}_k(t)$ this density represents a density centered at the origin which is then translated to be centered at $\vec{x}_k$. By virtue of depending on the magnitude $|\vec{x} - \vec{x}_k(t)|$ this density is spherically symmetric about its center, so rotational symmetry isn't broken. In

real life we know that the molecules comprising everyday matter are not point-like, they have finite nonzero size, and for everything but the simplest molecules they are also not spherically symmetric. However, in continuum mechanics we will require that the molecular size is much smaller than the scale of our averaging and much smaller than the distance between molecules. Consequently, on the averaged scales the molecules are effectively point-like and thus effectively spherically symmetric. This could be broken if the molecules had some appreciable directional internal structure, such as magnetic moments; we exclude that possibility from consideration here. The profile function is not to be taken literally as the mass distribution of an actual molecule but instead as a formal approximation of the Dirac delta that makes the averaging better behaved and consequently as the smoothened number density of a single molecule (meaning blurred out over the length scale resolution of the experiment). Because we intend the profile function to represent the number density of a single particle on the averaged scale, we need it to satisfy some basic properties. In particular, the density should be nonnegative so that only a positive fraction of the particle can be found in any region and it should integrate to one so that there is 1 total particle in space per particle considered:

$$R_0(|\vec{x}|) \geq 0 \quad \forall \vec{x} \quad (6.3.5)$$

$$\int_{\mathbb{S}} R_0(|\vec{x}|) d\mathbb{S} = 1. \quad (6.3.6)$$

Because $R_0(|\vec{x} - \vec{x}_k(t)|)$ is intended to represent the averaged number density of particle $\vec{x}_k(t)$, the number density for the full system of N particles is then:

$$n(t, \vec{x}) \stackrel{\text{def}}{=} \sum_{k=1}^N R_0(|\vec{x} - \vec{x}_k(t)|) = \sum_{k=1}^N R_k(t, \vec{x}). \quad (6.3.7)$$

Here in the last step we have introduced the notation $R_k(t, \vec{x}) = R_0(|\vec{x} - \vec{x}_k(t)|)$ as a shorthand because this combination will appear often. Because each particle has mass m , the corresponding mass density is immediately:

$$\rho_m(t, \vec{x}) = mn(t, \vec{x}) = \sum_{k=1}^N mR_k(t, \vec{x}). \quad (6.3.8)$$

Similarly the corresponding electric charge density is:

$$\rho_q(t, \vec{x}) = qn(t, \vec{x}) = \sum_{k=1}^N qR_k(t, \vec{x}) = \frac{q}{m} \rho_m. \quad (6.3.9)$$

We know from equation (6.1.12) that the number density must satisfy a continuity equation. We can verify this by differentiating the number density with respect to time:

$$\frac{\partial n}{\partial t} = \sum_{k=1}^N \frac{\partial}{\partial t} R_0(|\vec{x} - \vec{x}_k(t)|) = -\dot{\vec{x}}_k(t) \cdot \frac{\partial}{\partial \vec{x}} R_0(|\vec{x} - \vec{x}_k(t)|) = -\nabla \cdot \left(\sum_{k=1}^N \dot{\vec{x}}_k R_k(t, \vec{x}) \right). \quad (6.3.10)$$

So, in fact the number density does satisfy a continuity equation and comparing with equation (6.1.12) we see:

$$n(t, \vec{x}) \vec{v}(t, \vec{x}) = \sum_{k=1}^N \dot{\vec{x}}_k R_k(t, \vec{x}). \quad (6.3.11)$$

Immediately, it follows that the velocity field is given microscopically by:

$$\vec{v}(t, \vec{x}) \stackrel{\text{def}}{=} \frac{\sum_{k=1}^N \dot{\vec{x}}_k R_k(t, \vec{x})}{\sum_{k=1}^N R_k(t, \vec{x})}. \quad (6.3.12)$$

We can interpret this definition as the mass density weighted averaged velocity of the particles at $\vec{x}$. That is, this combination computes the average velocity of all the particles where the weights used in the averaging are just the mass density of each particle at the point being averaged about. Together we have the continuity equation:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0. \quad (6.3.13)$$

The definition of the velocity field $\vec{v}(t, \vec{x})$ makes it clear why we cannot exactly take the profile function to be the Dirac delta. If R_0 was exactly a Dirac delta then both the numerator and denominator in the

definition of the velocity field would be 0 at any points which are not exactly the locations of a particle. This gives a velocity field of 0/0 almost everywhere, which is complete nonsense. As well, where there is a particle it gives ∞/∞ and even if one regulates the Dirac deltas to give this quantity a meaning the result is only an “average” over that single particle. So, in order for $\vec{v}(t, \vec{x})$ to be well defined and smooth we need to take R_0 to be spread out enough in space for the denominator in equation (6.3.12) to be safely non-zero throughout the matter. If we want $\vec{v}(t, \vec{x})$ to be a good average we should in fact hope that anywhere in the matter the sum contains several terms which give a sizable contribution so that we aren’t “averaging over a single particle” (or worse, no particles almost everywhere in the case of a Dirac delta). Consequently, we need the support of our profile function to be wide enough so that our average contains enough particles. Exactly what width depends on the precision we need. If you need N_0 particles to contribute at least an amount δ to the sum to consider it a “good” average, then you need to select an R_0 so that if n_0 is the typical number density of the matter then $R_0 > \delta$ in a volume of at least size N_0/n_0 . The sufficiently large width of R_0 also explains why we can take the profile function to be spherically symmetric even for molecules which are not spherically symmetric. The width of R_0 is set by the typical molecular separation which is much larger than the molecular size, meaning that as the molecule rotates and vibrates its entire mass is safely contained within the sphere where R_0 is meaningfully different than 0. Within that sphere, the region where the molecule has nonzero mass density is effectively point-like.

6.3.2 Momentum Transfer

We see in the continuity equation for number density that the number current density of the particles is $n\vec{v}$. This combination has another nice interpretation. By equation (6.3.2) each particle carries a free linear momentum $m\dot{\vec{x}}_k$ and so the linear momentum density $\vec{\varphi}$ for this system should be:

$$\vec{\varphi}(t, \vec{x}) = \sum_{k=1}^N \vec{p}_k R_k(t, \vec{x}) = \sum_{k=1}^N m\dot{\vec{x}}_k R_k(t, \vec{x}) = mn(t, \vec{x})\vec{v}(t, \vec{x}) = \rho_m(t, \vec{x})\vec{v}(t, \vec{x}). \quad (6.3.14)$$

By the logic of section 6.1 we need an equation of motion for the momentum density to understand the evolution of the velocity field. So, let us differentiate the momentum density with respect to time:

$$\frac{\partial \vec{\varphi}}{\partial t} = \frac{\partial}{\partial t} \sum_{k=1}^N m\dot{\vec{x}}_k R_k(t, \vec{x}) = \sum_{k=1}^N m\ddot{\vec{x}}_k R_k(t, \vec{x}) + \sum_{k=1}^N m\dot{\vec{x}}_k \frac{\partial R_k}{\partial t} = \sum_{k=1}^N m\ddot{\vec{x}}_k R_k(t, \vec{x}) - \nabla \cdot \left(\sum_{k=1}^N m\dot{\vec{x}}_k \dot{\vec{x}}_k R_k \right). \quad (6.3.15)$$

Then, using equation (6.3.3):

$$\sum_{k=1}^N m\ddot{\vec{x}}_k R_k(t, \vec{x}) = \sum_{k=1}^N \vec{F}_k(t) R_k(t, \vec{x}) - \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} R_k(t, \vec{x}). \quad (6.3.16)$$

Because R_k represents the density of particle k , the total external force density $\vec{f}(t, \vec{x})$ on the system of particles is:

$$\vec{f}(t, \vec{x}) \stackrel{\text{def}}{=} \sum_{k=1}^N \vec{F}_k(t) R_k(t, \vec{x}). \quad (6.3.17)$$

Thus, with this we have an interpretation for the first term in equation (6.3.15). We can also develop an interpretation for the second term in equation (6.3.15) with a bit more work. Because $U_{kl} = U(|\vec{x}_k - \vec{x}_l|, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l)$, the only dependence on the particle positions is through $r_{kl} = |\vec{x}_k - \vec{x}_l|$. We will write U'_{kl} to indicate the derivative of U_{kl} with respect to this r_{kl} . That is:

$$U'_{kl} = \frac{\partial U}{\partial r}(r, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l) \Big|_{r=|\vec{x}_k - \vec{x}_l|} \implies \frac{\partial U_{kl}}{\partial \vec{x}_k} = U'_{kl} \frac{\vec{x}_k - \vec{x}_l}{|\vec{x}_k - \vec{x}_l|}. \quad (6.3.18)$$

Automatically $U'_{kl} = U'_{lk}$. This unit vector above will also appear often and so we define:

$$\vec{u}_{kl} = \frac{\vec{x}_k - \vec{x}_l}{|\vec{x}_k - \vec{x}_l|}. \quad (6.3.19)$$

With these we see:

$$\sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} R_k(t, \vec{x}) = \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} \vec{l}_{kl} R_k(t, \vec{x}) = \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} \vec{l}_{kl} R_k(t, \vec{x}) + \frac{1}{2} \sum_{l=1}^N \sum_{\substack{k=1 \\ k \neq l}}^N U'_{lk} \vec{l}_{lk} R_l(t, \vec{x}) \quad (6.3.20)$$

$$= \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} \vec{l}_{kl} (R_k(t, \vec{x}) - R_l(t, \vec{x})). \quad (6.3.21)$$

Nontrivially, we can write this vector expression as the divergence of a tensor expression. All of the $\vec{x}$ dependence is in the difference $R_k - R_l$. So, we seek a function $S_{kl}(t, \vec{x})$ so that:

$$\vec{l}_{kl} \cdot \nabla S_{kl} = R_k(t, \vec{x}) - R_l(t, \vec{x}). \quad (6.3.22)$$

As a boundary condition we will require that $S_{kl} \rightarrow 0$ as $|\vec{x}| \rightarrow \infty$. We specifically can apply this boundary condition by for any $\vec{x}$ decomposing it into a part $\vec{x}_\perp = \vec{x} - \vec{x} \cdot \vec{l}_{kl} \vec{l}_{kl}$ which is orthogonal to $\vec{l}_{kl}$ and a part $\vec{x} \cdot \vec{l}_{kl} \vec{l}_{kl}$ which is parallel to $\vec{l}_{kl}$; then, we require that if we keep the orthogonal part fixed and go toward $-\infty$ in the parallel part S_{kl} should go to 0. After this, we can simply integrate equation (6.3.22) along a straight line as a line integral from $-\infty$ to our desired $\vec{x}$ value. Doing so gives the explicit expression for S_{kl} :

$$S_{kl}(t, \vec{x}) = \int_{-\infty}^{\vec{l}_{kl} \cdot \vec{x}} (R_k(t, \vec{x} - \vec{l}_{kl} \vec{l}_{kl} \cdot \vec{x} + u \vec{l}_{kl}) - R_l(t, \vec{x} - \vec{l}_{kl} \vec{l}_{kl} \cdot \vec{x} + u \vec{l}_{kl})) du. \quad (6.3.23)$$

This function looks odd but its behavior can be understood by considering the limit that we take the profile functions to be Dirac deltas. If we are considering $\vec{x}$ which do not lie on the line connecting the two particles, this integral never crosses either Dirac delta and so is 0. If we are considering $\vec{x}$ which do lie on that line then when it crosses the first particle it ticks up by 1 and when it crosses the second particle it ticks back down by 0. Thus, when R_0 is taken to be a Dirac delta, this S_{kl} becomes:

$$R_0(|\vec{x}|) = \delta(\vec{x}) \implies S_{kl}(t, \vec{x}) = \delta_\perp(\vec{x}_\perp) \vartheta(\vec{x} \in L_{kl}) \quad (6.3.24)$$

where L_{kl} is the line segment connecting particles $\vec{x}_k$ and $\vec{x}_l$ and $\delta_\perp(\vec{x}_\perp)$ is a 2 dimensional Dirac delta for the directions perpendicular to $\vec{l}_{kl}$. This S_{kl} function essentially just selects out positions which lie on the line segment between the two particles. When the profile functions are only approximately Dirac deltas this gives a smoothened version of that selecting function. In general, we call this S_{kl} the selector function. It follows immediately from the explicit expression for S_{kl} that $S_{kl} = S_{lk}$. Automatically we can write:

$$\sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} R_k(t, \vec{x}) = \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} \vec{l}_{kl} \nabla \cdot (\vec{l}_{kl} S_{kl}) = \nabla \cdot \left(\sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{1}{2} U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl} \right). \quad (6.3.25)$$

Returning all of this to equation (6.3.16) gives:

$$\sum_{k=1}^N m \ddot{\vec{x}}_k R_k(t, \vec{x}) = \vec{f} - \nabla \cdot \left(\sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{1}{2} U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl} \right). \quad (6.3.26)$$

The final term in equation (6.3.15) can be written nicely by rewriting each velocity $\dot{\vec{x}}_k$ as the local average $\vec{v}(t, \vec{x})$ plus a deviation $\dot{\vec{x}}_k(t) - \vec{v}$ and then multiplying out keeping the $\dot{\vec{x}}_k(t) - \vec{v}$ pair always together, which is a common trick we will use repeatedly:

$$\sum_{k=1}^N m \dot{\vec{x}}_k \dot{\vec{x}}_k R_k = \sum_{k=1}^N m (\vec{v} + \dot{\vec{x}}_k - \vec{v}) (\vec{v} + \dot{\vec{x}}_k - \vec{v}) R_k = mn \vec{v} \vec{v} + \sum_{k=1}^N m (\dot{\vec{x}}_k - \vec{v}) (\dot{\vec{x}}_k - \vec{v}) R_k. \quad (6.3.27)$$

This decomposition is nice because the first term $mn \vec{v} \vec{v}$ does change under a Galilean boost but only depends on the averaged quantities $n, \vec{v}$ while the second term in the sum here does not change under a Galilean boost due to the difference $\dot{\vec{x}}_k - \vec{v}$. Returning this to equation (6.3.15) we have:

$$\frac{\partial}{\partial t} (\rho_m \vec{v}) + \nabla \cdot (\rho_m \vec{v} \vec{v}) = \vec{f} - \nabla \cdot \left(\sum_{k=1}^N m (\dot{\vec{x}}_k - \vec{v}) (\dot{\vec{x}}_k - \vec{v}) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl} \right). \quad (6.3.28)$$

Expanding the derivatives on the left hand side gives another simplification:

$$\frac{\partial}{\partial t}(\rho_m \vec{v}) + \nabla \cdot (\rho_m \vec{v} \vec{v}) = mn \frac{d\vec{v}}{dt} \quad (6.3.29)$$

$$\implies mn \frac{d\vec{v}}{dt} = \vec{f} - \nabla \cdot \left(\sum_{k=1}^N m(\dot{\vec{x}}_k - \vec{v})(\dot{\vec{x}}_k - \vec{v}) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl} \right). \quad (6.3.30)$$

If we consider the total force on a region $\mathbb{M}$ of matter, the averaged force on a matter element would be $m \frac{d\vec{v}}{dt} = m \ddot{\vec{z}}$ and so the force per unit volume on the matter would be $mn \frac{d\vec{v}}{dt}$. Then, the force on the region $\mathbb{M}$ is:

$$\vec{F}[\mathbb{M}] = \int_{\mathbb{M}} mn \frac{d\vec{v}}{dt} d\mathbb{S} \quad (6.3.31)$$

$$= \int_{\mathbb{M}} \vec{f} d\mathbb{S} - \int_{\partial \mathbb{M}} \left(\sum_{k=1}^N m(\dot{\vec{x}}_k - \vec{v})(\dot{\vec{x}}_k - \vec{v}) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl} \right) \cdot d\vec{\mathbb{A}}. \quad (6.3.32)$$

This first integral then represents the force on the interior of the matter and the surface integral represents the forces at the boundary of the matter. The integrand of the force on the boundary of matter is known as the stress tensor, exactly as used in problems 3.69, 3.78, 4.32, 4.33, 4.34, 4.35, and 4.82. Thus, the stress tensor $\hat{\sigma}$ for the matter is given by:

$$\hat{\sigma}(t, \vec{x}) \stackrel{\text{def}}{=} - \sum_{k=1}^N m(\dot{\vec{x}}_k - \vec{v})(\dot{\vec{x}}_k - \vec{v}) R_k - \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \vec{l}_{kl} \vec{l}_{kl}. \quad (6.3.33)$$

This results in the velocity equation of motion:

$$mn \frac{d\vec{v}}{dt} = \vec{f} + \nabla \cdot \hat{\sigma}. \quad (6.3.34)$$

Or, written more like a continuity equation, we reproduce (6.2.44):

$$\frac{\partial}{\partial t}(mn\vec{v}) + \nabla \cdot (mn\vec{v}\vec{v} - \hat{\sigma}) = \vec{f}. \quad (6.3.35)$$

While this gives us an equation of motion for the velocity field $\vec{v}$, it does so at the expense of introducing a new independent quantity in the stress tensor. And, while we were able to derive a microscopic expression for the stress tensor we have no expression for it in terms of our other averaged quantities like the velocity or the number density. So, it appears we need to keep going and differentiate our stress tensor with respect to time and see what equation of motion it satisfies. A thoughtful reader should suspect that it will have a reasonably nice equation of motion...after introducing yet further independent quantities which then need their own equations of motion. This is the trouble of kinetic theory. So far we have treated the underlying equations of motion of the particles exactly in deriving our expressions but the consequence of this exactness is that no finite system of equations of motion for the averaged quantities will close (be expressible in terms of just those averaged quantities). The fundamental approximations in kinetic theory come in forcing an approximate closure of the equations of motion.

6.3.3 Energy Transfer

We will return to the issue of forcing closure in a moment but first let us look at the final equation of motion we need which by the logic of section 6.1 is the equation of motion of the energy density. From the Hamiltonian we can write:

$$\mathcal{H} = \sum_{k=1}^N \left(\frac{|\vec{p}_k|^2}{2m} + h(q_k, p_k) \right) + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} = \int_{\mathbb{S}} \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k|^2 + h(q_k, p_k) + \frac{1}{2} \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \right) R_k d\mathbb{S}. \quad (6.3.36)$$

Thus we can take the energy density of our system to be:

$$\mathcal{E}(t, \vec{x}) = \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k|^2 + h(\mathbf{q}_k, \mathbf{p}_k) \right) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} R_k. \quad (6.3.37)$$

It is useful to write the energy density slightly differently using the $\dot{\vec{x}}_k = \dot{\vec{x}}_k - \vec{v} + \vec{v}$ trick:

$$\mathcal{E} = \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v} + \vec{v}|^2 + h(\mathbf{q}_k, \mathbf{p}_k) \right) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} R_k \quad (6.3.38)$$

$$= \frac{1}{2} mn |\vec{v}|^2 + \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h(\mathbf{q}_k, \mathbf{p}_k) \right) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} R_k. \quad (6.3.39)$$

The piece $\frac{1}{2} mn |\vec{v}|^2$ changes under a Galilean boost because $\vec{v}$ gets shifted. However, the remaining terms in the energy density do not change at all under a Galilean boost and so can be understood as the “internal energy density”, mean energy which remains even in the local instantaneous rest frame of the matter. We can then define the internal energy per matter element $\mathcal{U}$ so that $n\mathcal{U}$ is this internal energy density:

$$n\mathcal{U}(t, \vec{x}) = \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h(\mathbf{q}_k, \mathbf{p}_k) \right) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} R_k. \quad (6.3.40)$$

Then:

$$\mathcal{E} = \frac{1}{2} mn |\vec{v}|^2 + n\mathcal{U}. \quad (6.3.41)$$

It should be clear that $n\mathcal{U} = \rho u$ in our previous notation. Now we want an equation of motion for the energy density and so will take its time derivative and simplify. To do so it is algebraically simpler to look at a slightly different combination and to use the momentum equation of motion:

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E} \vec{v}) = \vec{v} \cdot \vec{f} + (\nabla \cdot \hat{\sigma}) \cdot \vec{v} + \frac{\partial}{\partial t} (n\mathcal{U}) + \nabla \cdot (n\mathcal{U} \vec{v}). \quad (6.3.42)$$

So this combination on the energy density reduces to some combination of predefined quantities plus the same derivative structure on the internal energy density. Now we will compute these individual pieces on the internal energy:

$$\begin{aligned} \frac{\partial}{\partial t} (n\mathcal{U}) &= \sum_{k=1}^N \left(m(\dot{\vec{x}}_k - \vec{v}) \cdot (\ddot{\vec{x}}_k - \dot{\vec{v}}) + \frac{\partial h_k}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial h_k}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) R_k + \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{R}_k \\ &\quad + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{R}_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot \dot{\vec{x}}_k + \frac{\partial U_{kl}}{\partial \vec{x}_l} \cdot \dot{\vec{x}}_l + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k + \frac{\partial U_{kl}}{\partial \mathbf{q}_l} \dot{\mathbf{q}}_l + \frac{\partial U_{kl}}{\partial \mathbf{p}_l} \dot{\mathbf{p}}_l \right) R_k. \end{aligned} \quad (6.3.43)$$

Using the equations of motion for the particles the first series in equation (6.3.43) becomes:

$$\begin{aligned} &\sum_{k=1}^N \left(m(\dot{\vec{x}}_k - \vec{v}) \cdot (\ddot{\vec{x}}_k - \dot{\vec{v}}) + \frac{\partial h_k}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial h_k}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) R_k \\ &= \sum_{k=1}^N \left((\dot{\vec{x}}_k - \vec{v}) \cdot \vec{F}_k + \dot{\mathbf{q}}_k \cdot \vec{f}_k \right) R_k - \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left((\dot{\vec{x}}_k - \vec{v}) \cdot \frac{\partial U_{kl}}{\partial \vec{x}_k} + \dot{\mathbf{q}}_k \frac{\partial U_{kl}}{\partial \mathbf{q}_k} + \dot{\mathbf{p}}_k \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \right) R_k \end{aligned} \quad (6.3.44)$$

The quantity $\dot{\vec{x}}_k - \vec{v}$ is the deviation of particle k 's velocity from the average and thus is a microscopic variable. This first sum then represents the rate of work done by external forces on all of the microscopic degrees of freedom of this system which is precisely the definition of the rate of heat transfer. Thus, the heat transfer

density to the matter is:

$$\Phi(t, \vec{x}) = \sum_{k=1}^N \left((\dot{\vec{x}}_k - \vec{v}) \cdot \vec{F}_k + \dot{q}_k f_k \right) R_k. \quad (6.3.45)$$

By definition then the heat added to a volume $\mathbb{M}$ of the matter from outside of that matter between times t_0 and t_f is:

$$\mathcal{Q} = \int_{t_0}^{t_f} \int_{\mathbb{M}} \Phi d^3 \vec{x} dt. \quad (6.3.46)$$

Then equation (6.3.44) becomes:

$$\sum_{k=1}^N \left(m(\dot{\vec{x}}_k - \vec{v}) \cdot (\ddot{\vec{x}}_k - \dot{\vec{v}}) + \frac{\partial h_k}{\partial \mathbf{q}_k} \dot{q}_k + \frac{\partial h_k}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) R_k = \Phi - \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left((\dot{\vec{x}}_k - \vec{v}) \cdot \frac{\partial U_{kl}}{\partial \vec{x}_k} + \dot{q}_k \frac{\partial U_{kl}}{\partial \mathbf{q}_k} + \dot{\mathbf{p}}_k \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \right) R_k. \quad (6.3.47)$$

Returning this to equation (6.3.43):

$$\begin{aligned} \frac{\partial}{\partial t} (n\mathcal{U}) &= \Phi + \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{R}_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{R}_k + \vec{v} \cdot \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} R_k \\ &\quad - \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot \dot{\vec{x}}_k - \frac{\partial U_{kl}}{\partial \vec{x}_l} \cdot \dot{\vec{x}}_l + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{q}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k - \frac{\partial U_{kl}}{\partial \mathbf{q}_l} \dot{q}_l - \frac{\partial U_{kl}}{\partial \mathbf{p}_l} \dot{\mathbf{p}}_l \right) R_k. \end{aligned} \quad (6.3.48)$$

The $\dot{R}_k$ terms can be simplified together:

$$\sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{R}_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{R}_k \quad (6.3.49)$$

$$= - \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{\vec{x}}_k \cdot \nabla R_k - \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{\vec{x}}_k \cdot \nabla R_k \quad (6.3.50)$$

$$= - \nabla \cdot \left(\sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{\vec{x}}_k R_k \right) + \sum_{k=1}^N R_k \dot{\vec{x}}_k \cdot \nabla \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 \right) - \nabla \cdot \left(\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{\vec{x}}_k R_k \right) \quad (6.3.51)$$

$$= - \nabla \cdot (n\mathcal{U}\vec{v}) - \nabla \cdot \left(\sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k + \frac{1}{2} \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \right) (\dot{\vec{x}}_k - \vec{v}) R_k \right) + \sum_{k=1}^N R_k \dot{\vec{x}}_k \cdot \nabla \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 \right). \quad (6.3.52)$$

The last piece here can be rewritten, with some effort:

$$\sum_{k=1}^N R_k \dot{\vec{x}}_k \cdot \nabla \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 \right) = - \partial_a v_b \sum_{k=1}^N R_k m (\dot{x}_k^a - v^a) (\dot{x}_k^b - v^b). \quad (6.3.53)$$

which is beginning to look like the stress tensor. This gives:

$$\begin{aligned} \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) \dot{R}_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \dot{R}_k &= - \nabla \cdot (n\mathcal{U}\vec{v}) - \partial_a v_b \sum_{k=1}^N R_k m (\dot{x}_k^a - v^a) (\dot{x}_k^b - v^b) \\ &\quad - \nabla \cdot \left(\sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k + \frac{1}{2} \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \right) (\dot{\vec{x}}_k - \vec{v}) R_k \right). \end{aligned} \quad (6.3.54)$$

The final term in the first line of equation (6.3.48) can be rewritten using equation (6.3.25):

$$\vec{v} \cdot \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} R_k(t, \vec{x}) = v_b \partial_a \left(\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \iota_{kl}^a \iota_{kl}^b \right) \quad (6.3.55)$$

$$= \nabla \cdot \left(\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot \vec{v} S_{kl} \vec{\iota}_{kl} \right) - \partial_a v_b \left(\frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \iota_{kl}^a \iota_{kl}^b \right). \quad (6.3.56)$$

Finally let us turn our attention to the second line of equation (6.3.48). Some terms in that expression are differentiated with respect to l indexed variables while others are differentiated with respect to k indexed variables. We can change them to both be k indexed by swapping the names l and k on those terms:

$$\begin{aligned} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot \dot{\vec{x}}_k - \frac{\partial U_{kl}}{\partial \vec{x}_l} \cdot \dot{\vec{x}}_l + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k - \frac{\partial U_{kl}}{\partial \mathbf{q}_l} \dot{\mathbf{q}}_l - \frac{\partial U_{kl}}{\partial \mathbf{p}_l} \dot{\mathbf{p}}_l \right) R_k \\ = \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \nabla \cdot \left(\left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot \dot{\vec{x}}_k + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) \vec{\iota}_{kl} S_{kl} \right). \end{aligned} \quad (6.3.57)$$

Returning equation (6.3.54), (6.3.56), and (6.3.57) back to equation (6.3.48):

$$\boxed{\frac{\partial}{\partial t} (n\mathcal{U}) + \nabla \cdot (n\mathcal{U}\vec{v}) = \Phi + \sigma^{ab} \partial_a v_b - \nabla \cdot \vec{q}} \quad (6.3.58)$$

where we defined the heat flux vector:

$$\boxed{\vec{q}(t, \vec{x}) \stackrel{\text{def}}{=} \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k + \frac{1}{2} \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \right) (\dot{\vec{x}}_k - \vec{v}) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot (\dot{\vec{x}}_k - \vec{v}) + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) \vec{\iota}_{kl} S_{kl}.} \quad (6.3.59)$$

By definition this is the sum over all particles of their individual internal energy times the deviation of their velocity from average times their density plus the sum of energy transfers between pairs of particles through their microscopic degrees of freedom $(\dot{\vec{x}}_k - \vec{v}, \mathbf{q}_k, \mathbf{p}_k)$. The interpretation of this vector then is that it is the current density of energy carried by the microscopic degrees of freedom of the matter, which is why it is called the heat flux or heat current vector. Then, the heat that flows across a surface $\mathbb{A}$ within the matter neglecting any heat added from external sources between a time t_0 and t_f is:

$$\mathcal{Q} = \int_{t_0}^{t_f} \int_{\mathbb{A}} \vec{q} \cdot d\vec{\mathbb{A}} dt. \quad (6.3.60)$$

Returning to equation (6.3.43), we find:

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot (\mathcal{E}\vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q}) = \vec{v} \cdot \vec{f} + \Phi. \quad (6.3.61)$$

Finally then using equation (6.3.41) we have:

$$\boxed{\frac{\partial}{\partial t} \left(\frac{1}{2} mn |\vec{v}|^2 + n\mathcal{U} \right) + \nabla \cdot \left(\frac{1}{2} mn |\vec{v}|^2 \vec{v} + n\mathcal{U}\vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q} \right) = \vec{v} \cdot \vec{f} + \Phi.} \quad (6.3.62)$$

Thus, we exactly reproduce equation (6.2.46) now with a precise definition of all the quantities in terms of microscopic variables.

Together then, all of our results from Kinetic Theory so far divide into two categories: the equations of motion for the number density, momentum density, and energy density which are again the nonrelativistic transport equations and the precise definitions of all the quantities appearing in those equations in terms of the microscopic properties of the matter which are called the kinetic definitions of those quantities. So, we have:

Theorem 6.2: Nonrelativistic Kinetic Theory

If a system of N identical nonrelativistic particles evolve microscopically according to the Hamiltonian:

$$\mathcal{H} = \sum_{k=1}^N \left(\frac{|\vec{p}_k|^2}{2m} + h(\mathbf{q}_k, \mathbf{p}_k) \right) + \sum_{k=1}^{N-1} \sum_{l=k+1}^N U(|\vec{x}_k - \vec{x}_l|, \mathbf{q}_k, \mathbf{p}_k, \mathbf{q}_l, \mathbf{p}_l) \quad (6.3.63)$$

under the influence of external forces $\vec{F}_k$ and $\mathbf{f}_k$ and each particle is described by a nonnegative profile function $R_k(t, \vec{x}) = R_0(|\vec{x} - \vec{x}_k(t)|)$ which integrates to 1 then the quantities of interest in continuum mechanics are defined microscopically by:

$$\text{Number Density:} \quad n(t, \vec{x}) = \sum_{k=1}^N R_k(t, \vec{x}), \quad (6.3.64)$$

$$\text{Average Velocity Field:} \quad \vec{v}(t, \vec{x}) = \frac{\sum_{k=1}^N \dot{\vec{x}}_k R_k}{\sum_{k=1}^N R_k}, \quad (6.3.65)$$

$$\text{Momentum Density:} \quad \vec{\rho}(t, \vec{x}) = mn(t, \vec{x})\vec{v}(t, \vec{x}), \quad (6.3.66)$$

$$\text{Force Density:} \quad \vec{f}(t, \vec{x}) \stackrel{\text{def}}{=} \sum_{k=1}^N \vec{F}_k(t) R_k(t, \vec{x}), \quad (6.3.67)$$

$$\text{Stress Tensor:} \quad \hat{\sigma}(t, \vec{x}) = - \sum_{k=1}^N m(\dot{\vec{x}}_k - \vec{v})(\dot{\vec{x}}_k - \vec{v}) R_k - \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U'_{kl} S_{kl} \vec{u}_{kl} \vec{u}_{kl}, \quad (6.3.68)$$

$$\text{Internal Energy Density:} \quad n\mathcal{U}(t, \vec{x}) = \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h(\mathbf{q}_k, \mathbf{p}_k) \right) R_k + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} R_k, \quad (6.3.69)$$

$$\text{Energy Density:} \quad \mathcal{E}(t, \vec{x}) = \frac{1}{2} mn|\vec{v}|^2 + n\mathcal{U}, \quad (6.3.70)$$

$$\text{Heat Transfer Density:} \quad \Phi(t, \vec{x}) = \sum_{k=1}^N \left((\dot{\vec{x}}_k - \vec{v}) \cdot \vec{F}_k + \dot{\mathbf{q}}_k \mathbf{f}_k \right) R_k, \quad (6.3.71)$$

$$\begin{aligned} \text{Heat Current Density:} \quad \vec{q}(t, \vec{x}) = & \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k + \frac{1}{2} \sum_{\substack{l=1 \\ l \neq k}}^N U_{kl} \right) (\dot{\vec{x}}_k - \vec{v}) R_k, \\ & + \frac{1}{2} \sum_{k=1}^N \sum_{\substack{l=1 \\ l \neq k}}^N \left(\frac{\partial U_{kl}}{\partial \vec{x}_k} \cdot (\dot{\vec{x}}_k - \vec{v}) + \frac{\partial U_{kl}}{\partial \mathbf{q}_k} \dot{\mathbf{q}}_k + \frac{\partial U_{kl}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) \vec{u}_{kl} S_{kl} \end{aligned} \quad (6.3.72)$$

where the function S_{kl} is defined by:

$$S_{kl}(t, \vec{x}) = \int_{-\infty}^{\vec{u}_{kl} \cdot \vec{x}} (R_k(t, \vec{x} - \vec{u}_{kl} \vec{u}_{kl} \cdot \vec{x} + u \vec{u}_{kl}) - R_l(t, \vec{x} - \vec{u}_{kl} \vec{u}_{kl} \cdot \vec{x} + u \vec{u}_{kl})) du. \quad (6.3.73)$$

These definitions lead to the exact nonrelativistic transport equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.3.74)$$

$$\frac{\partial}{\partial t} (mn\vec{v}) + \nabla \cdot (mn\vec{v}\vec{v} - \hat{\sigma}) = \vec{f} \quad (6.3.75)$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} mn|\vec{v}|^2 + n\mathcal{U} \right) + \nabla \cdot \left(\frac{1}{2} mn|\vec{v}|^2 \vec{v} + n\mathcal{U}\vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q} \right) = \vec{v} \cdot \vec{f} + \Phi. \quad (6.3.76)$$

6.4 Nonrelativistic Constitutive Relations

Now that we have the basic form of the equations of motion for continuum mechanics we need to address the issue of closing this system of equations. Everything contained in theorem 6.2 is exact for a Hamiltonian of the form equation (6.3.63). But, by the logic of section 6.1 we want to ultimately only have $n, \vec{v}, s$ be our independent variables and so we need to find a way to at least approximately write $\hat{\sigma}, \mathcal{U}$, and $\vec{q}$ in terms of these quantities. We do not need to write $\vec{f}$ or Φ in terms of our independent variables as because they are due to the external forces on the matter they must be supplied in addition to any established properties of the matter. The approximate equations we will find for $\hat{\sigma}, \mathcal{U}$, and $\vec{q}$ in terms of $n, \vec{v}$, and s are called constitutive relations and their precise form will depend on exactly what kind of matter we are attempting to describe.

Regardless of what type of matter we are describing the interpretation of $\mathcal{U}$ will be the internal energy (meaning energy of the microscopic degrees of freedom) per particle at location $\vec{x}$ at time t . In the quasidynamic approximation that these microscopic degrees of freedom (the deviations of each particle's velocity from the average and the internal $\mathbf{q}$ and $\mathbf{p}$ quantities) evolve much more quickly than the macroscopic degrees of freedom (the average velocity field, for example) then this $\mathcal{U}$ becomes the expected thermodynamic energy per particle. Essentially, each element of the matter acts locally as a thermodynamic system. This requirement of the quasidynamic approximation holding locally everywhere in the matter is known as the requirement of **local thermodynamic equilibrium**. Real matter is not generally everywhere all the time in thermodynamic equilibrium. Research on matter which is not in local thermodynamic equilibrium is actively ongoing and significantly more complicated than appropriate for us to analyze.

When assuming local thermodynamic equilibrium we then precisely mean that locally the system is acting as its own bath and so sampling locally from the system should follow the thermodynamic expectations. Locally the apparent probability of selecting a particular particle out of a sample is proportional to that particle's number density and so, if $\mathcal{O}_k$ is a time dependent quantity only depending on properties of particle k the requirement of local thermodynamic equilibrium is:

$$\frac{\sum_{k=1}^N R_k(t, \vec{x}) \mathcal{O}_k}{\sum_{k=1}^N R_k(t, \vec{x})} \approx \mathbb{E}[\mathcal{O}](t, \vec{x}) \quad (6.4.1)$$

where the expectation on the right is taken in the appropriate generalized Boltzmann distribution at the location being averaged over.

6.4.1 Gases

Gases are by far the easiest state of matter to describe, especially because often ideal gases are a sufficiently good approximation. In an ideal gas we simply set the interparticle potential $U = 0$ so that there are no interactions beyond the limiting to 0 weak amount of interaction necessary to locally bring the gas to equilibrium. Then, our Hamiltonian in equation (6.3.63) is precisely of the form of equation (5.9.49). By equation (5.9.62) the free energy of a nonrelativistic ideal gas in its rest frame is:

$$\mathcal{F} = -NT \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{1}{\gamma-1}} \frac{\mathbb{V}}{N} \right) - NT \quad (6.4.2)$$

where we have recalled the definition of the adiabatic ratio γ . Consequently, the entropy S , pressure p , and expected energy $\mathbb{E}$ are:

$$S = -\frac{\partial \mathcal{F}}{\partial T} = N \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{1}{\gamma-1}} \frac{\mathbb{V}}{N} \right) + \frac{\gamma}{\gamma-1} N, \quad (6.4.3)$$

$$p = -\frac{\partial \mathcal{F}}{\partial \mathbb{V}} = \frac{NT}{\mathbb{V}} \quad (6.4.4)$$

$$\mathbb{E} = \mathcal{F} + TS = \frac{NT}{\gamma-1}. \quad (6.4.5)$$

Letting $n = \frac{N}{\mathbb{V}}$ be the number density, $s = \frac{S}{N}$ be the entropy per particle, and $\mathcal{U} = \frac{\mathbb{E}}{N}$ be the internal energy per particle, we have:

$$s = \frac{\gamma}{\gamma-1} + \ln \left(\left(\frac{\kappa T}{2\pi} \right)^{\frac{1}{\gamma-1}} \frac{1}{n} \right) \quad (6.4.6)$$

$$p = nT \quad (6.4.7)$$

$$\mathcal{U} = \frac{T}{\gamma - 1}. \quad (6.4.8)$$

As well, from the fundamental thermodynamic relation for the gas:

$$dE = TdS - pdV \quad (6.4.9)$$

$$\implies Nd\mathcal{U} = NTds - pNd\left(\frac{1}{n}\right) \quad (6.4.10)$$

$$\implies d\mathcal{U} = Tds + \frac{p}{n^2}dn \quad (6.4.11)$$

which will serve as the local fundamental thermodynamic relation. Because this applies locally all of these quantities are functions of time and position. It is important to note that the free energy above gives an expected velocity of 0 and so is necessarily the free energy for the system in its local instantaneous rest frame. In a general frame then the velocities and consequently momenta are boosted. Consequently the single particle distribution function in general is:

$$f_1(\vec{x}_1, \vec{p}_1, q_1, p_1 | t, \vec{x}) = \frac{e^{-\beta(t, \vec{x}) \left(\frac{|\vec{p}_1 - m\vec{v}(t, \vec{x})|^2}{2m} + h(q_1, p_1) \right)}}{Z_1} \quad (6.4.12)$$

using the Hamiltonian in equation (6.3.63). By equations (6.3.68) and (6.4.1) we have that for an ideal gas:

$$\hat{\sigma}(t, \vec{x}) = - \sum_{k=1}^N m(\dot{\vec{x}}_k - \vec{v})(\dot{\vec{x}}_k - \vec{v})R_k \quad (6.4.13)$$

$$\implies \sigma^{ab}(t, \vec{x}) = -mn\mathbb{E}((\dot{x}^a - v^a)(\dot{x}^b - v^b)). \quad (6.4.14)$$

We can easily compute this expectation:

$$\mathbb{E}((\dot{x}^a - v^a)(\dot{x}^b - v^b)) = \frac{1}{m^2} \int_{\mathbb{P}} (p_1^a - mv^a)(p_1^b - mv^b) \frac{e^{-\beta \left(\frac{|\vec{p}_1 - m\vec{v}|^2}{2m} + h(q_1, p_1) \right)}}{Z} d\mathbb{P} = \frac{1}{m^2} \frac{\int_{\mathbb{R}^3} p_1^a p_1^b e^{-\frac{|\vec{p}_1|^2}{2mT}} d^3\vec{p}_1}{\int_{\mathbb{R}^3} e^{-\frac{|\vec{p}_1|^2}{2mT}} d^3\vec{p}_1}. \quad (6.4.15)$$

All of the integrals not over linear momentum end up canceling with the normalization factors in the partition function denominator. As well, we can shift away the $m\vec{v}$ in the momentum integration variables. This remaining integral is 0 if $a \neq b$ because then it is an odd integrand under inverting one of the coordinate axes and the integral of an odd function over the entire real line is 0. So, this integral can be written as:

$$\mathbb{E}((\dot{x}^a - v^a)(\dot{x}^b - v^b)) = A\delta^{ab} \quad (6.4.16)$$

for some A . Taking the trace of both sides:

$$\mathbb{E}|\dot{\vec{x}} - \vec{v}|^2 = 3A \quad (6.4.17)$$

$$\implies A = \frac{2}{3m} \mathbb{E} \frac{|\vec{p} - m\vec{v}|^2}{2m} = \frac{2}{3m} \left(-\frac{\partial}{\partial \beta} \right) \ln \left(\int_{\mathbb{R}^3} e^{-\frac{\beta|\vec{p}|^2}{2m}} d^3\vec{p} \right) = \frac{2}{3m} \left(-\frac{\partial}{\partial \beta} \right) \ln \left(\frac{2\pi m}{\beta} \right)^{\frac{3}{2}} = \frac{T}{m} \quad (6.4.18)$$

$$\implies \mathbb{E}((\dot{x}^a - v^a)(\dot{x}^b - v^b)) = \frac{T(t, \vec{x})}{m} \delta^{ab}. \quad (6.4.19)$$

Thus, the stress tensor for an ideal gas is (using equation (6.4.7)):

$$\hat{\sigma} = -mn \frac{T}{m} \mathbb{1} = -p(t, \vec{x}) \mathbb{1} \quad (6.4.20)$$

where $p(t, \vec{x}) = n(t, \vec{x})T(t, \vec{x})$ is the local thermodynamic pressure given by the ideal gas law. The final quantity we need a constitutive relation for is the heat flux vector. From equation (6.3.72) for an ideal gas it is given by:

$$\vec{q}(t, \vec{x}) = \sum_{k=1}^N \left(\frac{1}{2} m |\dot{\vec{x}}_k - \vec{v}|^2 + h_k \right) (\dot{\vec{x}}_k - \vec{v}) R_k. \quad (6.4.21)$$

In the rest frame then by equation (6.4.1):

$$\vec{q}(t, \vec{x}) = n\mathbb{E} \left(\frac{1}{2} m |\dot{\vec{x}}|^2 \dot{\vec{x}} + h \dot{\vec{x}} \right) = n\mathbb{E} \left(\frac{|\vec{p}|^2}{2m} \frac{\vec{p}}{m} + h \frac{\vec{p}}{m} \right). \quad (6.4.22)$$

Both terms are odd functions of the momentum but the single particle distribution is an even function of the momentum and so one can quickly compute this expectation to be 0:

$$\vec{q} = 0 \quad (6.4.23)$$

for an ideal gas.

Thus, for an ideal gas the equations of motion simplify to:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.4.24)$$

$$\frac{\partial}{\partial t} (mn\vec{v}) + \nabla \cdot (mn\vec{v}\vec{v}) = \vec{f} - \nabla p \quad (6.4.25)$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} mn|\vec{v}|^2 + n\mathcal{U} \right) + \nabla \cdot \left(\frac{1}{2} mn|\vec{v}|^2 \vec{v} + n\mathcal{U}\vec{v} + p\vec{v} \right) = \vec{v} \cdot \vec{f} + \Phi. \quad (6.4.26)$$

The relationships between $\mathcal{U}$, p , and s are given by the thermodynamic relations in equations (6.4.6)-(6.4.8). We can simplify these equations a bit further by expanding some of the derivatives and using our other equations of motion:

$$\frac{\partial}{\partial t} (n\mathcal{U}) + \nabla \cdot (n\mathcal{U}\vec{v}) = \Phi - p\nabla \cdot \vec{v} \quad (6.4.27)$$

$$\implies \mathcal{U} \left(\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) \right) + n \frac{d\mathcal{U}}{dt} = \Phi - p\nabla \cdot \vec{v} \quad (6.4.28)$$

$$\implies n \frac{\partial \mathcal{U}}{\partial s} \frac{ds}{dt} + n \frac{\partial \mathcal{U}}{\partial n} \frac{dn}{dt} = \Phi - p\nabla \cdot \vec{v} \quad (6.4.29)$$

$$\implies nT \frac{ds}{dt} + \frac{p}{n} \left(\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) \right) = \Phi \quad (6.4.30)$$

$$\implies nT \frac{ds}{dt} = \Phi. \quad (6.4.31)$$

Hence the energy equation of motion reduces to a simple statement about the rate at which entropy is produced when heat is supplied to the ideal gas. This is the local analog of equation (5.8.40). It happens to be convenient to look at the entropy equation of motion instead as an equation of motion for the pressure. By equation (6.4.8) we have:

$$n\mathcal{U} = \frac{nT}{\gamma - 1} = \frac{p}{\gamma - 1}. \quad (6.4.32)$$

Then, the energy equation becomes:

$$\frac{\partial}{\partial t} \left(\frac{p}{\gamma - 1} \right) + \nabla \cdot \left(\frac{p}{\gamma - 1} \vec{v} \right) = \Phi - p\nabla \cdot \vec{v} \quad (6.4.33)$$

$$\implies \frac{1}{\gamma - 1} \frac{\partial p}{\partial t} + \frac{1}{\gamma - 1} \vec{v} \cdot \nabla p + \frac{\gamma}{\gamma - 1} p \nabla \cdot \vec{v} = \Phi. \quad (6.4.34)$$

Using the continuity equation:

$$0 = \frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = \frac{dn}{dt} + n\nabla \cdot \vec{v} \implies \nabla \cdot \vec{v} = -\frac{1}{n} \frac{dn}{dt}. \quad (6.4.35)$$

Then:

$$\frac{1}{\gamma - 1} \frac{dp}{dt} - \frac{\gamma}{\gamma - 1} \frac{p}{n} \frac{dn}{dt} = \Phi \quad (6.4.36)$$

$$\implies \frac{d}{dt} (\ln p - \gamma \ln n) = (\gamma - 1) \frac{\Phi}{p}. \quad (6.4.37)$$

With this the pressure equation becomes:

$$\frac{d}{dt} (pn^{-\gamma}) = (\gamma - 1) \Phi n^{-\gamma} \quad (6.4.38)$$

Finally then we have a complete and closed reasonably simple set of equations of motion for an ideal gas:

Theorem 6.3: Ideal Gas (Euler) Equations of motion

The equations of motion for an ideal gas with number density $n(t, \vec{x})$, velocity field $\vec{v}(t, \vec{x})$, and pressure $p(t, \vec{x})$ are:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.4.39)$$

$$mn \frac{d\vec{v}}{dt} = \vec{f} - \nabla p \quad (6.4.40)$$

$$\frac{d}{dt} (pn^{-\gamma}) = (\gamma - 1)n^{-\gamma}\Phi \quad (6.4.41)$$

where m is the mass of each gas molecule, γ is the adiabatic ratio of the gas, $\vec{f}(t, \vec{x})$ is the force density on the gas and $\Phi(t, \vec{x})$ is the heat transfer density to the gas.

6.4.2 Fluids

Fluids are significantly more complicated than ideal gases. Whereas in an ideal gas we simply set the interparticle potential U to 0 and assumed local thermodynamic equilibrium, for a fluid that interparticle potential can be quite important and at best one can generally only expect approximate local thermodynamic equilibrium (and the deviation from equilibrium will cause extra terms in the equations of motion). For a fluid we assume that this potential decays to 0 for two particles which are “far” from each other but is very significant for particles which are sufficiently close to each other. This way the interactions in the fluid are still dominated by what is going on in the neighborhood of the fluid element.

Constitutive relations for fluids can be derived from either an effective theory or kinetic theory perspective. We will work from an effective theory perspective, because deriving constitutive relations from kinetic theory generally requires many assumptions about the material being considered and we would like to keep our analysis as general as possible. It is also typically much more painful. $\mathcal{U}$ needs to be supplied from thermodynamics. To model it, we need some thermodynamic model of a fluid, which we can get from treating (6.3.63) as a thermodynamic system. This is precisely what we did for the Van der Waals fluid, and so a reasonable approximation of the thermodynamic free energy can be given by (5.10.79) for weakly interacting fluids. For more complicated fluids, a more detailed calculation from an appropriate microscopic Hamiltonian would be necessary (where the interparticle potential needs to be carefully chosen as appropriate for the material under consideration).

To model $\hat{\sigma}$ in effective theory we simply use its transformation properties and make a series expansion assuming that the fluid velocity $\vec{v}(t, \vec{x})$ does not vary too quickly in space. This way, $\hat{\sigma}$ will be assumed to be some function of $n, T, \vec{v}$ and their derivatives. We already know the transformation properties of all of these quantities and $\hat{\sigma}$ under boosts and rotations. The number density and temperature are both scalars and so invariant under Galilean boosts and rotations. $\hat{\sigma}$ cannot depend on $\vec{v}$ directly because $\hat{\sigma}$ is invariant under Galilean boosts by $\vec{v}$ is not. However, $\hat{\sigma}$ can depend on $\nabla\vec{v}$ because under a Galilean boost $\vec{v}$ is shifted by a uniform vector (gradient 0) and so $\nabla\vec{v}$ is Galilean boost invariant. Therefore:

$$\hat{\sigma} = \hat{\sigma}(n, T, \nabla n, \nabla T, \nabla\vec{v}, \dots) \quad (6.4.42)$$

where the ... indicate possible dependence on higher derivatives of these quantities. In principle one could also allow the stress tensor to depend on the time derivatives of these quantities but these time derivatives can be iteratively eliminated using the equations of motion to be written in the way we have written here. The form (6.4.42) is reasonable for a wide variety of fluids, but in order to get some specific workable equations of motion we need to specify more about the function on the right hand side. Doing so will restrict the possible fluids under consideration.

A reasonable model for simple fluids is to assume that the field $n, T, \vec{v}$ do not vary too quickly in space, which means that the higher order derivatives $\nabla\nabla\vec{v}$ and higher, make negligible contributions to the fluid motion on the scale to which we are sensitive. Therefore, we model $\hat{\sigma} = \hat{\sigma}(n, T, \nabla n, \nabla T, \nabla\vec{v})$ and have that the first derivatives cannot be very large, so we further approximate $\hat{\sigma}$'s dependence on them as linear:

$$\sigma^{ab} = A^{ab}(n, T) + B^{abc}(n, T)\partial_c n + C^{abc}(n, T)\partial_c T + D^{abcd}(n, T)\partial_c v_d. \quad (6.4.43)$$

This model for $\hat{\sigma}$ is very restrictive and will not be good for all fluids. But, it gives good results for water and some other common fluids. We now need to determine the functions $A^{ab}(n, T)$, $B^{abc}(n, T)$, $C^{abc}(n, T)$,

and $D^{abcd}(n, T)$. Because $\hat{\sigma}$ must be a rank 2 tensor under rotations and $\nabla n, \nabla T$ are vectors and $\nabla \vec{v}$ is a rank 2 tensor, it follows that A^{ab} must form the components of a rank 2 tensor, B^{abc} and C^{abc} must form the components of a rank 3 tensor, and D^{abcd} must form the components of a rank 4 tensor, so that (6.4.43) remains valid under rotations. $A^{ab}(n, T)$ is unchanged by rotations because n, T are, and so it must form a rotationally invariant rank 2 tensor. $B^{abc}(n, T)$ and $C^{abc}(n, T)$ are also unchanged under rotations because n, T are, and so must form rotationally invariant rank 3 tensors. $D^{abcd}(n, T)$ is yet again unchanged by rotations, and so must form a rotationally invariant rank 4 tensor. By the results of problem 2.7, these conditions require A^{ab} to be proportional to δ^{ab} , B^{abc} and C^{abc} to be proportional to ϵ^{abc} and D^{abcd} to be a linear combination of $\delta^{ab}\delta^{cd}, \delta^{ac}\delta^{bd}, \delta^{ad}\delta^{bc}$. Therefore, for some scalar functions $A(n, T)$, $B(n, T)$, $C(n, T)$, $D(n, T)$, $E(n, T)$, and $F(n, T)$:

$$\sigma^{ab} = A(n, T)\delta^{ab} + B(n, T)\epsilon^{abc}\partial_c n + C(n, T)\epsilon^{abc}\partial_c T + D(n, T)\delta^{ab}\nabla \cdot \vec{v} + E(n, T)\partial^a v^b + F(n, T)\partial^b v^a. \quad (6.4.44)$$

We also know that σ^{ab} must be symmetric in exchanging a, b . Requiring this fixes $B(n, T) = C(n, T) = 0$ and $F(n, T) = E(n, T)$. The more common name for $A(n, T)$ is $-P(n, T)$, where P is called the **mechanical pressure**. The more common name for $E(n, T)$ is the **dynamic viscosity** $\mu(n, T)$ and the more common name for $D(n, T)$ is $\zeta(n, T) - \frac{2}{3}\mu(n, T)$ where $\zeta(n, T)$ is called the **bulk viscosity**. So, we can express our model for the stress tensor as:

$$\sigma^{ab} = -P(n, T)\delta^{ab} + \mu(n, T)\left(\partial^a v^b + \partial^b v^a - \frac{2}{3}\nabla \cdot \vec{v}\delta^{ab}\right) + \zeta(n, T)\nabla \cdot \vec{v}\delta^{ab}. \quad (6.4.45)$$

We can develop an understanding of P through studying how it enters the equations of motion. Suppose we have a locally uniform fluid so that we can approximate $\nabla \vec{v} = 0$. By equation (6.2.2) or (6.3.32), the force on a region $\mathbb{M}$ of the fluid due to internal stress is given by:

$$\vec{F}[\mathbb{M}] = \int_{\partial\mathbb{M}} \hat{\sigma} \cdot d\vec{A}. \quad (6.4.46)$$

Therefore, the mechanical pressure of the stress tensor, defined as in problem 4.38 by the force per unit area into that surface is given by (with $\vec{n}$ the unit normal to the surface):

$$\text{pressure} = -\vec{n} \cdot \hat{\sigma} \cdot \vec{n} = P(n, T) \quad (6.4.47)$$

using our formula for the stress tensor. This justifies the identification of P with the mechanical pressure. If the fluid is locally in thermodynamic equilibrium then the pressure can also be computed thermodynamically. Equilibrium requires the “external” mechanical pressure and the “internal” thermodynamic pressure to match, and so when local thermodynamic equilibrium is a good model, we take $P = p(n, T)$ where $p(n, T)$ is the thermodynamic pressure. (We will always assume this to be the case, but it may fail for complicated materials or on very short timescales.)

It is much harder to develop specific formulas for μ and ζ . Various different theoretical approaches predict that they should be independent of the number density n , and this is experimentally consistent for many different fluids. I do not have a good simple argument for why μ and ζ should be independent of n in general as to derive it theoretically in the ways I have seen more assumptions are necessary than should be, given how general of a phenomenon it is. We will always take $\mu = \mu(T)$ and $\zeta = \zeta(T)$ as an experimentally informed fact. The temperature dependence of the viscosities is much more complicated and does not seem to have a universal formula. One needs to compute it from the specific interparticle potential used for modeling the fluid¹. This can be done analytically or through a simulation, or one can try to fit the viscosity to some functional form from experimental data. All of these approaches are useful for different materials. We will not put stock in any particular formula for these as they depend strongly on the fluid at hand. Even qualitative features tend to be different with most interacting gases having increasing viscosity with temperature and most liquids have decreasing viscosity with temperature.

Therefore, our final model for the stress tensor for a simple fluid is:

$$\hat{\sigma} = -p(n, T)\mathbb{1} + \mu(T)\left(\nabla \vec{v} + (\nabla \vec{v})^T - \frac{2}{3}\nabla \cdot \vec{v}\mathbb{1}\right) + \zeta(T)\nabla \cdot \vec{v}\mathbb{1} \quad (6.4.48)$$

where $p(n, T)$ is the thermodynamic pressure and $\mu(T)$ and $\zeta(T)$ must be fit to some data (either experimental or simulation) or some kinetic theory calculation.

¹Most of the simplest derivations one can find for the temperature dependence of the viscosities gives that they should depend on temperature proportionally to $\sqrt{T}$. But, this dependence is generally a poor match to experiment.

We can perform the same type of analysis for $\vec{q}$. Again, we model $\vec{q}$ as being a function of $n, T, \vec{v}$, and their spatial derivatives. Because $\vec{q}$ is Galilean invariant, it cannot depend on $\vec{v}$ directly, only on $\nabla \vec{v}$. Then, again taking the dependence to only be on the quantities up to one order of differentiation, we have:

$$q_a = A_a(n, T) + B(n, T)\partial_a n + C(n, T)\partial_a T + D_{abc}(n, T)\partial^b v^c \quad (6.4.49)$$

for some vector function $A_a(n, T)$, scalar functions $B(n, T)$ and $C(n, T)$, and rank 3 tensor function $D_{abc}(n, T)$. There are no nonzero rotationally invariant vectors and so $A_a(n, T) = 0$. By the microscopic formula for $\vec{q}$ in (6.3.72) or from how it enters the transport equations in (6.2.46), we can see that $\vec{q}$ is parity odd. However, n and T are both parity even and so D_{abc} is automatically parity even. $\nabla \vec{v}$ is also parity even because both ∇ and $\vec{v}$ are parity odd and so $D_{abc}\partial^b v^c$ is parity even. Because $\vec{q}$ is parity odd, the only consistent choice for D_{abc} then is $D_{abc} = 0$. B and C are completely unrestricted by symmetry considerations and like μ and ζ are observed to quite often be independent of the density n . Going forward we will call $B(n, T) = -\iota(T)$ where $\iota(T)$ is the density conductivity and we will call $C(n, T) = -\kappa(T)$ where $\kappa(T)$ is the thermal conductivity. Thus, we have our model for $\vec{q}$:

$$\vec{q} = -\kappa(T)\nabla T - \iota(T)\nabla n. \quad (6.4.50)$$

Just like the viscosities, κ and ι have to be determined for the specific fluid at hand from experiment, simulation, or kinetic theory.

Combining all of our results:

Theorem 6.4: Simple Fluid (Navier-Stokes) Equations of motion

The equations of motion for simple fluid with number density $n(t, \vec{x})$, velocity field $\vec{v}(t, \vec{x})$, and pressure $p(t, \vec{x})$ are:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.4.51)$$

$$m n \frac{d\vec{v}}{dt} = \vec{f} - \nabla p + \nabla \cdot \left(\mu \nabla \vec{v} + \mu (\nabla \vec{v})^T + \left(\zeta - \frac{2}{3} \mu \right) \nabla \cdot \vec{v} \mathbb{1} \right) \quad (6.4.52)$$

$$n \frac{d\mathcal{U}}{dt} + p \nabla \cdot \vec{v} = \Phi + \mu \partial_a v_b \partial^a v^b + \mu \partial_a v_b \partial^b v^a + \left(\zeta - \frac{2}{3} \mu \right) (\nabla \cdot \vec{v})^2 + \nabla \cdot (\kappa \nabla T + \iota \nabla n). \quad (6.4.53)$$

where m is the mass of each molecule, $T(t, \vec{x})$ is the temperature of the fluid, $\mathcal{U}$ is the local thermodynamic internal energy per particle in the instantaneous local rest frame, $\mu(T)$ is the dynamic viscosity of the fluid, $\zeta(T)$ is the bulk viscosity of the fluid, $\kappa(T)$ is the thermal conductivity of the fluid, $\iota(T)$ is the density conductivity of the fluid, $\vec{f}(t, \vec{x})$ is the force density on the fluid, and $\Phi(t, \vec{x})$ is the heat transfer density to the fluid.

It is very common to consider certain special cases of the Navier-Stokes equations. In particular, incompressible solutions (meaning solutions with $n(t, \vec{x}) = n_0$ a constant) are often of interest due to them often correctly representing the behavior of water. As well, it is common to take $\zeta = \iota = 0$ and to take μ and κ to be effectively constant rather than functions of the temperature. For incompressible solutions:

$$0 = \frac{dn}{dt} = -n \nabla \cdot \vec{v} \implies \nabla \cdot \vec{v} = 0. \quad (6.4.54)$$

Thus, the velocity field for an incompressible fluid is always divergence free. Another simplifying assumption often made for the Navier-Stokes equations is that at fixed n the internal energy depends linearly on the temperature. This is typically best understood as a simple Taylor expansion of $\mathcal{U}$ in terms of T valid for small fluctuations of the temperature about a standard value. Then, let c_1 be the heat capacity per particle of the system so that by definition:

$$c_1 = \left. \frac{d\mathcal{U}}{dT} \right|_n \quad (6.4.55)$$

where this notation is to indicate that the derivative is taken at fixed n . With these simplifying assumptions we arrive at a very commonly used special case of the Navier-Stokes equations:

$$\rho_0 \frac{d\vec{v}}{dt} = \vec{f} - \frac{\rho_0}{m} \nabla T + \mu \nabla^2 \vec{v} \quad (6.4.56)$$

$$c_1 \frac{dT}{dt} = \Phi + \mu \partial_a v_b \partial^a v^b + \mu \partial_a v_b \partial^b v^a + \kappa \nabla^2 T. \quad (6.4.57)$$

Even though these “special Navier-Stokes equations” are much simpler than the fully general set, solving them in most cases is essentially impossible. Even understanding the existence and smoothness of solutions is an unsolved problem with a million dollar bounty on it.

There is a somewhat perplexing feature of the Navier-Stokes equations: they do not have time reversal symmetry. The reason this is interesting is that the underlying Hamiltonian in equation (6.3.63) does have time reversal symmetry automatically. How can macroscopic equations of motion which do not have time reversal symmetry be a good model for the averaged behavior of a microscopic theory which does have time reversal symmetry? The only place time reversal symmetry can be broken is in the averaging process. Mathematically, as established in chapter 5 interactions cause correlations. In order to derive the Navier-Stokes equations from kinetic theory one has to neglect any correlations and assume that at each stage the different particles can be treated as statistically independent. The time forward averaging assumes that just before interaction between two particles there is no correlation between them to compute the expectations. The time reversed version would assume that just after interacting there is no correlation. These two are not the same because in the interaction a correlation develops. So, this assumption of no correlation leading up to interactions is the source of when averaging breaks time reversal symmetry at the theoretical level. But, how experimentally is this a reasonable approximation to make? Experimentally where is the time reversal symmetry broken? It is broken by our inability to distinguish the particles from each other and our insensitivity to the correlations between them. Essentially, the experimentally accessible measurements of the fluid system are to measure the smoothened density over a finite length scale with a finite time resolution and to measure the smoothened velocity field over a finite length scale and with a finite time resolution. These averages are unable to track the locations of individual particles and throwing away this information at each time step going forward is not a time reversal symmetric procedure. Experimentally, which types of initial conditions we can prepare are not time reversal symmetric. For example, if we had two fluids of different colors in a container, it is not so hard to put one fluid in first and then the second and then watch them mix. In principle, if we reversed all of the final conditions of the fluid particles, they would unmix, but we don’t have the necessary control of the microscopic variables to do this. However, if the fluids are very viscous (paint) and they are mixed very slowly then we can actually unmix them very slowly, as a proof of principle (you can find videos of this online – search “Unmixing Color Machine”).

It should not be too surprising that $\mu, \zeta, \kappa, \iota$ are difficult to compute from microscopic considerations considering we know that if we work too microscopically, our model of matter is wrong (we know that point particles are not real, from both Earnshaw’s theorem and section 4.8). It turns out that the microscopic properties of $\mu, \zeta, \kappa, \iota$ can very much be directly affected by quantum mechanics, which is the corrected theory of what is really going on with matter microscopically that we will develop in Part II.

While the Navier-Stokes equations are useful for simple fluids, such as water, the constitutive relations used for $\vec{q}$ and $\hat{\sigma}$ fail to correctly predict the behavior of some more complicated fluids such as honey. One should understand the Navier-Stokes equations as a particular manifestation of the nonrelativistic transport equations which are often but not always valid. There are some materials like sand which under some circumstances flow like a fluid and in other circumstances are almost nothing like a fluid. The world of continuum mechanics is vast and complicated, relying on the detailed specifics of every material at hand to determine the correct expressions for $\vec{q}$ and $\hat{\sigma}$. Here we are only looking at the most basic and common models to understand the spirit of how continuum mechanics works. There is far too much to cover it all and a good amount of what could be asked has not been answered.

6.4.3 Solids

Solid matter is characterized by resisting having its shape stretched or deformed. Microscopically this manifests through a significantly strong attractive interparticle potential so that the particles resist being moved away from each other. Due to the specific interparticle potential used there will be some stable configuration of the particles. (For this to be true, one cannot simply assume point particles interacting via electrostatics or similar forces as due to Earnshaw’s theorem no such stable equilibrium exists. In reality the correct interparticle potential to use is far more complicated owing to that fact that the particles which comprise matter are not point-like and that there are interactions present we have not yet studied. These interactions are quantum mechanical and quantum physics is integral to the microscopic properties of solids. We will not need to know the details of how the matter stabilizes here, just the knowledge that it does.)

The stable multi particle configuration defines a lattice of points (the locations of the centers of each of the particles). Often but not always this lattice has a regularly repeating periodic structure, in which case it is called a crystal. Whenever the particles are displaced from their stable equilibria by a small amount, simple harmonic oscillations will develop by Hooke's law and the theorem of normal modes. The specific spring constants of the various oscillations are then predicted by the interparticle potential and the lattice structure it induces. The relationship between these is studied heavily in solid-state physics.

It is rarely possible to analytically express the stress tensor of a solid in terms of its microscopic interparticle potential due to the complicated induced lattice structure. For us, it is more useful to go with the effective theory approach and write down an expression for the stress tensor with the correct transformation properties. To determine the undetermined coefficients that appear in such an approach, one would need to fit the predictions of the theory to some experiment, simulation, or microscopic calculation. This is the most realistic way a comparison can be done in the status quo. In order to do this we need to know what the stress tensor can look like from bottom-up effective theory. So, what can it be?

For solids it is generally much more natural to describe the dynamics in Lagrangian coordinates. Previously we used the initial position to label Lagrangian coordinates but really any label is okay as long as it uniquely specifies one and only one matter element. We don't have to label by initial conditions, and in fact for solids it is more useful to label matter elements by labels $\vec{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$ which represent where they would be if the matter were in stable equilibrium. For this subsection assume we always do so. By equation (6.1.13) it immediately follows that the material momentum $\vec{p}(t, \vec{\alpha})$ is:

$$\vec{p}(t, \vec{\alpha}) = \frac{\vec{\varrho}(t, \vec{z})}{n(t, \vec{z})} = m \frac{d\vec{z}}{dt}(t, \vec{\alpha}). \quad (6.4.58)$$

The mass transfer equation in Lagrangian coordinates is simply equation (6.1.10):

$$n(t, \vec{z}) = \frac{n_0(\vec{\alpha})}{\det\left(\frac{\partial \vec{z}}{\partial \vec{\alpha}}\right)}. \quad (6.4.59)$$

The momentum transfer equation in Lagrangian coordinates is simply equation (6.2.45):

$$mn \frac{d^2 z^a}{dt^2} = f^a + \frac{\partial \sigma^{ab}}{\partial \alpha^c} \frac{\partial \alpha^c}{\partial z^b} \quad (6.4.60)$$

where we have expressed the spatial derivatives in terms of $\vec{\alpha}$ differentiation because in Lagrangian coordinates all quantities are properly expressed as functions of $t, \vec{\alpha}$. The matrix with components $\frac{\partial \alpha^a}{\partial z^b}$ here is to be understood as the matrix inverse of the derivative matrix with components $\frac{\partial z^a}{\partial \alpha^b}$. Similarly expanding the energy transfer equation in Lagrangian coordinates from equation (6.2.46):

$$n \frac{d\mathcal{U}}{dt} = \Phi + \sigma^{ab} \frac{\partial \alpha^c}{\partial z^a} \frac{\partial v_b}{\partial \alpha^c} - \frac{\partial q^a}{\partial \alpha^b} \frac{\partial \alpha^b}{\partial z^a}. \quad (6.4.61)$$

By definition the streamline function $\vec{z}(t, \vec{\alpha})$ gives the location at time t of the matter element which would be at $\vec{\alpha}$ in stable equilibrium. As established in section 2.9 when a body of matter moves rigidly the distance between any two points in the matter is exactly constant (by definition). In equilibrium the line element for measuring distances between matter elements is:

$$ds_0 = |d\vec{\alpha}| = \sqrt{d\vec{\alpha} \cdot d\vec{\alpha}} = \sqrt{(d\alpha^1)^2 + (d\alpha^2)^2 + (d\alpha^3)^2} = \sqrt{\delta_{ab} d\alpha^a d\alpha^b} \quad (6.4.62)$$

while when disturbed the line element for measuring distances between matter elements is:

$$ds = |d\vec{z}| = \sqrt{d\vec{z} \cdot d\vec{z}} = \sqrt{(dz^1)^2 + (dz^2)^2 + (dz^3)^2} = \sqrt{\delta_{ab} dz^a dz^b}. \quad (6.4.63)$$

Thus, the extent to which ds_0 and ds fail to coincide measures the amount by which the motion of matter has failed to be rigid. We can express the undisturbed line element in terms of the true displacements:

$$ds_0^2 = \delta_{ab} d\alpha^a d\alpha^b = \delta_{ab} \frac{\partial \alpha^a}{\partial z^c} \frac{\partial \alpha^b}{\partial z^d} dz^c dz^d. \quad (6.4.64)$$

It is common then to define the displacement gradient tensor:

$$F^a_b = \frac{\partial \alpha^a}{\partial z^b} \quad (6.4.65)$$

and the (left) Green deformation tensor or stretch tensor:

$$C_{ab} = \delta_{cd} F^c_a F^d_b = \delta_{cd} \frac{\partial \alpha^c}{\partial z^a} \frac{\partial \alpha^d}{\partial z^b} \quad (6.4.66)$$

$$\implies ds_0^2 = C_{ab} dz^a dz^b. \quad (6.4.67)$$

Thus, the matter is rigidly deformed only when $C_{ab} = \delta_{ab}$ everywhere. Locally then $C_{ab} - \delta_{ab}$ measures the extent to which the body has stretched (or compressed) as local distances have changed. The strain tensor E_{ab} is defined by this deviation:

$$E_{ab} = C_{ab} - \delta_{ab}. \quad (6.4.68)$$

We have called C_{ab} a tensor however we should be careful as to what space it is a tensor on. We have two coordinate systems, α^a and z^a . C_{ab} is a tensor with both of its indices corresponding to the z^a coordinate system. That is, $C_{ab} dz^a dz^b$ is a scalar invariant under rotations of the z^a coordinates. F^a_b has its upper index as an index in the α^a coordinate system and its lower index as an index in the z^a coordinate system. Because of this F^a_b should properly be called a bi-tensor as it is a tensor with indices corresponding to two different spaces. The combination $F^a_b d\alpha_a dz^b$ is a scalar but the quantity $F^a_b dz_a d\alpha^b$ is geometrically meaningless with no useful transformation property under changes of coordinates. Similarly, $C_{ab} d\alpha^a d\alpha^b$ is geometrically meaningless. This distinction is important because the stress tensor σ^{ab} is a spatial tensor and z^a corresponds to the spatial position. Thus, σ^{ab} should have its indices contracted with other quantities in the z^a coordinate system.

We will now try to find a model for the stress tensor of a solid. In principle, the viscosity terms from our fluid stress tensor can be included for a solid as well, as they have all of the correct transformation properties. For now we will neglect these additions but you may make them if you like. Because of the definition of stable equilibrium the transfer equations of motion should be trivially true with all vanishing time derivatives whenever $z(t, \vec{\alpha}) = \vec{\alpha}$ for all times. It follows that in such a case the stress tensor should vanish. Consequently $\delta\sigma^{ab}$ and $\delta\vec{q}$, the contributions which are added to the stress tensor and heat current density for a solid, should vanish in stable equilibrium, which occurs whenever $C_{ab} = \delta_{ab}$ everywhere for all times.

Simple solids are assumed to be isotropic (and so should have local rotational symmetry under redefining labels $\vec{\alpha}$), homogeneous (in that their constitutive relations should have no explicit position or time dependence), and linear (in that their constitutive relations should depend linearly on the difference $C_{ab} - \delta_{ab}$). By linearity then there exists a stiffness tensor S^{abcd} so that:

$$\delta\sigma^{ab} = S^{abcd}(C_{cd} - \delta_{cd}) = S^{abcd}E_{cd}. \quad (6.4.69)$$

The assumption of rotational symmetry means that S^{abcd} should be unchanged by rotations of the z^a coordinates. Thus, by the result of problem 2.7:

$$S^{abcd} = S^{1122}\delta^{ab}\delta^{cd} + S^{1212}\delta^{ac}\delta^{bd} + S^{1221}\delta^{ad}\delta^{bc}. \quad (6.4.70)$$

Because E_{ab} is a symmetric tensor $S^{1212} = S^{1221}$. Then, S^{abcd} can be written:

$$S^{abcd} = B(n, T)\delta^{ab}\delta^{cd} + G(n, T)\left(\delta^{ac}\delta^{bd} + \delta^{ad}\delta^{bc} - \frac{2}{3}\delta^{ab}\delta^{cd}\right) \quad (6.4.71)$$

for some coefficients B and G . B is called the **bulk modulus** of the solid and G is called the **shear modulus** of the solid. They are allowed to be generic functions of the density of and the temperature. Specific expressions for them have to be found empirically or computed from a specific interparticle potential through a matching calculation. Equivalently, the stress tensor can be written:

$$\delta\hat{\sigma} = B\text{Tr}(\hat{E})\mathbb{1} + 2G\left(\hat{E} - \frac{\text{Tr}(\hat{E})}{3}\mathbb{1}\right). \quad (6.4.72)$$

The stretch tensor is automatically parity even while the heat current vector is parity odd. Thus, there are no parity odd quantities available to make contributions to $\vec{q}$ and so we have for a simple solid:

$$\delta\vec{q} = 0. \quad (6.4.73)$$

There are possible terms which can be added if one allows derivatives of the stretch tensor, however because the stretch tensor already contains first derivatives and $\vec{q}$ is differentiated in the equations of motion, doing so would put third derivative or higher terms into the equations of motion. The equations of motion we typically use contain second derivatives or less, as always motivated by the logic after (3.2.35) that higher derivatives encode very short distance behavior we are generally insensitive to. So, we neglect the possibility of ∇C terms as an approximation.

Therefore, we have:

Theorem 6.5: Simple Solid (Cauchy-Green) Equations of motion

The equations of motion for a simple solid with equilibrium number density $n_0(\vec{\alpha})$ (where $\vec{\alpha}$ is the position of the matter element at equilibrium), streamlines $\vec{z}(t, \vec{\alpha})$, and element temperature $T(t, \vec{\alpha})$ are:

$$n(t, \vec{z}) = \frac{n_0(\vec{\alpha})}{\det\left(\frac{\partial \vec{z}}{\partial \vec{\alpha}}\right)} \quad (6.4.74)$$

$$mn \frac{d^2 z^a}{dt^2} = f^a + \frac{\partial \sigma^{ab}}{\partial z^b} \quad (6.4.75)$$

$$n \frac{d\mathcal{U}}{dt} = \Phi + \sigma^{ab} \frac{\partial \dot{z}_b}{\partial z^a} + \frac{\partial}{\partial z^a} \left(\kappa \frac{\partial T}{\partial z^a} + \iota \frac{\partial n}{\partial z^a} \right) \quad (6.4.76)$$

$$\sigma^{ab} = \frac{1}{2} \left(B \delta^{ab} \delta^{cd} + G \left(\delta^{ac} \delta^{bd} + \delta^{ad} \delta^{bc} - \frac{2}{3} \delta^{ab} \delta^{cd} \right) \right) \left(\delta_{ef} \frac{\partial \alpha^e}{\partial z^c} \frac{\partial \alpha^f}{\partial z^d} - \delta_{cd} \right) \quad (6.4.77)$$

where m is the mass of each molecule, $\mathcal{U}$ is the local thermodynamic internal energy per particle in the instantaneous local rest frame, $\kappa(T)$ is the thermal conductivity of the solid, $\iota(T)$ is the density conductivity of the solid, $B(n, T)$ is the bulk modulus of the solid, $G(n, T)$ is the shear modulus of the solid, $\vec{f}(t, \vec{x})$ is the force density on the solid and $\Phi(t, \vec{x})$ is the heat transfer density to the solid.

Here in discussing solids we have always assumed that our solid has one stable equilibrium which it will return to. This assumption is called elasticity. Many solids in fact have many stable equilibria and if pulled in the right way can permanently deform to a new equilibrium. This is called plasticity. The theoretical analysis of plastic solids is unfortunately even more complicated. We will not discuss it. As well, solids can be anisotropic, in which case the dependence of the stress tensor on the deformation gradient can be more complicated. We will not discuss this either.

6.4.4 Plasma

The final state of matter we will discuss in passing is plasma. A plasma is a state of matter in which a mixture of different species of electrically charged particles interact with each other through electromagnetism. The full theory of such a thing can essentially only be treated by coupling the full Liouville equation for all of the charged particles to Maxwell's equations for the fields. This is too complicated and deep for us to say much about. When considering relativistic effects one then also has to appropriately model the charges as non-point-like. Depending on the specific regime of physical interest significant simplifications can be made. Here we will study three simple cases of plasma though many other cases, of which some are significantly more complicated, exist.

For our first simple model we will consider only a single species of charged particles, each with charge q and mass m , moving slowly enough to ignore all relativistic effects with the only interactions between the particles mediated by electromagnetism. So, because the particles are noninteracting beyond what is necessary to bring them into local thermodynamic equilibrium, we can treat them as an ideal gas. This requires that the charges equilibrate with each other much more quickly than the time scale on which the electric and magnetic fields change appreciably. Because of our assumptions we will take the ideal gas constitutive relations:

$$\vec{q} = 0, \quad \hat{\sigma} = -p \mathbb{I}, \quad n\mathcal{U} = \frac{p}{\gamma - 1} \quad (6.4.78)$$

Consequently we have the ideal gas equations of motion and now we only need to find the appropriate expressions for Φ and $\vec{f}$ due to electromagnetism. We know the exact expression for the underlying force by using the Lorentz force law:

$$\vec{f} = \sum_{k=1}^N \vec{F}_k R_k = \sum_{k=1}^N q (\vec{E}(t, \vec{x}_k) + \dot{\vec{x}}_k \times \vec{B}(t, \vec{x}_k)) R_k \quad (6.4.79)$$

$$= q \left(\sum_{k=1}^N \vec{E}(t, \vec{x}_k) R_k \right) + q \left(\sum_{k=1}^N (\dot{\vec{x}}_k - \vec{v}) \times \vec{B}(t, \vec{x}_k) R_k \right) + q \vec{v} \times \left(\sum_{k=1}^N \vec{B}(t, \vec{x}_k) R_k \right). \quad (6.4.80)$$

It is tempting to make the replacements:

$$\sum_{k=1}^N \vec{E}(t, \vec{x}_k) R_k \stackrel{?}{\approx} n(t, \vec{x}) \vec{E}(t, \vec{x}), \quad \sum_{k=1}^N \vec{B}(t, \vec{x}_k) R_k \stackrel{?}{\approx} n(t, \vec{x}) \vec{B}(t, \vec{x}). \quad (6.4.81)$$

However, this is certainly not a good approximation in general. The exact microscopic $\vec{E}$ and $\vec{B}$ are determined by Maxwell's equations and don't necessarily agree with the results of our thermodynamic averaging in general. When this approximation holds and the middle term in equation (6.4.80) is negligible we have the “ideal” force density:

$$\vec{f}_{\text{ideal}} = qn(\vec{E} + \vec{v} \times \vec{B}). \quad (6.4.82)$$

The difference between the true force density and the ideal force density we will call $\delta \vec{f}$:

$$\delta \vec{f} = \vec{f} - \vec{f}_{\text{ideal}} \implies \vec{f} = qn(\vec{E} + \vec{v} \times \vec{B}) + \delta \vec{f}. \quad (6.4.83)$$

$\delta \vec{f}$ is generally called the “fluctuation” in the force. For simplicity, we will approximate $\delta \vec{f} \approx 0$ and $\Phi \approx 0$ as part of the definition of an ideal charged fluid. The electric charge density for the fluid is automatically qn . Consequently, the associated current density is $qn\vec{v}$. Thus, we have the equations of motion for an ideal charged fluid:

Theorem 6.6: Ideal Charged Fluid Equations of Motion

The equations of motion for an ideal charged fluid number density $n(t, \vec{x})$, velocity field $\vec{v}(t, \vec{x})$, and pressure $p(t, \vec{x})$ are:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.4.84)$$

$$mn \frac{d\vec{v}}{dt} = -\nabla p + qn(\vec{E} + \vec{v} \times \vec{B}) \quad (6.4.85)$$

$$\frac{d}{dt}(pn^{-\gamma}) = 0 \quad (6.4.86)$$

$$\nabla \cdot \vec{E} = \frac{qn}{\epsilon_0}, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (6.4.87)$$

$$\nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{B} = \mu_0 qn\vec{v} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t} \quad (6.4.88)$$

where m is the mass of each particle and q is the electric charge of each particle.

While for an ideal fluid we have approximated $\delta \vec{f}$ and Φ to 0 for many real situations they can be extremely important. These ideal equations of motion are often overly ideal. There is another issue with these equations; we have used the fully relativistic Maxwell's equations with nonrelativistic fluid equations. This fine if it is understood that these equations need corrections of order $\frac{1}{c^2}$ due to neglecting relativistic effects in the matter.

The next plasma approximation we will study is a mixture of two ideal charged fluids. We will assume that one fluid is positively charged (with charge q per particle, mass m_+ per particle, and adiabatic ratio γ_+) which we will call the ions and that the other fluid is negatively charged (with charge $-q$ per particle and mass m_- per particle, and adiabatic ratio γ_-) which we will call the electrons. It is not strictly necessary for the second fluid to be of actual electrons but it is the common enough case that it is reasonable to call it so. Because the two fluids do not directly interact, only indirectly through electromagnetism, there is no reason they ought to be in thermodynamic equilibrium with each other. So, each fluid will have its own independent pressure $p_{\pm}$ for which an equation of motion is needed. Together then for the fluids we have the two fluid equations:

$$\begin{aligned} \frac{\partial n_{\sigma}}{\partial t} + \nabla \cdot (n_{\sigma} \vec{v}_{\sigma}) &= 0, \\ m_{\sigma} n_{\sigma} \left(\frac{\partial \vec{v}_{\sigma}}{\partial t} + (\vec{v}_{\sigma} \cdot \nabla) \vec{v}_{\sigma} \right) &= -\nabla p_{\sigma} + \sigma q n_{\sigma} (\vec{E} + \vec{v}_{\sigma} \times \vec{B}), \\ \left(\frac{\partial}{\partial t} + (\vec{v}_{\sigma} \cdot \nabla) \right) (p_{\sigma} n_{\sigma}^{-\gamma_{\sigma}}) &= 0 \end{aligned} \quad (6.4.89)$$

where $\sigma = \pm 1$ (1 for the ions and -1 for the electrons).

The individual densities and velocities of the fluid species are typically not as directly experimentally accessible as the center of mass behavior of the fluid mixture and the total flow of charge. So, we define the total mass density ρ_m and total charge density ρ_q :

$$\rho_m = m_+ n_+ + m_- n_-, \quad \rho_q = q(n_+ - n_-) \quad (6.4.90)$$

as well as the center of mass velocity $\vec{v}$ and total electric current density $\vec{J}$:

$$\vec{v} = \frac{m_+ n_+ \vec{v}_+ + m_- n_- \vec{v}_-}{m_+ n_+ + m_- n_-}, \quad \vec{J} = q n_+ \vec{v}_+ - q n_- \vec{v}_-. \quad (6.4.91)$$

Then, it is useful to define the total mass per neutral pair M and electron mass fraction $\mathfrak{f}$:

$$M = m_+ + m_-, \quad \mathfrak{f} = \frac{m_-}{m_+ + m_-}. \quad (6.4.92)$$

Typically in applications the ions will be much more massive than the electrons ($m_+ \gg m_-$). Automatically $\mathfrak{f}$ is dimensionless and the approximation $m_+ \gg m_-$ is equivalent to $\mathfrak{f} \ll 1$ (but we will not make that approximation yet). From the continuity equations for the number densities one can find by weighted summing and weighted subtracting the continuity equations for ρ_m and ρ_q :

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{v}) = 0, \quad \frac{\partial \rho_q}{\partial t} + \nabla \cdot \vec{J} = 0 \quad (6.4.93)$$

which are exactly as we would expect.

Using the momentum equations of motion we can similarly compute equations of motion for $\vec{v}$ and $\vec{J}$. In particular, we find by differentiating the definitions of $\vec{v}$ and $\vec{J}$ with respect to time:

$$\begin{aligned} \rho_m \left(\frac{\partial}{\partial t} + (\vec{v} \cdot \nabla) \right) \vec{v} = & -\nabla \cdot \left(\frac{\rho_m M^2 \mathfrak{f} (1 - \mathfrak{f})}{(q \rho_m + M \mathfrak{f} \rho_q)(q \rho_m - (1 - \mathfrak{f}) M \rho_q)} (\vec{J} - \rho_q \vec{v})(\vec{J} - \rho_q \vec{v}) \right) \\ & - \nabla(p_+ + p_-) + \rho_q \vec{E} + \vec{J} \times \vec{B} \end{aligned} \quad (6.4.94)$$

$$\begin{aligned} \frac{\partial \vec{J}}{\partial t} + \nabla \cdot \left(\frac{\vec{J} \vec{J}}{\rho_q} \right) = & \nabla \cdot \left(\frac{q^2 \rho_m^2 (\vec{J} - \rho_q \vec{v})(\vec{J} - \rho_q \vec{v})}{\rho_q (q \rho_m + M \mathfrak{f} \rho_q)(q \rho_m - M(1 - \mathfrak{f}) \rho_q)} \right) + \nabla \cdot \left(\frac{q}{M} \frac{(1 - \mathfrak{f}) p_- - \mathfrak{f} p_+}{\mathfrak{f} (1 - \mathfrak{f})} \right) \\ & + \frac{q^2 \rho_m}{M^2 \mathfrak{f} (1 - \mathfrak{f})} (\vec{E} + \vec{v} \times \vec{B}) - \frac{q(1 - 2\mathfrak{f})}{M \mathfrak{f} (1 - \mathfrak{f})} (\rho_q \vec{E} + \vec{J} \times \vec{B}). \end{aligned} \quad (6.4.95)$$

We will assume that absent any interactions the fluids are completely uniform. Therefore, initially $p_+ n_+^{-\gamma_+}$ is completely uniform and so some constant κ_+ (and similarly so for the electrons). Then, because these quantities are constant along the flows of each fluid and they are initially uniform, they remain so for all time:

$$p_+ = \kappa_+ n_+^{\gamma_+}, \quad p_- = \kappa_- n_-^{\gamma_-}. \quad (6.4.96)$$

Often it is physically interesting to consider a quasineutral plasma, meaning a plasma in which $\rho_q = 0$ (it is called quasineutral because real such plasmas on sufficiently microscopic scales are not neutral, they only become neutral on average at the scale on which fluid mechanics is valid). This is relevant for most everyday matter as most everyday matter is electrically neutral on macroscopic scales. Quasineutrality implies:

$$\rho_q = q(n_+ - n_-) = 0 \implies n_+ = n_- \stackrel{\text{def}}{=} n(t, \vec{x}), \quad \frac{\partial \rho_q}{\partial t} = 0 \implies \nabla \cdot \vec{J} = 0 \quad (6.4.97)$$

$$\implies \rho_m = m_+ n_+ + m_- n_- = M n, \quad \frac{\partial n}{\partial t} + \nabla \cdot (n \vec{v}) = 0 \quad (6.4.98)$$

and from this the evolution of $\vec{v}$ and $\vec{J}$ can be simplified:

$$\begin{aligned} M n \left(\frac{\partial}{\partial t} + (\vec{v} \cdot \nabla) \right) \vec{v} = & \frac{M \mathfrak{f} (1 - \mathfrak{f})}{q^2 n^2} (\nabla n \cdot \vec{J}) \vec{J} - \nabla(p_+ + p_-) + \vec{J} \times \vec{B} \\ \frac{\partial \vec{J}}{\partial t} + (\vec{v} \cdot \nabla) \vec{J} + (\nabla \cdot \vec{v}) \vec{J} + (\vec{J} \cdot \nabla) \vec{v} = & \nabla \cdot \left(\frac{q}{M} \frac{(1 - \mathfrak{f}) p_- - \mathfrak{f} p_+}{\mathfrak{f} (1 - \mathfrak{f})} \right) + \frac{q^2 n}{M \mathfrak{f} (1 - \mathfrak{f})} (\vec{E} + \vec{v} \times \vec{B}) \\ & - \frac{q(1 - 2\mathfrak{f})}{M \mathfrak{f} (1 - \mathfrak{f})} \vec{J} \times \vec{B} - \frac{1 - 2\mathfrak{f}}{q n^2} (\nabla n \cdot \vec{J}) \vec{J}. \end{aligned} \quad (6.4.99)$$

The pressures then also become:

$$p_+ = \kappa_+ n^{\gamma_+}, \quad p_- = \kappa_- n^{\gamma_-}. \quad (6.4.100)$$

It is also common to approximate the matter as uniformly constantly massive. Then, we can take n to simply be a constant number. With that assumption the only dynamical equations remaining become:

$$Mn \left(\frac{\partial}{\partial t} + (\vec{v} \cdot \nabla) \right) \vec{v} = \vec{J} \times \vec{B}$$

$$\frac{\partial \vec{J}}{\partial t} + (\nabla \cdot \vec{v}) \vec{J} + (\vec{J} \cdot \nabla) \vec{v} = \frac{q^2 n}{M\ell(1-\ell)} (\vec{E} + \vec{v} \times \vec{B}) - \frac{q(1-2\ell)}{M\ell(1-\ell)} \vec{J} \times \vec{B}. \quad (6.4.101)$$

The center of mass velocity still has a completely safe equation of motion in the $\ell \rightarrow 0$ limit, but notice that the equation of motion for $\vec{J}$ contains a factor of $\frac{1}{\ell}$. We have said that most often ℓ is assumed to be small but due to the $\frac{1}{\ell}$ it seems dangerous to take a $\ell \approx 0$. The appearance of $\frac{1}{\ell}$ in the equation means that for small ℓ , $\frac{\partial \vec{J}}{\partial t}$ will generally be very large. In order for $\vec{J}$ to be large but $\vec{J}$ to not become large, $\vec{J}$ must oscillate very rapidly. We can in fact identify a characteristic frequency of this oscillation. Define the plasma frequency ω_p :

$$\omega_p \stackrel{\text{def}}{=} \sqrt{\frac{q^2 n}{m - \epsilon_0}} \implies \frac{1}{\ell} = \frac{\omega_p^2 M \epsilon_0}{q^2 n}. \quad (6.4.102)$$

We can isolate the $\frac{1}{\ell}$ behavior in the evolution of $\vec{J}$ by taking all other appearances of $\ell \rightarrow 0$ and leaving factors of the plasma frequency explicit. This self-consistently results in equations of motion which predict oscillations of the current density with a characteristic scale set by the plasma frequency. Together then we arrive at the quasineutral, uniformly dense, large mass ratio, ideal two fluid plasma equations:

$$\boxed{\begin{aligned} Mn \left(\frac{\partial}{\partial t} + (\vec{v} \cdot \nabla) \right) \vec{v} &= \vec{J} \times \vec{B} \\ \frac{\partial \vec{J}}{\partial t} + (\nabla \cdot \vec{v}) \vec{J} + (\vec{J} \cdot \nabla) \vec{v} &= \epsilon_0 \omega_p^2 \left(\vec{E} + \left(\vec{v} - \frac{\vec{J}}{qn} \right) \times \vec{B} \right). \end{aligned}} \quad (6.4.103)$$

The final simple plasma approximation we will study is called magnetohydrodynamics or MHD. For magnetohydrodynamics we assume that there is an electrically neutral but electrically conducting fluid (with conductivity σ) consisting of particles which have some internal electromagnetic structure so they carry a current density $\vec{J}$ while carrying a vanishing charge density. (For example, our fluid could consist of neutral atoms, themselves consisting of positive and negative charges. The fluid is overall charge neutral above the atomic scale but can still have noticeable electric current because the atoms are not point particles. Some of the charge may flow around with the overall charge density still being essentially 0.) With these approximations we still take the ideal gas constitutive relations for $\mathcal{U}, \hat{\sigma}, \vec{q}$ and similarly take the ideal expression for the force density:

$$\vec{f}_{\text{ideal}} = \rho_q \vec{E} + \vec{J} \times \vec{B} = \vec{J} \times \vec{B} \quad (6.4.104)$$

where the last equation follows because we assume we have a neutral fluid. The transport equations then become:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}) = 0 \quad (6.4.105)$$

$$mn \frac{d\vec{v}}{dt} = -\nabla p + \vec{J} \times \vec{B} \quad (6.4.106)$$

$$\frac{d}{dt} (pn^{-\gamma}) = 0. \quad (6.4.107)$$

Here we will properly make the nonrelativistic approximation so that we consider the $c \rightarrow \infty$ limit of Maxwell's equations (which simply reduces the Maxwell-Ampere law back to Ampere's law):

$$\nabla \cdot \vec{E} = 0, \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{B} = \mu_0 \vec{J} \quad (6.4.108)$$

and finally we have Ohm's law as derived in problem 3.62 to relate the current density to the fields. We found in problem 3.62 that in a body's instantaneous rest frame the current density is related to the electric field by:

$$\vec{J}_{\text{rest}} = \sigma \vec{E}_{\text{rest}} \quad (6.4.109)$$

for a material conductivity σ . Using the Galilean boost properties of the current density and the electromagnetic

fields derived in chapter 3 we have:

$$\vec{J} = \vec{J}_{\text{rest}} + \rho_{\text{rest}} \vec{v} = \vec{J}_{\text{rest}} \quad (6.4.110)$$

$$\vec{B} = \vec{B}_{\text{rest}} \quad (6.4.111)$$

$$\vec{E} = \vec{E}_{\text{rest}} - \vec{v} \times \vec{B}_{\text{rest}} \implies \vec{E}_{\text{rest}} = \vec{E} + \vec{v} \times \vec{B}. \quad (6.4.112)$$

In the frame in which the fluid is moving then we have:

$$\vec{J} = \sigma(\vec{E} + \vec{v} \times \vec{B}). \quad (6.4.113)$$

Using Ampere's law we can eliminate $\vec{J}$ from the equations of motion in favor of $\vec{B}$. Using Ohm's law we can eliminate $\vec{E}$ from the equations of motion in favor of $\vec{B}$ (and $\vec{J}$) as well. So, in the end we are left with only equations of motion for n , $\vec{v}$, p , and $\vec{B}$. The force density can be rewritten as:

$$\vec{J} \times \vec{B} = \nabla \cdot \left(\frac{\vec{B}\vec{B}}{\mu_0} - \frac{|\vec{B}|^2}{2\mu_0} \mathbb{1} \right) \quad (6.4.114)$$

by using the Solenoid law and Ampere's law. Faraday's law then gives an equation of motion for $\vec{B}$:

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} = -\nabla \times \left(\frac{\vec{J}}{\sigma} - \vec{v} \times \vec{B} \right) = \frac{1}{\mu_0 \sigma} \nabla^2 \vec{B} + \nabla \times (\vec{v} \times \vec{B}). \quad (6.4.115)$$

Together then we have the equations of motion for MHD:

Theorem 6.7: Magnetohydrodynamic Equations of Motion

The equations of motion for a nonrelativistic neutral conducting ideal fluid of conductivity σ are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (6.4.116)$$

$$\rho \frac{d\vec{v}}{dt} = \nabla \cdot \left(-p \mathbb{1} + \frac{\vec{B}\vec{B}}{\mu_0} - \frac{|\vec{B}|^2}{2\mu_0} \mathbb{1} \right) \quad (6.4.117)$$

$$\frac{d}{dt}(p\rho^{-\gamma}) = 0 \quad (6.4.118)$$

$$\frac{\partial \vec{B}}{\partial t} = \frac{\nabla^2 \vec{B}}{\mu_0 \sigma} + \nabla \times (\vec{v} \times \vec{B}). \quad (6.4.119)$$

Exercises

Problem 6.3: Sound waves in Air. Consider the air as (approximately) an ideal gas with some adiabatic ratio γ . Suppose that the air is nearly uniformly constantly dense and pressured and only barely moving so that the number density, pressure, and velocity field can be written as:

$$n(t, \vec{x}) = n_0 + \delta n(t, \vec{x}), \quad p(t, \vec{x}) = p_0 + \delta p(t, \vec{x}), \quad \vec{v}(t, \vec{x}) = \delta \vec{v}(t, \vec{x})$$

where n_0 and p_0 are constants and $\delta n, \delta p, \delta \vec{v}$ are small. Assume the air is initially in equilibrium (so that all of the δ quantities are 0) and that then an external force acts briefly on the air without transferring any heat to the air. After that force is applied, we can set $\vec{f} = 0$ and $\Phi = 0$. Show then that after the force is applied to lowest order in the δ quantities, the equations of motion for the air become:

$$\frac{\partial \delta n}{\partial t} + n_0 \nabla \cdot \delta \vec{v} = 0, \quad mn_0 \frac{\partial \delta \vec{v}}{\partial t} = -\nabla \delta p, \quad \delta p = \gamma T_0 \delta n$$

where T_0 is the temperature of the unperturbed gas. Use these to show that the pressure fluctuation δp satisfies the wave equation with wave speed c_s given by:

$$\frac{\partial^2 \delta p}{\partial t^2} - c_s^2 \nabla^2 \delta p = 0, \quad c_s^2 = \frac{\gamma T_0}{m}.$$

Because c_s is the speed at which pressure fluctuations propagate in the air, it is the speed of sound. Thus, because the chemical composition of air is known (and thus the average mass of air molecules m and adiabatic ratio γ can be determined) and we have established how to measure temperature, this makes a prediction for the speed of sound in air that can be tested experimentally (and it works!).

Problem 6.4: Atmospheric Power Laws. In this question we will make the absolute simplest model of the atmosphere, neglecting many interesting and significant effects. The result will be pretty accurate for pressure and density at higher altitudes than you would naively expect but not very accurate for temperature at altitudes over 15 km.

- (a) Consider the air as a fluid which satisfies the special Navier-Stokes equations everywhere in space outside of the Earth and which is essentially at rest without any heat source (obviously neglecting the sun here is not a very good approximation). Show that temperature $T(t, \vec{x})$ satisfies the diffusion equation:

$$\frac{c_1}{\kappa} \frac{\partial T}{\partial t} = \nabla^2 T.$$

Now consider the equilibrium temperature solution so that $\frac{\partial T}{\partial t} = 0$. Assume that the atmosphere is spherically symmetric with the center of the Earth as the origin of the coordinate system. Show that $T = T(r)$ and that for some constants A, B :

$$\nabla^2 T = 0 \implies T(r) = A + \frac{B}{r}.$$

Let R be the radius of the Earth treated as a sphere and T_0 be the surface temperature of the Earth. Approximate that far away space is at 0 temperature. Show that:

$$T(r) = \frac{T_0 R}{r}.$$

This is by far the poorest approximation we will find in this model compared to the actual atmospheric temperature of the Earth (which fluctuates up and down with altitude due to many more complex effects).

- (b) Show that the conditions that the average air velocity be 0 and air density be constant require that the air pressure satisfies:

$$\nabla p = \vec{f} = -\frac{GM\rho(r)}{r^2} \vec{e}_r$$

where G is the gravitational constant, M is the mass of the Earth, and $\rho(r)$ is the mass density of the air. Use the ideal gas law and our solution for the temperature to show that the air pressure satisfies:

$$\frac{\partial p}{\partial r} + \frac{GMm}{RT_0} \frac{p}{r} = 0$$

where m is the mass of a molecule of air. Thus, show that:

$$p(r) = Cr^{-\frac{GMm}{RT_0}}$$

for some constant r .

- (c) Let $h = r - R$ be the altitude above the surface of the Earth, g be the surface gravitational acceleration on Earth, c_s be the speed of sound in air on the surface, γ the adiabatic ratio of air, and ρ_0 the average density of air at the surface of the Earth. Show that our solutions imply that the atmospheric temperature, pressure, and air density can be written as:

$$T(h) = \frac{T_0}{1 + \frac{h}{R}}, \quad p(h) = \frac{c_s^2 \rho_0}{\gamma} \left(1 + \frac{h}{R}\right)^{-\frac{gR\gamma}{c_s^2}}, \quad \rho(h) = \rho_0 \left(1 + \frac{h}{R}\right)^{1 - \frac{gR\gamma}{c_s^2}}.$$

Thus, these provide definite predictions for the atmospheric behavior of these quantities in terms of parameters that are measurable at the surface. For pressure and density these are reasonably accurate formulas, but not for temperature.

Problem 6.5: Bernoulli's Principle. Consider a nondissipative fluid ($\hat{\sigma} = -p\mathbf{1}$ and $\vec{q} = 0$) which is unheated ($\Phi = 0$).

- (a) Assume that initially the fluid is in equilibrium before being disturbed and assume that disturbance is adiabatic. Show that the entropy field of the fluid is a uniform constant. Thus, for the rest of this problem we will suppress the entropy dependence of any quantities. Justify from thermodynamics that consequently the pressure p is a function only of the density of the fluid $p(\rho)$ and that that function is given by:

$$p(\rho) = \rho^2 \frac{\partial u}{\partial \rho}$$

where u is the thermodynamic internal energy of the fluid per unit mass. Such a fluid is called barotropic.

- (b) Suppose the fluid is irrotational (meaning $\nabla \times \vec{v} = 0$). Explain that there exists a velocity potential $\varphi(t, \vec{x})$ so that $\vec{v} = \nabla\varphi$ which is only defined up to the addition of a function of t only. Assume further that the external forces on the fluid $\vec{f}$ are due to a scalar potential $\phi(t, \vec{x})$ so that $\vec{f} = -\rho\nabla\phi$ (as would be the case for gravity or electrostatics). Show that the velocity potential $\varphi(t, \vec{x})$ can be chosen to satisfy the Bernoulli equation:

$$\frac{\partial\varphi}{\partial t} + \frac{1}{2}|\nabla\varphi|^2 + \phi(t, \vec{x}) + u(\rho) + \rho\frac{\partial u}{\partial\rho} = 0.$$

- (c) Justify that the Bernoulli equation is simply the Hamilton-Jacobi equation with $S(t, \vec{x}) = m\varphi$ and Hamiltonian $\mathcal{H} = \frac{|\vec{p}|^2}{2m} + m\phi + mu + m\rho\frac{\partial u}{\partial\rho}$.
- (d) Show that the Lagrangian:

$$\mathcal{L} = \int_{\mathbb{S}} \left(-\rho\frac{\partial\varphi}{\partial t} - \frac{1}{2}\rho|\nabla\varphi|^2 - \rho u - \rho\phi \right) d^3\vec{x}$$

produces the Bernoulli equation and the continuity equation as its equations of motion. Finally, show that the Hamiltonian derived from this Lagrangian through the Legendre transformation is equal to the combined energy of the fluid and the external potential ϕ .

Problem 6.6: Kelvin's Circulation Theorem. Consider a nondissipative fluid which is unheated and barotropic.

- (a) Let $\vec{\omega}(t, \vec{x}) = \nabla \times \vec{v}$ (known as the vorticity of the fluid). Show by directly taking the curl of the velocity equation of motion for the fluid that the vorticity satisfies:

$$\frac{\partial\vec{\omega}}{\partial t} + \nabla \cdot (\vec{v}\vec{\omega} - \vec{\omega}\vec{v}) = \nabla \times \left(\frac{\vec{f}}{\rho} \right).$$

- (b) Consider a closed loop $\gamma(t)$ which evolves in time by following the velocity field of the fluid. Define the circulation $C[\gamma]$ of that curve by:

$$C[\gamma] = \int_{\gamma(t)} \vec{v}(t, \vec{x}) \cdot d\vec{x}.$$

Show that the time derivative of the circulation is given by:

$$\frac{dC}{dt} = \int_{\gamma} \frac{\vec{f}}{\rho} \cdot d\vec{x}.$$

This is known as Kelvin's Circulation Theorem.

- (c) Suppose that the external forces on the fluid elements are due to a scalar potential field so that $\vec{f} = -\rho\nabla\phi$ for some ϕ . Show that under such forces the circulation of any regular loop $\gamma(t)$ is conserved.

Problem 6.7: Basics of Vortices. Consider a nondissipative fluid ($\hat{\sigma} = -p\mathbb{1}$ and $\vec{q} = 0$) which is unheated ($\Phi = 0$), under no external forces ($\vec{f} = 0$), and incompressible ($\rho(t, \vec{x}) = \rho_0$) in two spatial dimensions (take the z component of all velocities to be 0).

- (a) Consider a velocity field for this fluid which has a Dirac delta curl with the center of that Dirac delta having coordinates $(a(t), b(t))$. That is:

$$\nabla \times \vec{v}(t, \vec{x}) = \kappa(t)\vec{e}_z\delta(x - a(t))\delta(y - b(t))$$

for some function $\kappa(t)$. Show that incompressibility combined with this curl condition and the requirement that the velocity field should go to 0 when far away from (a, b) gives the solution:

$$\vec{v}(t, \vec{x}) = \frac{\kappa(t)}{2\pi} \frac{(-y + b(t), x - a(t))}{(x - a)^2 + (y - b)^2}.$$

- (b) Use Kelvin's circulation theorem to justify that $\kappa(t)$ is constant. Assuming that there is no other source of motion in the fluid and that the appropriate value to take for the velocity at the point (a, b) is the average value of $\vec{v}$ over a small circle containing (a, b) , show that $a(t)$ and $b(t)$ are constant. The result is known as a stationary vortex solution.
- (c) Consider two vortices with centers $(a_1(t), b_1(t))$ and $(a_2(t), b_2(t))$ and strengths κ_1 and κ_2 (still conserved

due to the circulation theorem) so that the total velocity field is:

$$\vec{v}(t, \vec{x}) = \frac{\kappa_1}{2\pi} \frac{(-y + b_1(t), x - a_1(t))}{(x - a_1)^2 + (y - b_1)^2} + \frac{\kappa_2}{2\pi} \frac{(-y + b_2(t), x - a_2(t))}{(x - a_2)^2 + (y - b_2)^2}.$$

Show that the vortex centers move according to the equations of motion:

$$\begin{pmatrix} \kappa_1 \dot{a}_1 \\ \kappa_1 \dot{b}_1 \end{pmatrix} = - \begin{pmatrix} \kappa_2 \dot{a}_2 \\ \kappa_2 \dot{b}_2 \end{pmatrix} = \frac{\kappa_1 \kappa_2}{2\pi} \frac{1}{(a_1 - a_2)^2 + (b_1 - b_2)^2} \begin{pmatrix} b_2 - b_1 \\ a_1 - a_2 \end{pmatrix}.$$

(d) Assume $\kappa_1 \neq -\kappa_2$. Let $\vec{X}$ be the “center of circulation” of the system:

$$\vec{X}(t) = \frac{1}{\kappa_1 + \kappa_2} \begin{pmatrix} \kappa_1 a_1 + \kappa_2 a_2 \\ \kappa_1 b_1 + \kappa_2 b_2 \end{pmatrix}.$$

Show that $\dot{\vec{X}} = 0$. Let $\kappa = \kappa_1 + \kappa_2$, $a = a_2 - a_1$, and $b = b_2 - b_1$. Show that:

$$\dot{a} = -\frac{\kappa}{2\pi} \frac{b}{a^2 + b^2}, \quad \dot{b} = \frac{\kappa}{2\pi} \frac{a}{a^2 + b^2}.$$

Show that $\ell = \sqrt{a^2 + b^2}$ is constant and that $a(t)$ and $b(t)$ are given by:

$$a(t) = \ell \cos \left(\frac{\kappa t}{2\pi \ell^2} + \varphi \right), \quad b(t) = \ell \sin \left(\frac{\kappa t}{2\pi \ell^2} + \varphi \right)$$

for a constant φ . Geometrically interpret these solutions in terms of the motion of the vortices.

(e) Assume $\kappa_1 = -\kappa_2$. Show that $c = a_2(t) - a_1(t)$ and $d = b_2(t) - b_1(t)$ are constant. Show that $a_1(t)$ and $b_1(t)$ are given by:

$$a_1(t) = -\frac{\kappa_1}{2\pi} \frac{d}{c^2 + d^2} t + a_1(0), \quad b_1(t) = \frac{\kappa_1}{2\pi} \frac{c}{c^2 + d^2} t + b_1(0).$$

Geometrically interpret these solutions in terms of the motion of the vortices.

Problem 6.8: Bubble Collapse. In this question we will make the simplest model of a spherically symmetric bubble. Consider a spherically symmetric solution of the Navier-Stokes equations for an incompressible fluid of density ρ_0 and temperature independent dynamic and bulk viscosities. The fluid is assumed to fill all of space outside of a ball (the bubble) of radius $R(t)$ at the origin. Due to spherical symmetry, $\vec{v}(t, \vec{x}) = v(t, r)\vec{r}_r$ and $p(t, \vec{x}) = p(t, r)$.

(a) Show that the continuity equation and boundary condition at the edge of the bubble imply:

$$v(t, r) = \frac{R^2(t)}{r^2} \dot{R}(t).$$

(This assumes the interior of the bubble is empty.)

(b) Assume that there are no external forces on the fluid. Show that the momentum equation of motion for the fluid becomes:

$$\frac{R^2 \ddot{R} + 2R\dot{R}^2}{r^2} - \frac{2R^4 \dot{R}^2}{r^5} + \frac{\partial p}{\partial r} = 0.$$

Let p_0 be the pressure of the fluid very far away from the bubble. Show that:

$$p(t, R(t)) = p_0 + \rho_0 \left(R\ddot{R} + \frac{3}{2}\dot{R}^2 \right).$$

(c) Surface tension is an effect at the surfaces of materials that causes them to resist increases in their area. Let γ be the surface tension of the fluid (γ is the force conjugate to the surface area variable) and assume it is constant. Because γ is conjugate to the surface area, a work $\gamma d\mathbb{A}$ is necessary to increase the surface area of the bubble by $d\mathbb{A}$. Show that the force per unit surface area due to surface tension at the surface of the bubble is $-\frac{2\gamma}{R}\vec{r}_r$. Then, use that the interior of the bubble is empty to show that the pressure at the surface is given by:

$$p(t, R(t)) = -\frac{4\mu}{R} \dot{R} - \frac{2\gamma}{R}.$$

Return this to our previous result to show that the radius of the bubble satisfies the Rayleigh-Plesset equation:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 + \frac{4\mu}{\rho_0} \frac{\dot{R}}{R} + \frac{2\gamma}{\rho_0} \frac{1}{R} + \frac{p_0}{\rho_0} = 0.$$

- (d) For simplicity, let us study the case that we neglect surface tension and viscosity. Show that the Rayleigh-Plesset equation simplifies to:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 + \frac{p_0}{\rho_0} = 0.$$

Simplify this equation using the change of variables:

$$a(t) = R^{\frac{5}{2}}(t)$$

and show that $a(t)$ satisfies:

$$\ddot{a} = -\frac{5p_0}{2\rho_0}a^{\frac{1}{5}}.$$

- (e) Assume that the bubble begins with an initial radius of ℓ and $\dot{R} = 0$. Show by solving the equation of motion of the previous part that the bubble collapses in a critical time:

$$\tau = \frac{\Gamma\left(\frac{5}{6}\right)}{\Gamma\left(\frac{4}{3}\right)} \sqrt{\frac{\pi\rho_0}{6p_0}} \ell.$$

To do so it will be useful to remember the definition of the beta function.

Problem 6.9: Newton's Law of Cooling.

- (a) Consider a fluid which is uniformly dense and at rest but with a non-uniform temperature and with no heat transfer density to the fluid on the interior of the fluid. Show that the temperature equation of motion becomes:

$$n \frac{\partial \mathcal{U}}{\partial t} = \nabla \cdot (\kappa \nabla T).$$

Suppose the fluid is in a region $\mathbb{V}$. Show that the total rate of heat transfer to the fluid is:

$$\frac{dQ}{dt} = \int_{\partial\mathbb{V}} \kappa \nabla T \cdot d\vec{\mathbb{A}}.$$

- (b) Consider two fluids which are both uniformly dense and at rest in two non-overlapping regions $\mathbb{V}_1$ and $\mathbb{V}_2$ with a wall between them of “small” thickness ℓ and contact area $\mathbb{A}$. Assume that the temperature of each fluid is essentially uniform over the surface of the contact wall. Show that the net heat transfer rate from fluid 1 to fluid 2 is:

$$\frac{dQ_{1 \rightarrow 2}}{dt} = \frac{(\kappa_1 + \kappa_2)\mathbb{A}}{\ell} (T_2 - T_1).$$

Thus, the rate of heat transfer between the bodies is (under these approximations) proportional to their temperature difference. This is known as Newton's Law of Cooling.

Problem 6.10: Surface Water Waves. Here we will make the simplest model for waves at the surface of water. Consider a nondissipative fluid which is unheated, barotropic, with irrotational flow, subject only to a constant uniform gravitational force in the z direction so that the velocity field is given as the gradient of a velocity potential $\vec{v}(t, \vec{x}) = \nabla\varphi_1(t, \vec{x})$ and so that that potential satisfies the Bernoulli equation:

$$\frac{\partial\varphi_1}{\partial t} + \frac{1}{2}|\nabla\varphi_1|^2 + gz + u(\rho) + \rho \frac{\partial u}{\partial \rho} = 0.$$

Assume further that the fluid is incompressible with density ρ_0 and pressure p_0 and that the fluid is infinite in extent in the x and y directions but only exists between $z = -h$ up to a surface $z = \zeta(t, x, y)$. That surface represents the actual water wave and the purpose of this question is to seek an equation of motion for ζ .

- (a) Show that incompressibility guarantees we can define a velocity potential $\varphi(t, x, y, z)$ so that $\vec{v} = \nabla\varphi$ but which satisfies:

$$\nabla^2\varphi = 0, \quad \frac{\partial\varphi}{\partial t} + \frac{1}{2}|\nabla\varphi|^2 + gz = 0.$$

As well, show that the surface function ζ must satisfy:

$$\frac{\partial\zeta}{\partial t} + \frac{\partial\zeta}{\partial x} \frac{\partial\varphi(t, x, y, \zeta)}{\partial x} + \frac{\partial\zeta}{\partial y} \frac{\partial\varphi(t, x, y, \zeta)}{\partial y} = \frac{\partial\varphi}{\partial z}(t, x, y, \zeta)$$

and that the requirement that no water flows through the bottom of the container implies:

$$\frac{\partial \varphi}{\partial z}(t, x, y, -h) = 0.$$

Explain how this set of conditions in principle determines the equation of motion for ζ (though it is badly nonlinear).

- (b) Show that because φ satisfies the Laplace equation with the given boundary conditions, there exists a function $\eta(t, k_x, k_y)$ so that:

$$\varphi(t, x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \eta(t, k_x, k_y) e^{ik_x x + ik_y y} \cosh\left(\sqrt{k_x^2 + k_y^2}(z + h)\right) dk_x dk_y.$$

- (c) Linearize the equations of motion for ζ for small waves (meaning ζ is only barely different from 0) and low speeds to show that at linear order it satisfies:

$$\zeta(t, x, y) = -\frac{1}{g} \frac{\partial \varphi}{\partial t}(t, x, y, 0), \quad \frac{\partial \zeta}{\partial t} = \frac{\partial \varphi}{\partial z}(t, x, y, 0).$$

- (d) Let $\tilde{\zeta}(t, k_x, k_y)$ be the spatial Fourier transform of $\zeta(t, x, y)$. Show that (at linearized order) it satisfies the equations of motion:

$$\frac{\partial^2 \tilde{\zeta}(t, k_x, k_y)}{\partial t^2} + g \sqrt{k_x^2 + k_y^2} \tanh\left(h \sqrt{k_x^2 + k_y^2}\right) \tilde{\zeta}(t, k_x, k_y) = 0.$$

Thus, show that small water waves propagate with the dispersion relation:

$$\Omega(k_x, k_y) = \sqrt{g \sqrt{k_x^2 + k_y^2} \tanh\left(h \sqrt{k_x^2 + k_y^2}\right)}.$$

Finally, show that in the limit of very deep water ($h \rightarrow \infty$) the dispersion relation becomes:

$$\Omega(k_x, k_y) = \sqrt{g} (k_x^2 + k_y^2)^{\frac{1}{4}}.$$

Explain qualitatively the differences in propagation of long versus short wavelength waves according to this dispersion relation.

Problem 6.11: Waves on a guitar string.

- (a) Consider a system of N identical masses m with positions $\vec{x}_1(t), \dots, \vec{x}_N(t)$ which are arranged so that for each n , mass n is attached to mass $n+1$ by a spring of spring constant k and unstretched length L . Additionally, mass 1 is attached by another identical such spring to a fixed post at the origin $\vec{x}_0 = (0, 0, 0)$ and mass N is attached again by such a spring to a fixed post at the position $\vec{x}_{N+1} = (\ell, 0, 0)$. Show that the Lagrangian for such a system is:

$$\mathcal{L} = \sum_{n=1}^N \frac{1}{2} m |\dot{\vec{x}}_n|^2 - \sum_{n=0}^N \frac{1}{2} k (|\vec{x}_{n+1} - \vec{x}_n| - L)^2.$$

- (b) We will now want to take the number of masses $N \rightarrow \infty$ so that the system becomes a continuous guitar string. For each mass at finite n , let $\alpha = \frac{n}{N}$ label points on the string and define $\vec{x}(t, \alpha) = \vec{x}_n(t)$. Let M be the total mass of the string, K be the total end-to-end spring constant of the string when unstretched, and ℓ_0 be the total length of the string when unstretched. Show that if M , K , and ℓ_0 are held fixed in the $N \rightarrow \infty$ limit, the Lagrangian becomes:

$$\mathcal{L} = \int_0^1 \left(\frac{1}{2} M |\dot{\vec{x}}(t, \alpha)|^2 - \frac{1}{2} K \left(\left| \frac{\partial \vec{x}}{\partial \alpha} \right| - \ell_0 \right)^2 \right) d\alpha.$$

Show that this Lagrangian produces the equations of motion:

$$\frac{\partial^2 \vec{x}}{\partial t^2} = \frac{K}{M} \frac{\partial}{\partial \alpha} \left(\left(1 - \frac{\ell_0}{\left| \frac{\partial \vec{x}}{\partial \alpha} \right|} \right) \frac{\partial \vec{x}}{\partial \alpha} \right).$$

- (c) Show that the equilibrium solution to the equation of motion gives:

$$\vec{x}_{\text{eq}}(\alpha) = (\ell \alpha, 0, 0).$$

Then, consider perturbations $\delta \vec{x}(t, \alpha)$ of this solution. Show that to linear order they satisfy:

$$\frac{\partial^2 \delta x}{\partial t^2} = \frac{K}{M} \frac{\partial^2 \delta x}{\partial \alpha^2}, \quad \frac{\partial^2 \delta y}{\partial t^2} = \frac{K(\ell - \ell_0)}{M\ell} \frac{\partial^2 \delta y}{\partial \alpha^2}, \quad \frac{\partial^2 \delta z}{\partial t^2} = \frac{K(\ell - \ell_0)}{M\ell} \frac{\partial^2 \delta z}{\partial \alpha^2}.$$

- (d) Show that to linear order in the perturbation we can define $y(t, x)$ (or equivalently $z(t, x)$) as the displacement in the y direction at the horizontal position x and that it satisfies the wave equation:

$$\frac{\partial^2 y}{\partial t^2} = \frac{K(\ell - \ell_0)\ell}{M} \frac{\partial^2 y}{\partial x^2}.$$

Show that when the string is in equilibrium the tension T in the string and mass density μ of the string are:

$$T = K(\ell - \ell_0), \quad \mu = \frac{M}{\ell}.$$

Show that the wavespeed c on the string is:

$$c = \sqrt{\frac{T}{\mu}}.$$

Show that the lowest frequency f_0 (not angular frequency) of waves on the guitar string is:

$$f_0 = \frac{c}{2\ell}.$$

This lowest frequency determines the perceived pitch of the string to the human ear when the guitar is played. The higher harmonic content makes a guitar sound different from a piano.

6.5 Nonrelativistic Continuum Mechanical Actions

Like everything else in physics, continuum mechanics can be understood very nicely through an action. We will see that if there is no heat transfer from outside the matter or between different matter elements, then the entropy of each matter element is conserved and a traditional action for $\vec{z}(t, \vec{x}_0)$ without anything special can be formulated. If there is heat transfer between the different matter elements or from the outside, then the entropy of each matter element is not conserved and instead the entropy evolution is supplemented to the traditional action for $\vec{z}$ through a nonholonomic constraint. This is a local generalization of (5.8.66) where we found before that it is possible to write an effective action for thermodynamically averaged quantities and include entropy evolution through a simple variation condition on the entropy.

We will label each matter element by a label $\vec{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$ in the same way we did for solids. There still must be 3 labels because these labels are equivalent to supplying the initial conditions. The associated space of all matter labels we will call A . Then, we are looking to describe the evolution of $\vec{z}(t, \vec{\alpha})$ which is a function of time and a point within A to physical space $\mathbb{S}$. We will define the function $n_0(\vec{\alpha})$ so that by definition the number of particles in a subset M of A is given by the integral of that function over that set within A :

$$N[M] = \int_M n_0(\vec{\alpha}) d^3 \vec{\alpha}. \quad (6.5.1)$$

The function $\vec{z}(t, \vec{\alpha})$ tells the location of particle $\vec{\alpha}$ in space at time t . We can also define the inverse $\vec{\alpha}(t, \vec{x})$ which returns which particle is at location $\vec{x}$ at time t . Consequently:

$$\vec{z}(t, \alpha(t, \vec{x})) = \vec{x}, \quad \vec{\alpha}(t, \vec{z}(t, \vec{\alpha})) = \vec{\alpha}. \quad (6.5.2)$$

Then, we can define the region $\vec{z}(t, M)$, which is notational abuse that means the set of all positions in space corresponding to the particles with labels in $\vec{\alpha}$. Using this region we have that the number of particles in M can be equivalently written:

$$N[M] = \int_{\vec{z}(t, M)} n_0(\vec{\alpha}) \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right) d^3 \vec{x} \quad (6.5.3)$$

and so we can see that the number density $n(t, \vec{x})$ is given in terms of the label functions as:

$$n(t, \vec{x}) = n_0(\vec{\alpha}) \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right). \quad (6.5.4)$$

Alternatively, we can write:

$$n(t, \vec{z}(t, \vec{\alpha})) = \frac{n_0(\vec{\alpha})}{\det \left(\frac{\partial \vec{z}}{\partial \vec{\alpha}} \right)}. \quad (6.5.5)$$

The only other condition we will put on the labeling scheme $\vec{\alpha}$ is that when the matter is in the “default” configuration, meaning $\vec{z}(t, \vec{\alpha}) = \vec{\alpha}$, the line element is simply given by:

$$ds_0^2 = \delta_{ab} d\alpha^a d\alpha^b \quad (6.5.6)$$

just as with the definition of the $\vec{\alpha}$ labels when we did solids.

6.5.1 Active Formulation

In the active formulation we seek an action for $\vec{z}(t, \vec{\alpha})$. By the logic of equation (5.8.41), we will need a separate equation of motion for the entropy $S(t, \vec{\alpha})$ as well and it will be specified by knowledge of how heat is transferred in the system. Let $\mathcal{U}$ retain its previous meaning as the thermodynamic internal energy in the local instantaneous rest frame of the matter. Because $\vec{z}$ transforms exactly like the position of an ordinary particle under Galilean transformations, we can follow directly from theorem 2.1 that for some functions $\vec{K}$ and U , the Lagrangian per matter element is:

$$\mathcal{L}_1 = \frac{1}{2} m |\dot{\vec{z}}|^2 + \vec{K}(t, \vec{z}) \cdot \dot{\vec{z}} - U(t, \vec{z}). \quad (6.5.7)$$

The energy per matter element is then:

$$E = \frac{\partial \mathcal{L}_1}{\partial \dot{\vec{z}}} \cdot \dot{\vec{z}} - \mathcal{L} = \frac{1}{2} m |\dot{\vec{z}}|^2 + U \quad (6.5.8)$$

and the linear momentum is:

$$\vec{p} = \frac{\partial \mathcal{L}_1}{\partial \vec{z}} = m\dot{\vec{z}} + \vec{K}. \quad (6.5.9)$$

If we consider no external forces on the matter element then our matter element is a local average over free particles. Then, the total linear momentum of the free particles points along the direction of their center of mass velocity and so in the instantaneous local rest frame $\vec{p}$ should be 0. Consequently:

$$\vec{K} = 0. \quad (6.5.10)$$

Similarly, in the instantaneous local rest frame the energy should simply be the per particle thermodynamic internal energy $\mathcal{U}$:

$$U = \mathcal{U}. \quad (6.5.11)$$

So, the nonrelativistic Lagrangian per matter element for free matter is:

$$\mathcal{L}_1 = \frac{1}{2}m|\dot{\vec{z}}|^2 - \mathcal{U}. \quad (6.5.12)$$

Consequently the total Lagrangian, integrating over all labels weighted by the number of particles per label volume, is:

$$\mathcal{L} = \int_A \left(\frac{1}{2}m|\dot{\vec{z}}|^2 - \mathcal{U} \right) n_0 d^3\vec{\alpha}. \quad (6.5.13)$$

In general $\mathcal{U}$ may be a function of any of the local quantities that can be made out of $\vec{z}$ and which are invariant under Galilean boost. As well, it will depend on the entropy per matter element $S(t, \vec{\alpha})$, as expected from statistical mechanics. Due to translational symmetry of a free particle system, we have that $\mathcal{U}$ just considering possibilities up to first derivatives is some function:

$$\mathcal{U} = \mathcal{U} \left(\dot{\vec{z}}, \frac{\partial \vec{z}}{\partial \vec{\alpha}}, S \right). \quad (6.5.14)$$

In the local instantaneous rest frame, $\dot{\vec{z}} = 0$ and so the Galilean invariance of $\mathcal{U}$ implies it is not a function directly of $\dot{\vec{z}}$:

$$\mathcal{U} = \mathcal{U} \left(0, \frac{\partial \vec{z}}{\partial \vec{\alpha}}, S \right) = \mathcal{U} \left(\frac{\partial \vec{z}}{\partial \vec{\alpha}}, S \right). \quad (6.5.15)$$

There is an important symmetry which further restricts what is possible in the Lagrangian and consequently the function $\mathcal{U}$. Our labeling scheme is required to satisfy equation (6.5.6) but any redefinition of the particle labels which preserves this changes nothing physically. The reason nothing physical is affected by such a redefinition is that because the line element is preserved, the distance between any particles is unchanged and we assume that microscopically the interactions have rotational symmetry and thus are fixed by the distances between particles. Thus, there is a relabeling symmetry given by:

$$\alpha'^a = \alpha^a(\alpha) \quad (6.5.16)$$

where it is required that:

$$ds_0^2 = \delta_{ab} d\alpha'^a d\alpha'^b \stackrel{!}{=} \delta_{ab} d\alpha^a d\alpha^b. \quad (6.5.17)$$

Because this should be true for all $d\alpha^a$:

$$\delta_{cd} \frac{\partial \alpha'^c}{\partial \alpha^a} \frac{\partial \alpha'^d}{\partial \alpha^b} d\alpha^a d\alpha^b \stackrel{!}{=} \delta_{ab} d\alpha^a d\alpha^b \quad (6.5.18)$$

$$\implies \delta_{ab} = \delta_{cd} \frac{\partial \alpha'^c}{\partial \alpha^a} \frac{\partial \alpha'^d}{\partial \alpha^b}. \quad (6.5.19)$$

Due to this relabeling symmetry, we only consider relabeling invariant $\mathcal{U}$. The stretch tensor is relabeling invariant:

$$C'_{ab} = \delta_{cd} \frac{\partial \alpha'^c}{\partial z^a} \frac{\partial \alpha'^d}{\partial z^b} = \delta_{cd} \frac{\partial \alpha'^c}{\partial \alpha^e} \frac{\partial \alpha'^d}{\partial \alpha^f} \frac{\partial \alpha^e}{\partial z^a} \frac{\partial \alpha^f}{\partial z^b} = \delta_{ef} \frac{\partial \alpha^e}{\partial z^a} \frac{\partial \alpha^f}{\partial z^b} = C_{ab}. \quad (6.5.20)$$

The relabeling symmetry condition in equation (6.5.19) can be rewritten in matrix form by defining the matrix $\hat{R}$ with components:

$$R^a_b = \frac{\partial \alpha'^a}{\partial \alpha^b} \implies \hat{R}^T \hat{R} = \mathbb{1}. \quad (6.5.21)$$

Then, we see that $\hat{R}$ must be an orthogonal matrix (a composition of rotations and -1). It is useful to recall the definition of the displacement gradient:

$$F^a{}_b = \frac{\partial \alpha^a}{\partial z^b}. \quad (6.5.22)$$

Letting $\hat{C}$ be the matrix form of the stretch tensor and $\hat{F}$ be the matrix form of the displacement gradient:

$$\hat{C} = \hat{F}^T \hat{F}. \quad (6.5.23)$$

Suppose we have can identify a particular matrix $\hat{F}_0$ so that:

$$\hat{C} = \hat{F}_0^T \hat{F}_0. \quad (6.5.24)$$

Define then $\hat{G}$ by:

$$\hat{G} = \hat{F} \hat{F}_0^{-1}. \quad (6.5.25)$$

It follows that:

$$\hat{G}^T \hat{G} = \hat{F}_0^{-T} \hat{F}^T \hat{F} \hat{F}_0^{-1} = \hat{F}_0^{-T} \hat{C} \hat{F}_0^{-1} = \hat{F}_0^{-T} \hat{F}_0^T \hat{F}_0 \hat{F}_0^{-1} = \mathbb{1}. \quad (6.5.26)$$

Thus, $\hat{G}$ is an orthogonal matrix. So, the displacement gradient matrix $\hat{F}$ can always be written as an orthogonal matrix $\hat{G}$ times any matrix $\hat{F}_0$ which satisfies $\hat{F}_0^T \hat{F}_0 = \hat{C}$:

$$\hat{F} = \hat{G} \hat{F}_0. \quad (6.5.27)$$

Because $\hat{F}_0$ is determined by $\hat{C}$, we see that $\hat{F}$ is determined by $\hat{C}$ up to an orthogonal matrix. However, under a change of labels that orthogonal matrix is transformed:

$$\hat{F}' = \hat{R} \hat{F} = \hat{R} \hat{G} \hat{F}_0 = \hat{G}' \hat{F}_0 \implies \hat{G}' = \hat{R} \hat{G} \quad (6.5.28)$$

and so $\hat{C}$ determines $\hat{F}$ precisely up to the orthogonal group of matrices which represent our ability to relabel the α 's. Consequently, anything relabel invariant (and thus $\hat{R}$ and correspondingly $\hat{G}$ independent) is actually determined by $\hat{C}$. So, the stretch tensor contains all relabeling invariant information in the deformation gradient. Because of this we have that $\mathcal{U}$ only depends on the deformation gradient through the stretch tensor:

$$\mathcal{U} = \mathcal{U}(\hat{C}, S). \quad (6.5.29)$$

The stretch tensor is a 3x3 symmetric matrix and thus is diagonalizable by a rotation matrix. Its 3 eigenvalues are invariant under rotations but any other matrix with the same eigenvalues is related to $\hat{C}$ by a compositions of rotations and parity transformations. Because we have symmetry under both rotations and parity in the Galilean theory, the only invariant quantities that can be formed out of the stretch tensor are its eigenvalues. Thus, we can take $\mathcal{U}$ to depend only on the eigenvalues of $\hat{C}$. Because there are three of them, we can equivalently use any three independent functions of the eigenvalues. We can do this with the traces of the first three powers of $\hat{C}$, letting $\lambda_1, \lambda_2, \lambda_3$ be the eigenvalues of $\hat{C}$:

$$\text{Tr}(\hat{C}) = \lambda_1 + \lambda_2 + \lambda_3, \quad \text{Tr}(\hat{C}^2) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \quad \text{Tr}(\hat{C}^3) = \lambda_1^3 + \lambda_2^3 + \lambda_3^3. \quad (6.5.30)$$

Or, instead of using $\text{Tr}(\hat{C}^3)$, we can use the determinant of $\hat{C}$:

$$\det \hat{C} = \lambda_1 \lambda_2 \lambda_3 = \det(\hat{F}^T \hat{F}) = (\det \hat{F})^2 = \left(\det \frac{\partial \vec{\alpha}}{\partial \vec{z}} \right)^2 \quad (6.5.31)$$

$$\implies n(t, \vec{x}) = n_0(\vec{\alpha}) \sqrt{\det \hat{C}}. \quad (6.5.32)$$

So, defining:

$$C^{(1)} = \text{Tr}(\hat{C}) = C_{ab} \delta^{ab}, \quad C^{(2)} = \text{Tr}(\hat{C}^2) = C_{ab} C^{ab} \quad (6.5.33)$$

we can express all of the $\hat{C}$ dependence of $\mathcal{U}$ in terms of $C^{(1)}$, $C^{(2)}$, and n :

$$\mathcal{U} = \mathcal{U}(n, C^{(1)}, C^{(2)}, S) \quad (6.5.34)$$

Explicitly separating out the number density like this is convenient as for fluids the internal energy only depends on the stretch tensor through the number density while for solids the internal energy is allowed to depend on $C^{(1)}$ and $C^{(2)}$ as well. Together then we have that in the absence of any external forces or interactions:

$$\mathcal{L} = \int_A \left(\frac{1}{2} m |\dot{\vec{z}}|^2 - \mathcal{U}(n, C^{(1)}, C^{(2)}, S) \right) n_0 d^3 \vec{\alpha}. \quad (6.5.35)$$

It is possible for us to add back in electromagnetic interactions to our matter quite easily so long as the electromagnetic fields do not vary significantly over the length scale on which the continuum mechanical averaging is performed (really this means the potentials and fields entering here will be smoothed out over the fluid length scale rather than being the exact microscopic fields). If the potentials are smoothed out in this way then we can take the exact electromagnetic interaction terms and approximate them by the smoothed out interaction:

$$\mathcal{L}_{\text{int}} = \sum_{k=1}^N \left(q\dot{\vec{x}}_k \cdot \vec{A}(t, \vec{x}_k) - q\phi(t, \vec{x}_k) \right) \approx \int_A \left(q\dot{\vec{z}} \cdot \vec{A}(t, \vec{z}) - q\phi(t, \vec{z}) \right) n_0 d^3 \vec{\alpha}. \quad (6.5.36)$$

Alternatively, this become exactly equal when n_0 is taken to be a sum of Dirac deltas at the appropriate locations for the point particles at the time of labeling. However, we then need to smooth n_0 appropriately in order to have continuous, differentiable, well-defined matter equations.

Together then, we take the Lagrangian for nonrelativistic charged matter to be:

$$\mathcal{L} = \int_A \left(\frac{1}{2} m |\dot{\vec{z}}|^2 - \mathcal{U}(n, C^{(1)}, C^{(2)}, S) + q\dot{\vec{z}} \cdot \vec{A} - q\phi \right) n_0 d^3 \vec{\alpha}. \quad (6.5.37)$$

Conventionally, we would like to simply vary this to find the Euler-Lagrange equations of motion for $\vec{z}$. However, we should be careful. The reason the entropy $S(t, \vec{\alpha})$ appears in our Lagrangian is because we have assumed the matter is locally in thermodynamic equilibrium. Consequently, we should use the quasidynamic equations of motion:

$$\frac{dQ^a}{dt} = \frac{\partial E}{\partial P_a}, \quad \frac{dP_a}{dt} = -\frac{\partial E}{\partial Q^a} + F_{Ma}, \quad \frac{\partial E}{\partial S} \frac{dS}{dt} = \frac{dQ}{dt} \quad (6.5.38)$$

However, these equations of motion should each apply locally (meaning at each $\vec{\alpha}$) because we have assumed local thermodynamic equilibrium at each $\vec{\alpha}$. Consequently, our equations of motion should read:

$$\frac{dz^a}{dt} = \frac{\delta E}{\delta p_a}, \quad \frac{dp_a}{dt} = -\frac{\delta E}{\delta z^a} + f_{Ma}, \quad \frac{\delta E}{\delta S} \frac{dS}{dt} = \frac{dq}{dt} \quad (6.5.39)$$

where f_{Ma} is the force density per unit matter element on the matter which is external to the matter element at $\vec{\alpha}$ and $\frac{dq}{dt}$ is the heat transfer per unit time and volume to the matter element at $\vec{\alpha}$. All of the matter elements at $\vec{\alpha}' \neq \vec{\alpha}$ are external to the matter element at $\vec{\alpha}$. Therefore, f_{Ma} not only contains terms which are due to forces external to the whole matter but also forces between different matter elements. Similarly, $\frac{dq}{dt}$ not only contains heat transfer from outside of the whole matter but also heat transfer from one matter element to another. This is a bit annoying because it means that matter-to-matter interactions enter the equations of motion through f_{Ma} , which is supplied in addition to our action rather than derived from it. However, by the entropy-varied formulation of the quasidynamic equations of motion we can incorporate these forces into our variational principle by considering appropriate variations of the entropy.

The forces between the matter elements exist as some contribution to the stress tensor (by looking at equation (6.2.45) the forces on a given matter element are comprised of contributions from complete external sources and the divergence of the stress tensor). So, let $\hat{d}$ be the part of the stress tensor which is to be captured by f_{Ma} and consequently our entropy varied formulation. The force density due to $\hat{d}$ is then $\nabla \cdot \hat{d}$ and so the force per matter element due to $\hat{d}$ is:

$$\vec{f}_M = \frac{\nabla \cdot \hat{d}}{n}. \quad (6.5.40)$$

By equation (5.8.66) then we consider entropy variations which satisfy:

$$nT\delta S + \delta z_a \partial_b d^{ab} = 0. \quad (6.5.41)$$

The time evolution of the entropy should still be given by equation (6.2.46), which we shall return to shortly. Using this variation in equation (6.5.37) gives (integrating the Lagrangian with respect to time to form an action $\mathcal{S}$):

$$\delta \mathcal{S} = \int \int_A \left(m\dot{\vec{z}} \cdot \delta \dot{\vec{z}} - \frac{\partial \mathcal{U}}{\partial n} \delta n - \frac{\partial \mathcal{U}}{\partial C^{(1)}} \delta C^{(1)} - \frac{\partial \mathcal{U}}{\partial C^{(2)}} \delta C^{(2)} - \frac{\partial \mathcal{U}}{\partial S} \delta S + q\vec{A} \cdot \delta \dot{\vec{z}} + q\dot{\vec{z}} \cdot \partial_a \vec{A} \delta z^a - q\partial_a \phi \delta z^a \right) n_0 d^3 \vec{\alpha} dt \quad (6.5.42)$$

$$= \int \int_A \left(\frac{d}{dt} \left((m\dot{\vec{z}} + q\vec{A}) \cdot \delta \vec{z} \right) - m\ddot{\vec{z}} \cdot \delta \vec{z} - \frac{\partial \mathcal{U}}{\partial n} \delta n - \frac{\partial \mathcal{U}}{\partial C^{(1)}} \delta C^{(1)} - \frac{\partial \mathcal{U}}{\partial C^{(2)}} \delta C^{(2)} \right)$$

$$-\frac{\partial \mathcal{U}}{\partial S} \delta S + q \left(\vec{E} + \dot{\vec{z}} \times \vec{B} \right) \cdot \delta \vec{z} \Big) n_0 d^3 \vec{\alpha} dt. \quad (6.5.43)$$

We will as always assume that the initial and final variations are 0 and so the total time derivative will vanish.

We can compute and simplify the variations δn , $\delta C^{(1)}$, $\delta C^{(2)}$. Using the definition of n and the variation of the determinant from equation (5.2.30):

$$\delta n = -\frac{n_0}{\det \left(\frac{\partial \vec{z}}{\partial \vec{\alpha}} \right)^2} \delta \det \left(\frac{\partial \vec{z}}{\partial \vec{\alpha}} \right) = -n \frac{\partial \alpha^b}{\partial z^a} \frac{\partial \delta z^a}{\partial \alpha^b} = -n \nabla \cdot \delta \vec{z}. \quad (6.5.44)$$

Thus as always assuming the field variations go to 0 at infinity:

$$\int_A \frac{\partial \mathcal{U}}{\partial n} \delta n n_0 d^3 \vec{\alpha} = - \int_A \frac{\partial \mathcal{U}}{\partial n} n \nabla \cdot \delta \vec{z} n_0 d^3 \vec{\alpha} = - \int_S \frac{\partial \mathcal{U}}{\partial n} n^2 \nabla \cdot \delta \vec{z} d^3 \vec{x} \quad (6.5.45)$$

$$= - \int_{\partial S} \frac{\partial \mathcal{U}}{\partial n} n^2 \delta \vec{z} \cdot d\vec{A} + \int_{\partial S} \nabla \left(n^2 \frac{\partial \mathcal{U}}{\partial n} \right) \cdot \delta \vec{z} dS \quad (6.5.46)$$

$$= \int_A \frac{1}{n} \nabla \left(n^2 \frac{\partial \mathcal{U}}{\partial n} \right) \cdot \delta \vec{z} n_0 d^3 \vec{\alpha}. \quad (6.5.47)$$

Let us do the same for the variation of the stretch tensor. By definition:

$$\delta C_{ab} = \delta_{cd} \delta \left(\frac{\partial \alpha^c}{\partial z^a} \right) \frac{\partial \alpha^d}{\partial z^b} + \delta_{cd} \frac{\partial \alpha^c}{\partial z^a} \delta \left(\frac{\partial \alpha^d}{\partial z^b} \right). \quad (6.5.48)$$

We can compute the variation of $\frac{\partial \alpha}{\partial z}$ by using that it is the inverse of $\frac{\partial z}{\partial \alpha}$:

$$\frac{\partial z^a}{\partial \alpha^c} \frac{\partial \alpha^c}{\partial z^b} = \delta_b^a \implies \frac{\partial \delta z^a}{\partial \alpha^c} \frac{\partial \alpha^c}{\partial z^b} + \frac{\partial z^a}{\partial \alpha^c} \delta \left(\frac{\partial \alpha^c}{\partial z^b} \right) = 0 \implies \delta \left(\frac{\partial \alpha^c}{\partial z^a} \right) = -\frac{\partial \alpha^c}{\partial z^d} \frac{\partial \delta z^d}{\partial z^a}. \quad (6.5.49)$$

Returning this to the variation of the stretch tensor:

$$\delta C_{ab} = -C_{cb} \frac{\partial \delta z^c}{\partial z^a} - C_{ac} \frac{\partial \delta z^c}{\partial z^b} \quad (6.5.50)$$

$$\implies \delta C^{(1)} = \delta^{ab} \delta C_{ab} = -2C^a{}_b \frac{\partial \delta z^b}{\partial z^a}, \quad \delta C^{(2)} = 2C^{ab} \delta C_{ab} = -4C^{ab} C_{bc} \frac{\partial \delta z^c}{\partial z^a}. \quad (6.5.51)$$

So, the term the stretch tensor variation contributes to the Lagrangian is (following corresponding manipulations to those done for the number density):

$$\int_A \left(\frac{\partial \mathcal{U}}{\partial C^{(1)}} \delta C^{(1)} + \frac{\partial \mathcal{U}}{\partial C^{(2)}} \delta C^{(2)} \right) n_0 d^3 \vec{\alpha} = \int_A \delta z^a \partial_b \left(2n \frac{\partial \mathcal{U}}{\partial C^{(1)}} C^b{}_a + 4n \frac{\partial \mathcal{U}}{\partial C^{(2)}} C^{bc} C_{ca} \right) \frac{n_0}{n} d^3 \vec{\alpha}. \quad (6.5.52)$$

Returning these to the variation of the action along with the entropy variation:

$$\begin{aligned} \delta S = \int \int_A \left(-m \ddot{\vec{z}} \cdot \delta \vec{z} - \frac{1}{n} \nabla \left(n^2 \frac{\partial \mathcal{U}}{\partial n} \right) \cdot \delta \vec{z} - \delta z^a \frac{2}{n} \partial_b \left(n \frac{\partial \mathcal{U}}{\partial C^{(1)}} C^b{}_a + 2n \frac{\partial \mathcal{U}}{\partial C^{(2)}} C^{bc} C_{ca} \right) \right. \\ \left. + \frac{1}{n} \partial_b d^{ab} \delta z_a + q \left(\vec{E} + \dot{\vec{z}} \times \vec{B} \right) \cdot \delta \vec{z} \right) n_0 d^3 \vec{\alpha}. \end{aligned} \quad (6.5.53)$$

Thus, requiring this to be true for all allowed variations $\delta \vec{z}$, the equation of motion produced for the streamlines is:

$$mn \frac{d^2 z_a}{dt^2} = -\partial_a \left(n^2 \frac{\partial \mathcal{U}}{\partial n} \right) - \partial^b \left(2n \frac{\partial \mathcal{U}}{\partial C^{(1)}} C_{ab} + 4n \frac{\partial \mathcal{U}}{\partial C^{(2)}} C^c{}_a C_{cb} \right) + \partial^b d_{ab} + qn \left(E_a + (\dot{\vec{z}} \times \vec{B})_a \right). \quad (6.5.54)$$

This is our usual momentum equation of motion identifying the force density and stress tensor to be:

$$\vec{f} = qn(\vec{E} + \vec{v} \times \vec{B}), \quad \sigma_{ab} = -n^2 \frac{\partial \mathcal{U}}{\partial n} \delta_{ab} - 2n \frac{\partial \mathcal{U}}{\partial C^{(1)}} C_{ab} - 4n \frac{\partial \mathcal{U}}{\partial C^{(2)}} C^c{}_a C_{cb} + d_{ab}. \quad (6.5.55)$$

The continuity equation for n follows automatically from its definition in terms of $\frac{\partial \vec{z}}{\partial \vec{\alpha}}$. We have already recovered the momentum equation of motion. Now in order to know how the entropy evolves we need to supply equation (6.2.46) (as the entropy evolution in the quasidynamic formulation is supplied in addition to the variational principle using energy evolution). Expanding out the derivatives in equation (6.2.46) and simplifying using the continuity and momentum equations:

$$\frac{\partial}{\partial t} \left(\frac{1}{2} mn |\vec{v}|^2 + n\mathcal{U} \right) + \nabla \cdot \left(\frac{1}{2} mn |\vec{v}|^2 \vec{v} + n\mathcal{U} \vec{v} - \hat{\sigma} \cdot \vec{v} + \vec{q} \right) = \vec{v} \cdot \vec{f} + \Phi \quad (6.5.56)$$

$$\implies n \frac{d\mathcal{U}}{dt} - \sigma^{ab} \partial_a v_b + \nabla \cdot \vec{q} = \Phi. \quad (6.5.57)$$

Now let us put in the explicit variable dependence of $\mathcal{U}$ and the form we have derived for the stress tensor. To do so we will need the time derivatives of n and C_{ab} . These follow directly from their variations:

$$\frac{dn}{dt} = -n \nabla \cdot \vec{v}, \quad \frac{dC_{ab}}{dt} = -\partial_a v^c C_{cb} - \partial_b v^c C_{ca}. \quad (6.5.58)$$

Then the energy equation simplifies to:

$$\boxed{nT \frac{dS}{dt} - d^{ab} \partial_a v_b + \nabla \cdot \vec{q} = \Phi.} \quad (6.5.59)$$

This is the equation of motion the entropy must satisfy to produce the continuity of energy. All that must be supplied now is the heat transfer Φ , the heat flux vector $\vec{q}$, and the “dissipative stress tensor” $\hat{d}$ which is the part of the stress due to inter-matter element heat exchange. For $\vec{q}$ and $\hat{d}$ one typically takes the Navier-Stokes form, but other forms may be of relevance for different materials.

It is very straightforward to find the Hamiltonian formulation of our system by the usual way. By now, you can likely predict the answer at a glance. The conjugate momentum $\vec{p}(t, \vec{\alpha})$ to the position of each matter element is:

$$\vec{p} = \frac{\delta \mathcal{L}}{\delta \dot{\vec{z}}} = mn_0 \dot{\vec{z}} + qn_0 \vec{A} \quad (6.5.60)$$

and so by the Legendre transformation gives the Hamiltonian:

$$\mathcal{H}[z, p, S] = \int_A \vec{p} \cdot \dot{\vec{z}} d^3 \vec{\alpha} - \mathcal{L} = \int_A \left(\frac{|\vec{p} - qn_0 \vec{A}|^2}{2mn_0} + n_0 \mathcal{U} + qn_0 \phi \right) d^3 \vec{\alpha}. \quad (6.5.61)$$

Altogether then:

Theorem 6.8: Active Nonrelativistic Continuum Field Theory

The equations of motion for nonrelativistic continuum mechanics are given by varying the position fields $\vec{z}(t, \vec{\alpha})$ in the action:

$$S = \int \int_A \left(\frac{1}{2} m |\dot{\vec{z}}|^2 - \mathcal{U}(n, C^{(1)}, C^{(2)}, S) + q \dot{\vec{z}} \cdot \vec{A} - q\phi \right) n_0 d^3 \vec{\alpha} dt \quad (6.5.62)$$

where the number density n and stretch tensor C are given by:

$$n(t, \vec{z}(t, \vec{\alpha})) = \frac{n_0(\vec{\alpha})}{\det \left(\frac{\partial \vec{z}}{\partial \vec{\alpha}} \right)}, \quad C_{ab} = \delta_{cd} \frac{\partial \alpha^c}{\partial z^a} \frac{\partial \alpha^d}{\partial z^b}, \quad C^{(1)} = C_{ab} \delta^{ab}, \quad C^{(2)} = C^{ab} C_{ab} \quad (6.5.63)$$

and the entropy per matter element $S(t, \vec{\alpha})$ is varied as:

$$n \frac{\partial \mathcal{U}}{\partial S} \delta S + \delta z_a \partial_b d^{ab} = 0 \quad (6.5.64)$$

where d^{ab} is the dissipative contribution to the stress tensor (supplied as a constitutive relation). The entropy evolution is given by the additional equation:

$$n \frac{\partial \mathcal{U}}{\partial S} \frac{dS}{dt} - d^{ab} \partial_a v_b + \nabla \cdot \vec{q} = \Phi \quad (6.5.65)$$

where the heat flux vector $\vec{q}$ and heat transfer Φ need to be supplied.

This action, for appropriate choice of $\mathcal{U}$, $\hat{d}$, and $\vec{q}$ can reproduce all of the cases of a gas, liquid, solid, or plasma. Therefore, this action provides a general formulation of nonrelativistic continuum mechanics.

6.5.2 Passive Formulation

It is very nice to formulate the variational principle in passive coordinates as well. In the passive coordinates we use the label fields $\vec{\alpha}(t, \vec{x})$ and the entropy field $s(t, \vec{x})$ which is defined so that $s(t, \vec{z}(t, \vec{\alpha})) = S(t, \vec{\alpha})$. By definition, the label fields automatically satisfy (by taking a time derivative):

$$\vec{z}(t, \vec{\alpha}(t, \vec{x})) = \vec{x} \implies \dot{z}^a(t, \vec{\alpha}(t, \vec{x})) + \frac{\partial z^a}{\partial \alpha^b} \frac{\partial \alpha^b}{\partial t} = 0. \quad (6.5.66)$$

Using the label fields it is convenient to define the notation $\frac{\partial \vec{x}}{\partial \vec{\alpha}}$ as the matrix inverse of $\frac{\partial \vec{z}}{\partial \vec{\alpha}}$ at the spatial position $\vec{x}$. Then:

$$v^a(t, \vec{x}) = -\frac{\partial x^a}{\partial \alpha^b} \dot{\alpha}^b(t, \vec{x}) \quad (6.5.67)$$

where the dot above α^a indicates partial t time differentiation (at fixed $\vec{x}$). The action in equation (6.5.62) can then be rewritten as a spatial integral as:

$$\mathcal{S} = \int \int_{\mathbb{S}} \left(\frac{1}{2} m \frac{\partial x^a}{\partial \alpha^b} \frac{\partial x_a}{\partial \alpha^c} \dot{\alpha}^b \dot{\alpha}^c - \mathcal{U}(n, C^{(1)}, C^{(2)}, s) - q A_a \frac{\partial x^a}{\partial \alpha^b} \dot{\alpha}^b - q \phi \right) n d^3 \vec{x} dt. \quad (6.5.68)$$

This looks quite gross, but because we have simply changed coordinates from the streamlines to the label fields we will arrive at the same equations of motion. The presence of the matrix inverse $\frac{\partial \vec{x}}{\partial \vec{\alpha}}$ all over the place makes this action not very nice. Let $\beta_a(t, \vec{x})$ be the conjugate momentum fields to the label fields. Immediately we have:

$$\beta_a = \frac{\delta \mathcal{L}}{\delta \dot{\alpha}^a} = m \frac{\partial x^c}{\partial \alpha^a} \frac{\partial x_c}{\partial \alpha^b} \dot{\alpha}^b - q n A_b \frac{\partial x^b}{\partial \alpha^a} \quad (6.5.69)$$

$$\implies -\frac{\partial \alpha^b}{\partial x^a} \beta_b = m n v_a + q n A_a = \wp_a. \quad (6.5.70)$$

From here we can solve for $\dot{\alpha}^a$ to perform the Legendre transformation:

$$\dot{\alpha}^a = -\frac{\partial \alpha^a}{\partial x^b} v^b = \frac{1}{m} \frac{\partial \alpha^a}{\partial x^b} \left(\frac{\beta_c \partial^b \alpha^c}{n} + q A^b \right). \quad (6.5.71)$$

This gives (after a little simplification) the Hamiltonian:

$$\mathcal{H} = \int_{\mathbb{S}} \beta_a \dot{\alpha}^a d^3 \vec{x} - \mathcal{L} \quad (6.5.72)$$

$$\implies \mathcal{H} = \int_{\mathbb{S}} \left(\frac{\left| \frac{\beta_a \nabla \alpha^a}{n} + q \vec{A} \right|^2}{2m} + q \phi + \mathcal{U}(n, C^{(1)}, C^{(2)}, s) \right) n d^3 \vec{x}. \quad (6.5.73)$$

This Hamiltonian is very easy to remember as we see that the energy per particle (which is given by everything inside the large parentheses) is the single particle energy with the replacement of $\vec{p} = -\frac{1}{n} \beta_a \nabla \alpha^a$. If we take this Hamiltonian and write the associated Hamiltonian action we have:

$$\mathcal{S}[\vec{\alpha}, \vec{\beta}] = \int \int_{\mathbb{S}} \left(\beta_a \dot{\alpha}^a - \frac{\left| \beta_a \nabla \alpha^a + q n \vec{A} \right|^2}{2nm} - q n \phi - n \mathcal{U} \right) d^3 \vec{x} dt. \quad (6.5.74)$$

This is much nicer as it has eliminated any direct use of the matrix inverse in the action.

We should not include the entropy as an independent field to be varied in the action because its variation is dependent on the variation of α . In order to use this action to compute equations of motion we will need that precise relationship. By varying equation (6.5.66) we see:

$$\delta z^a + \frac{\partial z^a}{\partial \alpha^b} \delta \alpha^b = 0. \quad (6.5.75)$$

Then, the variation of the entropy (using equation (6.5.64)) becomes:

$$s(t, \vec{z}(t, \vec{\alpha})) = S(t, \vec{\alpha}) \implies \delta s + \frac{\partial s}{\partial x^a} \delta z^a = \delta S \quad (6.5.76)$$

$$\implies n T \delta s = \left(n T \frac{\partial s}{\partial x^a} + \partial^b d_{ab} \right) \frac{\partial x^a}{\partial \alpha^c} \delta \alpha^c. \quad (6.5.77)$$

We can make the action a little nicer by introducing the velocity field $\vec{v}(t, \vec{x})$ as its own field which needs to be varied. Consider the action:

$$\mathcal{S}[\vec{\alpha}, \vec{\beta}, \vec{v}] = \int \int_{\mathbb{S}} \left(\beta_a \left(\frac{\partial \alpha^a}{\partial t} + \frac{\partial \alpha^a}{\partial x^b} v^b \right) + \frac{1}{2} m n |\vec{v}|^2 + q n \vec{A} \cdot \vec{v} - q n \phi - n \mathcal{U} \right) d^3 \vec{x} dt. \quad (6.5.78)$$

Here we treat $\vec{v}$ as a completely independent quantity not defined in terms of the position fields. Because no derivatives appear on $\vec{v}$, requiring the action to have vanishing variation with respect to it imposes an

algebraic condition:

$$\frac{\delta \mathcal{S}}{\delta v^a} = \beta_b \frac{\partial \alpha^b}{\partial x^a} + mn v_a + qn A_a \stackrel{!}{=} 0 \quad (6.5.79)$$

which recovers the correct condition from equation (6.5.70). Replacing this expression for $\vec{v}$ back into the action reduces it to equation (6.5.74). Thus, this action is completely equivalent!

Theorem 6.9: Passive Nonrelativistic Continuum Field Theory

The equations of motion for nonrelativistic continuum mechanics are given by varying the label fields $\vec{\alpha}(t, \vec{x})$, their conjugate fields $\vec{\beta}(t, \vec{x})$, and the velocity field $\vec{v}(t, \vec{x})$ independently in the action:

$$S[\vec{\alpha}, \vec{\beta}, \vec{v}] = \int_{\mathbb{S}} \left(\beta_a \left(\frac{\partial \alpha^a}{\partial t} + v^b \frac{\partial \alpha^a}{\partial x^b} \right) + \frac{1}{2} mn |\vec{v}|^2 + qn \vec{A} \cdot \vec{v} - qn \phi - n \mathcal{U}(n, C^{(1)}, C^{(2)}, s) \right) d^3 \vec{x} dt \quad (6.5.80)$$

where the number density n and stretch tensor C are given by:

$$n(t, \vec{x}) = n_0(\vec{\alpha}) \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right), \quad C_{ab} = \delta_{cd} \frac{\partial \alpha^c}{\partial x^a} \frac{\partial \alpha^d}{\partial x^b}, \quad C^{(1)} = C_{ab} \delta^{ab}, \quad C^{(2)} = C^{ab} C_{ab} \quad (6.5.81)$$

and the entropy field $s(t, \vec{x})$ is varied as:

$$nT \delta s = \left(nT \frac{\partial s}{\partial x^a} + \partial^b d_{ab} \right) \frac{\partial x^a}{\partial \alpha^c} \delta \alpha^c \quad (6.5.82)$$

where d^{ab} is the dissipative contribution to the stress tensor which must be supplied by a constitutive relation. The entropy evolution is given by the additional equation:

$$n \frac{\partial \mathcal{U}}{\partial s} \left(\frac{\partial s}{\partial t} + v^a \frac{\partial s}{\partial x^a} \right) - d^{ab} \partial_a v_b + \nabla \cdot \vec{q} = \Phi \quad (6.5.83)$$

where the heat flux vector $\vec{q}$ and heat transfer Φ need to be supplied.

Exercises

Problem 6.12: Relabeling Gauge Symmetry and Circulation Conservation.

(a) Show that the active formulation action is invariant under the coordinate transformation:

$$\vec{z}'(t, \vec{\alpha}') = \vec{z}(t, \vec{\alpha}), \quad \vec{\alpha}' = \hat{R}(\vec{\alpha}) \vec{\alpha} + \vec{b}(\vec{\alpha})$$

for an $\vec{\alpha}$ dependent rotation matrix $\hat{R}(\vec{\alpha})$ and vector field $\vec{b}(\vec{\alpha})$.

(b) Because the action is invariant under the above arbitrary functions of transformations, the action has gauge symmetry under such transformations. Show that the resulting conservation laws from these symmetries are the local conservation of linear and angular momentum. Then, show that the integrated form of the angular momentum law predicts the conservation of circulation of the momentum field $\vec{p}_1 = m\vec{z} + q\vec{A}$. Show that in the case of no magnetic field this reduces to Kelvin's circulation theorem. Because in the presence of a magnetic field the circulation of the momentum is conserved and not of the velocity, it is useful to define a noncirculating fluid as a fluid for which $\nabla \times \vec{p}_1 = 0$. In the absence of a magnetic field this is the same as an irrotational fluid.

Problem 6.13: ★ Noncirculating flow, the Hamilton-Jacobi Equation, and the Schrödinger equation. Consider an isobaric fluid which has $\mathcal{U} = \mathcal{U}(n)$ (because it is a fluid, it only resists rescaling and not any other kind of deformation and so does not depend on $C^{(1)}$ or $C^{(2)}$, because it is isobaric s is a uniform constant and so we suppress the dependence of $\mathcal{U}$ on it) which is also noncirculating ($\nabla \times \vec{p}_1 = 0$).

(a) Let $\varphi(t, \vec{x})$ be a potential for the momentum. That is:

$$\vec{p}_1 = \nabla \varphi.$$

Explain that $\nabla \times \vec{p}_1 = 0$ ensures such a potential exists. Show that φ has the same units as the action and that it is related to the label fields α^a and their conjugate momenta β_a by:

$$\beta_a \nabla \alpha^a = -n \nabla \varphi.$$

(b) Show that it is possible using relabeling symmetry to choose a labeling scheme so that $\alpha^1 = \varphi, \beta_1 =$

$-n, \beta_2 = \beta_3 = 0$. Show that with this labeling scheme the action can simply be rewritten as:

$$S = \int \int_{\mathbb{S}} \left(-\frac{\partial \varphi}{\partial t} - \frac{|\nabla \varphi - q\vec{A}|^2}{2m} - q\phi - \mathcal{U} \right) nd^3\vec{x}dt.$$

Show that the equations of motion derived from this action generalize Bernoulli's principle to the case of an electromagnetically charged fluid.

- (c) Show that the fluid of the previous part has gauge symmetry under the transformation:

$$\varphi' = \varphi + qf(t, \vec{x}), \quad \vec{A}' = \vec{A} + \nabla f, \quad \phi' = \phi - \frac{\partial f}{\partial t}.$$

- (d) Consider the fluid to be cold (to have negligible internal energy, so that we can approximate $\mathcal{U} = 0$). Show that for such a fluid φ exactly satisfies the Hamilton-Jacobi equation for the canonical action with the familiar single particle Hamiltonian:

$$\mathcal{H} = \frac{|\vec{p} - q\vec{A}|^2}{2m} + q\phi.$$

- (e) Consider the cold fluid from the previous part. Let $\hbar$ be a (for now arbitrary) positive constant with units of the action. Define the complex field:

$$\psi(t, \vec{x}) = \sqrt{n(t, \vec{x})} e^{i\frac{\varphi(t, \vec{x})}{\hbar}}.$$

Show that the action can nicely be rewritten in terms of ψ as (up to a total time derivative):

$$S = \int \int_{\mathbb{S}} \left(i\hbar\psi^*\dot{\psi} - \frac{|i\hbar\nabla\psi + q\vec{A}\psi|^2}{2m} - q\phi|\psi|^2 + \frac{\hbar^2|\nabla|\psi||^2}{2m} \right) d^3\vec{x}dt.$$

- (f) Show that the action of the previous part has gauge symmetry under the transformation:

$$\psi' = e^{i\frac{q}{\hbar}f(t, \vec{x})}\psi, \quad \vec{A}' = \vec{A} + \nabla f, \quad \phi' = \phi - \frac{\partial f}{\partial t}$$

and that this can be interpreted as the freedom to rotate ψ by an arbitrary angle in the complex plane at each point in spacetime.

- (g) Let ℓ_n be a characteristic length scale on which the density and momentum of the fluid change appreciably (this could be estimated by $\ell_n \approx \frac{n}{|\nabla n|}$). We can estimate the length scale on which φ varies appreciably relative to our constant $\hbar$ by defining the length scale $\ell_\varphi = \frac{\hbar}{|\nabla\varphi|}$. Assume that we have chosen the value of $\hbar$ so that everywhere in our fluid the length scale ℓ_φ is much smaller than ℓ_n . Explain that this means φ appears like a quickly oscillating phase with a slowly changing wavenumber and that consequently the action above can be approximated as:

$$S \approx \int \int_{\mathbb{S}} \left(i\hbar\psi^*\dot{\psi} - \frac{|i\hbar\nabla\psi + q\vec{A}\psi|^2}{2m} - q\phi|\psi|^2 \right) d^3\vec{x}dt.$$

Show that the resulting equation of motion for ψ is a linear differential equation for ψ :

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{1}{2m}(\hbar\nabla - iq\vec{A})^2\psi + q\phi\psi.$$

This is known as the Schrödinger equation. Although we have found here that it can be derived from a sequence of approximations of fluids, it will turn out to be a fundamental equation of motion for describing the microscopic behavior of single particles.

Problem 6.14: Reproducing the Cauchy-Green Equations. Show by expanding the stress tensor in (6.5.55) for small strain tensor that the Cauchy-Green equations of motion are reproduced and identify the precise expressions for the bulk modulus and shear modulus as derived from the Lagrangian.

6.6 Relativistic Transport Equations

In principle, one can use the same degrees of freedom for describing relativistic continuum mechanics as we did for nonrelativistic continuum mechanics. However, doing so directly is inefficient and for non-ideal matter they are generally insufficient to make relativistically convenient closed equations of motion. Instead, it is better to mildly reorganize our fields so that our description plays more nicely with relativity. As well later we will find that for non-ideal matter some additional degrees of freedom are helpful. We previously used $\vec{z}(t, \vec{\alpha})$ to indicate the position of the matter element with label $\vec{\alpha}$ at time t . We can still do this. Alternatively, we found we can invert this relationship to define $\vec{\alpha}(t, \vec{x})$ which gives the identity of the matter element located at position $\vec{x}$ at the time t . The label functions are nicer relativistically because $\alpha^a(t, \vec{x})$ for $a \in \{1, 2, 3\}$ is a Lorentz scalar field and the system has a symmetry under relabelings $\alpha'^a = \alpha'^a(\alpha)$ which leave the stretch tensor unchanged. Therefore, we will treat the α^a fields as our fundamental fields unless stated otherwise (it is nicer to use the “passive formulation”). As well, we have the Lorentz scalar field $s(t, \vec{x})$ corresponding to the entropy per matter element in the instantaneous local rest frame (as that is the frame in which we can have local thermodynamic equilibrium). We then need transport equations to determine the evolution of s and the α^a .

The continuity equation for particle number remains valid in relativity as the only ingredient in its derivation was the local conservation of particle number. However, the number density (like charge density) is not a Lorentz scalar but instead the 0 component of a number current 4-vector. This follows immediately from the fact that the charge density should be q times the number density and the electric charge q of a single particle is simply a number (and so Lorentz invariant). Thus, the charge density and number density must have the same Lorentz transformation property and the electric current density and number current density must have the same Lorentz transformation property. When discussing relativistic materials, we will let J^μ be the **number current 4-vector**. Then, the electric current 4-vector is qJ^μ in this notation (rather than J^μ being the electric current 4-vector as we usually have written).

By (6.5.4) then we immediately have:

$$J^0(t, \vec{x}) = n_0(\alpha(t, \vec{x})) \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right) \quad (6.6.1)$$

which is just the solution implied by the continuity equation. We will retire the use of the symbol $n(t, \vec{x})$ for the number density J^0 in a general frame. Instead, we will use n to mean the number density in the instantaneous local rest frame of the matter, so that it is Lorentz invariant. The 3-velocity field is still given by (6.5.67):

$$v^a = -\frac{\partial x^a}{\partial \alpha^b} \frac{\partial \alpha^b}{\partial t} \quad (6.6.2)$$

where again the matrix $\frac{\partial \vec{x}}{\partial \vec{\alpha}}$ is meant as the matrix inverse of the spatial derivative matrix $\frac{\partial \vec{\alpha}}{\partial \vec{x}}$. By comparing the continuity equation to the covariant form of the continuity equation we can identify the appropriate expression for J^a :

$$\frac{\partial J^0}{\partial t} + \nabla \cdot (J^0 \vec{v}) = \partial_0 J^0 + \partial_a (J^0 v^a) = \partial_\mu J^\mu = 0, \quad J^a = J^0 v^a. \quad (6.6.3)$$

In the instantaneous local rest frame $v^a = 0$ by definition and so in that frame we trivially have:

$$n = \sqrt{-J^\mu J_\mu} \quad (6.6.4)$$

because the only contribution is from J^0 . However, this equation is Lorentz invariant and so because it is true in one frame it is true in any frame. (Again, n now means the number density in the instantaneous local rest frame). It follows that in a general frame:

$$n = \sqrt{-J^\mu J_\mu} = \frac{J^0}{\gamma} = n_0 \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right) \sqrt{1 - \frac{\partial x^a}{\partial \alpha^b} \frac{\partial x_a}{\partial \alpha^c} \dot{\alpha}^b \dot{\alpha}^c}. \quad (6.6.5)$$

Above γ is the usual Lorentz factor in terms of the velocity v^a .

These expressions for the current density are correct, but inconvenient in that they are not obviously covariant. Notice that J^0 can equivalently be written (using the expression for the determinant in terms of the Levi-Civita symbol):

$$J^0(t, \vec{x}) = -\frac{n_0}{6} \epsilon_{abc} \epsilon^{0\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} \quad (6.6.6)$$

where recall that $\epsilon_{\mu\nu\rho\sigma}$ is defined so that $\epsilon_{0123} = 1$ and that this fixes $\epsilon^{0abc} = -\epsilon^{abc}$. This suggests a possible formula for J^μ :

$$J^\mu_{\text{test}} = -\frac{n_0}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma}. \quad (6.6.7)$$

We have already established that this is the correct formula for J^0 . For $\mu = a \neq 0$ one can expand the 4 dimensional Levi-Civita into cases for which each index either is or isn't 0 and find with a little effort that in fact:

$$J^a_{\text{test}} = -n_0 \frac{\partial x^a}{\partial \alpha^b} \dot{\alpha}^b \det \left(\frac{\partial \vec{\alpha}}{\partial \vec{x}} \right) = J^0 v^a = J^a. \quad (6.6.8)$$

Therefore, the proper covariant expression for the number current density is:

$$J^\mu(X) = -\frac{n_0(\vec{\alpha})}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma}. \quad (6.6.9)$$

We should verify that the continuity equation holds.

$$\begin{aligned} \partial_\mu J^\mu = & -\frac{1}{6} \frac{\partial n_0}{\partial \alpha^d} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^d}{\partial x^\mu} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} - \frac{n_0(\alpha)}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial^2 \alpha^a}{\partial x^\mu \partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} \\ & - \frac{n_0(\alpha)}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial^2 \alpha^b}{\partial x^\mu \partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} - \frac{n_0(\alpha)}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial^2 \alpha^c}{\partial x^\mu \partial x^\sigma}. \end{aligned} \quad (6.6.10)$$

In the first term, the factor of $\epsilon^{\mu\nu\rho\sigma}$ contracted with the four factors of $\frac{\partial \alpha^a}{\partial x^\nu}$ (and other appropriate indices) forms a completely antisymmetric tensor of rank 4 but with indices a, b, c, d that can only take values 1, 2, 3. By being completely antisymmetric it is only nonzero when all of its indices are distinct. Because there are only three possible values for each index, there is no way 4 of them can be distinct. Therefore, the first term is 0. All of the other terms contain a second derivative of α which is then contracted into the 4-dimensional Levi-Civita. However, the second derivative matrix is always symmetric and the Levi-Civita is fully antisymmetric and so when the second derivative matrix is fully contracted into the Levi-Civita, the result is 0. Therefore, each of the other terms are 0 on their own as well. Thus:

$$\partial_\mu J^\mu = 0 \quad (6.6.11)$$

automatically, without the need to supply it as an equation of motion (which was also true in the nonrelativistic case). It is useful to introduce the local average 4-velocity field u^μ defined by:

$$u^\mu = \frac{J^\mu}{n} \implies J^\mu = n u^\mu. \quad (6.6.12)$$

This 4-velocity is often called the Eckart 4-velocity (some sources define an additional 4-velocity called the Landau velocity, which is the velocity of the center of momentum frame; we will generally not have a direct use for this). Automatically, $u^\mu u_\mu = -1$. This is the 4-velocity corresponding to the 3-velocity v^a . That is, one can quickly see that:

$$u^0 = \gamma = \frac{1}{\sqrt{1 - v^a v_a}}, \quad u^a = \gamma v^a. \quad (6.6.13)$$

In terms of u^μ , the continuity equation for J^μ becomes:

$$\partial_\mu (n u^\mu) = 0. \quad (6.6.14)$$

It is useful to introduce an analog of the worldline timelike parameter λ for the matter. Consider a function $\lambda(X)$ which has the property that $\frac{\partial \lambda}{\partial x^\mu}$ is everywhere timelike and that $\frac{\partial \lambda}{\partial x^0} > 0$ (λ is an increasing function of time). Because the 3-velocity in equation (6.6.2) must have speed less than c , it immediately follows that each of the label fields α^a have derivatives $\frac{\partial \alpha^a}{\partial x^\mu}$ which are spacelike:

$$\frac{\partial \alpha^a}{\partial x^\mu} \frac{\partial \alpha^a}{\partial x_\mu} > 0. \quad (6.6.15)$$

Because the relationship between the label fields and positions $\vec{z}(t, \vec{\alpha})$ is invertible, the label field derivatives $\frac{\partial \alpha^a}{\partial x^\mu}$ are linearly independent vector fields for different values of a . As well, because they are all spacelike and $\frac{\partial \lambda}{\partial x^\mu}$ is timelike, the set $\{\frac{\partial \lambda}{\partial x}, \frac{\partial \alpha^1}{\partial x}, \frac{\partial \alpha^2}{\partial x}, \frac{\partial \alpha^3}{\partial x}\}$ is linearly independent. Then, because these vectors are linearly independent the determinant of the matrix of derivatives of $(\lambda, \alpha^1, \alpha^2, \alpha^3)$ with respect to x^μ is nonzero. Consequently, the relationship between $\lambda, \alpha^1, \alpha^2, \alpha^3$ and x^0, x^1, x^2, x^3 is invertible. The inverse defines the

covariant position fields $z^\mu(\lambda, \vec{\alpha})$:

$$z^\mu(\lambda(X), \vec{\alpha}(X)) = x^\mu. \quad (6.6.16)$$

These covariant position fields are the more convenient relativistic generalization of the position fields $\vec{z}(t, \vec{\alpha})$ we used previously.

The current density can be given a nice expression in terms of the covariant position fields. Because the set $\{\frac{\partial \lambda}{\partial x}, \frac{\partial \alpha^1}{\partial x}, \frac{\partial \alpha^2}{\partial x}, \frac{\partial \alpha^3}{\partial x}\}$ is a linearly independent set of 4 vectors in 4 dimensional spacetime, they span the Minkowski space. Consequently, the inverses $\{\frac{\partial z}{\partial \lambda}, \frac{\partial z}{\partial \alpha^1}, \frac{\partial z}{\partial \alpha^2}, \frac{\partial z}{\partial \alpha^3}\}$ are also a spanning set. So, for some coefficients A^0, A^a :

$$J^\mu = A^0 \frac{\partial z^\mu}{\partial \lambda} + A^a \frac{\partial z^\mu}{\partial \alpha^a}. \quad (6.6.17)$$

Contracting both sides with $\frac{\partial \lambda}{\partial x^\mu}$ and using the chain rule:

$$J^\mu \frac{\partial \lambda}{\partial x^\mu} = A^0 \frac{\partial z^\mu}{\partial \lambda} \frac{\partial \lambda}{\partial x^\mu} + A^a \frac{\partial z^\mu}{\partial \alpha^a} \frac{\partial \lambda}{\partial x^\mu} = A^0 \frac{\partial \lambda}{\partial \lambda} + A^a \frac{\partial \lambda}{\partial \alpha^a} = A^0. \quad (6.6.18)$$

Or, instead contracting both sides with $\frac{\partial \alpha^a}{\partial x^\mu}$:

$$J^\mu \frac{\partial \alpha^a}{\partial x^\mu} = A^0 \frac{\partial z^\mu}{\partial \lambda} \frac{\partial \alpha^a}{\partial x^\mu} + A^b \frac{\partial z^\mu}{\partial \alpha^b} \frac{\partial \alpha^a}{\partial x^\mu} = A^0 \frac{\partial \alpha^a}{\partial \lambda} + A^b \frac{\partial \alpha^a}{\partial \alpha^b} = A^a. \quad (6.6.19)$$

Additionally, we can compute these contractions using the expression for J^μ (recall that $\epsilon^{0123} = -1$):

$$J^\mu \frac{\partial \lambda}{\partial x^\mu} = -\frac{n_0(\vec{\alpha})}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \lambda}{\partial x^\mu} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} \quad (6.6.20)$$

$$= -n_0(\vec{\alpha}) \epsilon^{\mu\nu\rho\sigma} \frac{\partial \lambda}{\partial x^\mu} \frac{\partial \alpha^1}{\partial x^\nu} \frac{\partial \alpha^2}{\partial x^\rho} \frac{\partial \alpha^3}{\partial x^\sigma} \quad (6.6.21)$$

$$= n_0(\vec{\alpha}) \det \left(\frac{\partial(\lambda, \vec{\alpha})}{\partial X} \right). \quad (6.6.22)$$

$$J^\mu \frac{\partial \alpha^a}{\partial x^\mu} = -\frac{n_0(\vec{\alpha})}{6} \epsilon_{bcd} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \lambda}{\partial x^\mu} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} \frac{\partial \alpha^d}{\partial x^\sigma} = 0. \quad (6.6.23)$$

The last line is 0 because there are not four linearly independent vectors that can be made out of the first derivatives of the α fields (as there are only 3 of them). Returning these expressions to the current density, we have:

$$J^\mu = n_0 \det \left(\frac{\partial(\lambda, \vec{\alpha})}{\partial X} \right) \frac{\partial z^\mu}{\partial \lambda}. \quad (6.6.24)$$

As well, this gives a nice formula for the number density:

$$n = \sqrt{-J^\mu J_\mu} = n_0 \det \left(\frac{\partial(\lambda, \vec{\alpha})}{\partial X} \right) \sqrt{-\frac{\partial z^\mu}{\partial \lambda} \frac{\partial z_\mu}{\partial \lambda}}. \quad (6.6.25)$$

Finally, this gives a simple formula for the Eckart velocity:

$$u^\mu = \frac{J^\mu}{n} = \frac{\frac{\partial z^\mu}{\partial \lambda}}{\sqrt{-\frac{\partial z^\nu}{\partial \lambda} \frac{\partial z_\nu}{\partial \lambda}}}. \quad (6.6.26)$$

The continuity equation determines the evolution of n from u^μ . We need an equation of motion to determine the evolution of u^μ . We can repeat much of the argument given in section 6.2 to identify the form of our transport equations. In fact, the arguments for space translational symmetry, time translational symmetry, and rotational symmetry can be repeated identically and so from section 6.2 we have:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{\rho}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{f}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \hat{\sigma}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.6.27)$$

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \mathcal{E}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \mathcal{P}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \vec{\mathcal{I}}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.6.28)$$

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{j}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{\tau}(t, \vec{x}) d\mathbb{S} + \int_{\partial \mathbb{M}(t)} \hat{M}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.6.29)$$

with the interpretation of each symbol completely unchanged. For Lorentz boost symmetry we will instead

have that the free dynamic energy moment density $\vec{\mathcal{K}}$ satisfies an equation of the form:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} \vec{\mathcal{K}}(t, \vec{x}) d\mathbb{S} = \int_{\mathbb{M}(t)} \vec{B}(t, \vec{x}) d\mathbb{S} + \int_{\partial\mathbb{M}(t)} \hat{N}(t, \vec{x}) \cdot d\vec{\mathbb{A}} \quad (6.6.30)$$

for some vector $\vec{B}$ and tensor $\hat{N}$.

For all of these we can recycle (6.2.8) as it also was true regardless of which theory was used for a general function $g(t, \vec{x})$:

$$\frac{d}{dt} \int_{\mathbb{M}(t)} g(t, \vec{x}) d^3\vec{x} = \int_{\mathbb{M}(t)} \left(\frac{\partial g}{\partial t} + \partial_a (g v^a) \right) d^3\vec{x}. \quad (6.6.31)$$

Therefore, the local versions of our transport equations are only changed to now give:

$$\frac{\partial \mathcal{E}}{\partial t} + \partial_a (\mathcal{E} v^a) = \mathcal{P} + \partial_a \mathcal{I}^a \quad (6.6.32)$$

$$\frac{\partial \wp^a}{\partial t} + \partial_b (\wp^a v^b) = f^a + \partial_b \sigma^{ab} \quad (6.6.33)$$

$$\frac{\partial j^a}{\partial t} + \partial_b (j^a v^b) = \tau^a + \partial_b M^{ab} \quad (6.6.34)$$

$$\frac{\partial \mathcal{K}^a}{\partial t} + \partial_b (\mathcal{K}^a v^b) = B^a + \partial_b N^{ab}. \quad (6.6.35)$$

Like with the Galilean case, let us begin with the last of these. The free dynamic energy moment carried by a mass m is $t\vec{p} - E\vec{x}$ where $E = \sqrt{m^2 + |\vec{p}|^2}$ is the free energy of that mass. Because the dynamic energy moment is a linear function of the momentum and energy, the locally averaged dynamic energy moment density will simply be:

$$\vec{\mathcal{K}} = t\vec{\wp} - \mathcal{E}\vec{x}. \quad (6.6.36)$$

The time derivative of $\vec{\mathcal{K}}$ for a mass under an external force $\vec{F}$ is $t\vec{F} - P\vec{x}$ where $P = \vec{F} \cdot \dot{\vec{x}}$ is the power delivered to the mass by that force. This is also a linear function of the force and power and so behaves well under the local averaging to give that $\vec{B}$ (which is the density corresponding to $\vec{\mathcal{K}}$) and $\hat{N}$ (which is the surface density corresponding to $\vec{\mathcal{K}}$) are:

$$\vec{B} = t\vec{f} - P\vec{x}, \quad \hat{N} \cdot d\vec{\mathbb{A}} = t\hat{\sigma} \cdot d\vec{\mathbb{A}} - \vec{x} \cdot \hat{\mathcal{I}} \cdot d\vec{\mathbb{A}}. \quad (6.6.37)$$

Returning these to equation (6.6.35) gives:

$$\wp^a - \mathcal{E} v^a + \mathcal{I}^a + t \left(\frac{\partial \wp^a}{\partial t} + \partial_b (\wp^a v^b) - \partial_b \sigma^{ab} - f^a \right) - x^a \left(\frac{\partial \mathcal{E}}{\partial t} + \partial_b (\mathcal{E} v^b) - \mathcal{P} - \partial_b \mathcal{I}^b \right) = 0. \quad (6.6.38)$$

Using equations (6.6.32) and (6.6.33) we have:

$$\mathcal{I}^a = \mathcal{E} v^a - \wp^a. \quad (6.6.39)$$

Returning this to equation (6.6.32), it becomes:

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \vec{\wp} = \mathcal{P}. \quad (6.6.40)$$

Therefore, unlike in the Galilean case, Lorentz boost symmetry is insufficient to determine a relationship between $\vec{\wp}$ and $\vec{v}$. Consequently, we must continue to consider them as independent. This can be understood by thinking about the relationship between $\vec{p}$ and $\dot{\vec{x}}$ for a single relativistic particle, $\vec{p} = \frac{m\dot{\vec{x}}}{\sqrt{1-|\dot{\vec{x}}|^2}}$. Because this is a nonlinear function of $\dot{\vec{x}}$, the local average momentum over particles of different velocities will **NOT** be given by $\frac{m\vec{v}}{\sqrt{1-|\vec{v}|^2}}$ because averages and nonlinear functions do not commute. So, there is no reason to believe that $\vec{\wp}$ points in the same direct as the local average velocity. The relationship between $\vec{\wp}$ and $\vec{v}$ is a constitutive relation in the relativistic theory.

The free orbital angular momentum carried by a mass m is $\vec{x} \times \vec{p}$ independent of the theory (as this follows from the fact that orbital angular momentum generates rotations of the position vector). The same scaling argument (up to a single factor of γ) which excluded an independent spin density in the nonrelativistic theory applies to the relativistic case so that again we can simply take:

$$\vec{j} = \vec{x} \times \vec{\wp}. \quad (6.6.41)$$

The torque on a point particle is simply $\vec{x} \times \vec{F}$ where $\vec{F}$ is the force acting on the particle. Therefore, because

this applies locally to each force element, we have:

$$\vec{\tau} = \vec{x} \times \vec{f}, \quad \hat{M} \cdot d\vec{A} = \vec{x} \times (\hat{\sigma} \cdot d\vec{A}). \quad (6.6.42)$$

In components:

$$j^a = \epsilon^a_{bc} x^b \wp^c, \quad \tau^a = \epsilon^a_{bc} x^b f^c, \quad M^{ab} = \epsilon^a_{cd} x^c \sigma^{db}. \quad (6.6.43)$$

Returning these to equation (6.6.34):

$$\epsilon^a_{bc} x^b \left(\frac{\partial \wp^c}{\partial t} + \partial_d (\wp^c v^d) \right) + \epsilon^a_{bc} v^b \wp^c = \epsilon^a_{bc} x^b f^c + \partial_d (\epsilon^a_{bc} x^b \sigma^{cd}). \quad (6.6.44)$$

Because we cannot assume $\vec{\wp}$ and $\vec{v}$ point in the same direction, we cannot set the $\vec{\wp} \times \vec{v}$ term to 0 the way we did in the Galilean case. Now use equation (6.6.33):

$$\implies \epsilon^a_{bc} (\sigma^{bc} + v^b \wp^c) = 0. \quad (6.6.45)$$

Contracting with ϵ_{ade} and simplifying gives that:

$$\sigma^{ab} - \sigma^{ba} = \wp^a v^b - \wp^b v^a. \quad (6.6.46)$$

Hence, in the relativistic case, σ^{ab} will generally not be symmetric. Instead, it is useful to define the symmetric part of σ^{ab} :

$$\sigma_+^{ab} = \frac{\sigma^{ab} + \sigma^{ba}}{2}. \quad (6.6.47)$$

Then, σ^{ab} can be written as:

$$\sigma^{ab} = \frac{\sigma^{ab} + \sigma^{ba}}{2} + \frac{\sigma^{ab} - \sigma^{ba}}{2} = \sigma_+^{ab} + \frac{1}{2} \wp^a v^b - \frac{1}{2} \wp^b v^a. \quad (6.6.48)$$

Returning this equation (6.6.33):

$$\frac{\partial \wp^a}{\partial t} = f^a + \partial_b \left(\sigma_+^{ab} - \frac{\wp^a v^b + \wp^b v^a}{2} \right). \quad (6.6.49)$$

Thus, this is the required form of the moment equation of motion due to rotational symmetry. Because σ_+^{ab} is just some symmetric rotational tensor which needs to be modeled, we can just as usefully define:

$$T^{ab} = -\sigma_+^{ab} + \frac{\wp^a v^b + \wp^b v^a}{2} \quad (6.6.50)$$

as a different symmetric 3x3 rank-2 rotational tensor which needs to modeled, but then our momentum equation is simpler:

$$\frac{\partial \wp^a}{\partial t} = f^a - \partial_b T^{ab}. \quad (6.6.51)$$

Thus (6.6.51) and (6.6.40) are the resultant forms of the energy and momentum transport equations when rotational symmetry and Lorentz boost symmetry are enforced.

Just as with the Galilean case, to further understand the energy and momentum equations of motion it is useful to study their boost properties. Because the volume element dS is not Lorentz invariant, quantities and their densities do not have the same Lorentz transformation properties. However, by using the number density $J^0(t, \vec{x})$, we can make quantities with more familiar transformation properties than energy density or linear momentum density. Let $E_1 = \frac{\mathcal{E}}{J^0}$ be the local average energy density per particle and $\vec{p}_1 = \frac{\vec{\mathcal{E}}}{J^0}$ be the local average linear momentum density per particle. Then, E_1 and $\vec{p}_1$ have the usual Lorentz transformation properties of energy and momentum and so form a four vector p_1^μ :

$$p_1^\mu = (E_1, \vec{p}_1)^\mu, \quad \mathcal{E} = J^0 p_1^0, \quad \wp^a = J^0 p_1^a. \quad (6.6.52)$$

Written in terms of $\vec{p}_1$, T^{ab} becomes:

$$T^{ab} = -\sigma_+^{ab} + \frac{1}{2} (p_1^a J^b + p_1^b J^a). \quad (6.6.53)$$

Then, the energy and momentum transport equations become:

$$\partial_0 (J^0 p_1^0) + \partial_a (J^0 p_1^a) = \mathcal{P} \quad (6.6.54)$$

$$\partial_0 (J^0 p_1^a) + \partial_b \left(-\sigma_+^{ab} + \frac{1}{2} p_1^a J^b + \frac{1}{2} p_1^b J^a \right) = f^a. \quad (6.6.55)$$

The left hand side of the first of these can rewritten as $\partial_\mu (J^0 p_1^\mu)$ which looks like the 0 component of a

covariant equation of motion (which is unsurprising given that this is the energy equation). The right hand side of the second of these can be rewritten as a 4-divergence as well and so let us package these equations into a manifestly covariant form by defining the **energy-momentum tensor** $T^{\mu\nu}$:

$$T^{00} = \mathcal{E}, \quad T^{0a} = T^{a0} = \wp^a, \quad T^{ab} = -\sigma_+^{ab} + \frac{1}{2}(\wp^a v^b + \wp^b v^a) \quad (6.6.56)$$

and the force density 4-vector f^μ :

$$f^0 = \mathcal{P}, \quad f^a = \text{same as before.} \quad (6.6.57)$$

Then, they become:

$$\boxed{\partial_\nu T^{\mu\nu} = f^\mu, \quad T^{\mu\nu} = T^{\nu\mu}.} \quad (6.6.58)$$

If we define σ_+^{ab} to transform as the spatial part of a rank-2 tensor under Lorentz transformations, then $T^{\mu\nu}$ is automatically a symmetric rank-2 tensor. Thus, the Poincare symmetries together require that the transport equations take the form of (6.6.58). For relativistic continuum mechanics the model of the matter in question will determine an explicit formula for the energy-momentum tensor. The fact that the local conservation laws of a Poincare symmetric theory can be cast as a continuity equation for a symmetric energy-momentum tensor should be no surprise given the result of theorem 4.9.

In the nonrelativistic case the instantaneous local rest frame of the matter ($\vec{v} = 0$) and the instantaneous local center of momentum frame ($\vec{\wp} = 0$) coincide. This is not generally true in the relativistic case because the relationship between momentum and velocity for a single particle is nonlinear and so doesn't pass through the averaging over multiple particles in such a simple way. We identified u^μ (the Eckart frame 4-velocity) as the local average 4-velocity of the matter, and therefore it is also the 4-velocity at which the instantaneous local rest frame is moving. The 4-velocity at which the instantaneous local center of momentum frame is moving is called the Landau frame. In the center of momentum frame then, $u_L^\mu = \delta_0^\mu$. As well, in the center of momentum frame:

$$\wp^a = T^{a0} = 0. \quad (\text{center of momentum frame}). \quad (6.6.59)$$

However, in the rest frame, $u^\mu = \delta_0^\mu$ and the momentum density is nonzero. We call that rest frame momentum density q^a :

$$\wp^a = T^{a0} = q^a. \quad (\text{rest frame}). \quad (6.6.60)$$

By (6.6.40), the rest frame momentum density corresponds exactly with the rest frame energy current density which is precisely what we mean by the heat current density. We can then define the vector q^μ so that in the rest frame $q^0 = 0$ and the q^a components are given as above. Then, we can generalize q^μ to an arbitrary frame through boosting. In the rest frame:

$$u \cdot q = 0 \quad (6.6.61)$$

and because this is true in the rest frame and u and q are 4-vectors, this is true in any frame. Therefore, q^μ is the covariant meaning of the heat current density.

Let $\varepsilon = T^{00}$ be the energy density of the matter in the rest frame. Then, it automatically follows that in the rest frame:

$$\varepsilon = T^{\mu\nu} u_\mu u_\nu. \quad (6.6.62)$$

However, the above equation is Lorentz covariant and so because it is true in one frame it is true in any frame. Combining the definitions of ε and q^μ we find

$$T^{\mu\nu} u_\nu = -\varepsilon u^\mu - q^\mu. \quad (6.6.63)$$

in the rest frame and then again in any frame because this equation is Lorentz covariant. Because ε is the energy density of the matter in its rest frame, we can identify it with the rest frame internal energy density $n\mathcal{U}$ where n is the rest frame number density and $\mathcal{U}$ is the thermodynamic internal energy per particle in the rest frame:

$$\varepsilon = n\mathcal{U}. \quad (6.6.64)$$

It is useful to define the projector orthogonal to u^μ :

$$\perp^{\mu\nu} = \eta^{\mu\nu} + u^\mu u^\nu. \quad (6.6.65)$$

This projector when contracted with a vector kills any component of the vector parallel to u^μ and leaves

untouched the pieces orthogonal to u^μ . It satisfies the properties:

$$\perp^{\mu\nu} = \perp^{\nu\mu}, \quad \perp^\mu{}_\mu = 3, \quad \perp^{\mu\nu} u_\nu = 0, \quad \perp^\mu{}_\rho \perp^\rho{}_\nu = \perp^\mu{}_\nu, \quad \perp^\mu{}_\nu q^\nu = q^\mu. \quad (6.6.66)$$

We also define the mechanical pressure P :

$$P = \frac{1}{3} \perp_{\mu\nu} T^{\mu\nu} \quad (6.6.67)$$

and the deviatoric stress tensor:

$$\sigma^{\mu\nu} = - \left(\perp^\mu{}_\rho \perp^\nu{}_\sigma - \frac{1}{3} \perp^{\mu\nu} \perp_{\rho\sigma} \right) T^{\rho\sigma}. \quad (6.6.68)$$

Then:

$$\perp^\mu{}_\rho \perp^\nu{}_\sigma T^{\rho\sigma} = -\sigma^{\mu\nu} + P \perp^{\mu\nu} \quad (6.6.69)$$

$$\sigma^{\mu\nu} = \sigma^{\nu\mu}, \quad \sigma^\mu{}_\mu = 0, \quad \sigma^{\mu\nu} u_\nu = 0. \quad (6.6.70)$$

With $\perp^{\mu\nu}$, we can rewrite $T^{\mu\nu}$ as:

$$T^{\mu\nu} = (\perp^\mu{}_\rho - u^\mu u_\rho) (\perp^\nu{}_\sigma - u^\nu u_\sigma) T^{\rho\sigma} \quad (6.6.71)$$

$$\Rightarrow \boxed{T^{\mu\nu} = n\mathcal{U}u^\mu u^\nu + q^\mu u^\nu + u^\mu q^\nu + P \perp^{\mu\nu} - \sigma^{\mu\nu}}. \quad (6.6.72)$$

It is also useful to decompose the force density 4-vector. Let $\mathfrak{f}^\mu$ be defined so that it is the spatial part of the force density 4-vector in the matter rest frame:

$$\mathfrak{f}^\mu = \perp^\mu{}_\nu f^\nu \quad (6.6.73)$$

and let Φ be defined so that it is the power density delivered to the matter in its rest frame:

$$\Phi = -u_\mu f^\mu. \quad (6.6.74)$$

Thus, Φ is the heat transfer density to the matter and f^μ can be expressed as:

$$\boxed{f^\mu = \mathfrak{f}^\mu + \Phi u^\mu}. \quad (6.6.75)$$

Equations (6.6.72) and (6.6.75) give generic but convenient decompositions of the energy-momentum tensor and force density and (6.6.58) gives the relativistic transport equations. If we want to follow the same thinking used in the nonrelativistic case, in order to complete the set of equations of motion we should find constitutive relations giving $q^\mu, P, \sigma^{\mu\nu}$ in terms of the entropy field $s(X)$ and label fields $\alpha^a(X)$. Unfortunately, this is not as straightforward as in the nonrelativistic case. The key source of this difficulty is that in the nonrelativistic case our constitutive relations expressed the stress tensor in terms of spatial derivatives of our fields; due to Lorentz invariance we can't simply have only spatial derivatives involved in a generic frame. Instead, we can make it a function of only the spatial derivatives in a specific frame and then relate that expression to other frames using Lorentz transformations (which from the perspective of the new frame would make it a function of both spatial and time derivatives). However, when one does so, the wave dispersion relations derived from linearized fluctuations in the resulting equation of motion generically allow faster than light propagation of waves. This should not be surprising as in the nonrelativistic case the Navier-Stokes equations produce the diffusion equation for small fluctuations and our solution to the diffusion equation shows that it propagates infinitely quickly (an infinitely localized Dirac delta in arbitrarily short time becomes a Gaussian which is nonzero at any finite distance). If we apply the same strategy to the relativistic theory then when we expand for small velocities, it will necessarily be equivalent to the nonrelativistic theory at small velocities and so will also have diffusion. While this was not an issue in the nonrelativistic case, in the relativistic theory we know infinite propagation speed is fundamentally at odds with causality. Therefore, the critical difficulty of relativistic continuum mechanics is generalizing the logic used in deriving the Navier-Stokes equations in a Lorentz invariant and causal way.

For an ideal material where we ignore dissipative effects and assume the validity of local thermodynamic equilibrium, we would have $q^\mu = 0$ due to the rotational symmetry of the rest frame, $P = p$ where p is the thermodynamic pressure predicted by $\mathcal{U}$ due to thermodynamic equilibrium, and $\sigma^{\mu\nu}$ be determined by stretch tensors derivatives of $\mathcal{U}$. For non-ideal materials, we will consider only weakly non-ideal materials so that we can take perturbations of these relations:

$$P = p + \Pi, \quad \sigma^{\mu\nu} = \sigma_{\text{ideal}}^{\mu\nu} + d^{\mu\nu} \quad (6.6.76)$$

where $\Pi, q^\mu, d^{\mu\nu}$ are all considered to be of the same order as perturbations. Π is called the dissipative pressure and $d^{\mu\nu}$ is called the dissipative stress. Imposing instantaneous exact constitutive relations for Π, q, d

is a poor approximation because it leads to noncausal diffusion. Instead, in the relativistic theory the most we can ask for is that Π, q, d have equations of motion which relax over time to some constitutive relations. Before looking for such equations of motion, we will study ideal continuum mechanics through a variational principle.

Exercises

Problem 6.15: Consistent use of Pressure. Recall the definition of the pressure on a surface as the force per unit area directed into the surface and that for a force given by a stress tensor $\hat{\sigma}$ onto a surface with unit normal $\vec{n}$ that pressure is given by $-\vec{n} \cdot \hat{\sigma} \cdot \vec{n}$. Show that P as defined in this section is the precisely this pressure in the instantaneous local rest frame of the matter.

Problem 6.16: Soliton Solutions. Many systems admit soliton solutions. A soliton is a solution to the equations of motion which is only nonnegligible in a region of finite size which (at least after a long time) retains its shape and simply moves by translating along in space. Because soliton solutions are localized to a finite region and maintain a steadily moving profile, from far away they essentially appear to look like a point particle. (“Far” here means on a length scale much larger than the size of the region on which the soliton is nonzero.) As an example of a system with solitons, consider the “Sine-Gordon Lagrangian” in 1 spatial dimension:

$$\mathcal{L} = \int_{-\infty}^{\infty} \left(\frac{1}{2} \dot{\phi}^2 - \frac{c^2}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 - \frac{c^2}{\ell^2} (1 - \cos \alpha \phi) \right) \frac{\hbar}{c} dx$$

where $c, \ell, \alpha, \hbar$ are positive constants.

- (a) Show that the equation of motion implied by the above Lagrangian is the Sine-Gordon equation:

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} + \frac{\alpha c^2}{\ell^2} \sin(\alpha \phi) = 0.$$

- (b) Show that if c is interpreted as the speed of light (which we will do so for the rest of this question) and ϕ is taken as a Lorentz invariant scalar function then the Sine-Gordon Lagrangian has Lorentz boost symmetry.
- (c) We will now look for a soliton solution which moves to the right with velocity v . Explain that a function $\phi(t, x)$ which moves with velocity v at fixed shape can be written as a function of only $x - vt$. For γ an at the moment unchosen factor, consider a solution:

$$\phi(t, x) = \psi(\gamma(x - vt))$$

for some function ψ . Show that if γ is chosen to be the usual Lorentz factor for v , then $\psi(y)$ satisfies the equation:

$$\frac{\partial^2 \psi(y)}{\partial y^2} = \frac{\alpha}{\ell^2} \sin(\alpha \psi(y)).$$

- (d) Assume that ψ is a solution to the above equation. Show that in the rest frame of the solution ($v = 0$ frame), the energy density of the solution is:

$$\mathcal{E}(x) = \frac{\hbar c}{2} \left(\frac{\partial \psi(x)}{\partial x} \right)^2 + \frac{\hbar c}{\ell^2} (1 - \cos(\alpha \psi)).$$

Thus explain that if the solution is to be a soliton (and so have localized energy density), at large $|x|$ we must have ψ limit to $\frac{2\pi n}{\alpha}$ for some integer n . (The value of n for $x \rightarrow \infty$ and the value for $x \rightarrow -\infty$ do not need to be the same.)

- (e) With the established boundary conditions, solve the equations for ψ to show:

$$\psi(y) = \frac{4}{\alpha} \arctan \left(e^{\frac{\alpha \sigma}{\ell} (y - y_0)} \right) + \frac{4\pi n}{\alpha}$$

where $\sigma \in \pm 1$, y_0 is a constant real number, and n is a constant integer.

- (f) Show that in the rest frame the energy density of this solution is:

$$\mathcal{E}(x) = \frac{4\hbar c}{\ell^2 \cosh^2 \left(\frac{\alpha(x - y_0)}{\ell} \right)}.$$

Explain that this energy density decays exponentially to 0 away from $x = y_0$ with a characteristic length

scale $\frac{\ell}{\alpha}$. As well, show that the total energy of the solution in the rest frame is:

$$E = \frac{8\hbar c}{\ell\alpha}.$$

- (g) Show that in a general frame (by computing the total energy and linear momentum of the field ϕ from the original Sine-Gordon Lagrangian) the energy and linear momentum of the soliton are:

$$E = \frac{8\hbar c}{\ell\alpha}\gamma, \quad p = \frac{8\hbar}{\ell\alpha c}\gamma v.$$

Explain that these results shown that on length scales much larger than $\frac{\ell}{\alpha}$ the soliton is effectively a free relativistic point particle with mass:

$$m = \frac{8\hbar}{\ell\alpha c}.$$

- (h) Consider time and spatial translations of ϕ to find expressions for the energy and momentum density for this theory. Show that they satisfy continuity equations and that they can be packaged into:

$$\partial_\nu T^{\mu\nu} = 0$$

where the energy-momentum tensor of the theory is given by:

$$T_{\mu\nu} = \hbar\partial_\mu\phi\partial_\nu\phi - \frac{\hbar}{2}\left(\partial^\rho\phi\partial_\rho\phi + \frac{4}{\ell^2}\sin^2\left(\frac{\alpha\phi}{2}\right)\right)\eta_{\mu\nu}.$$

- (i) Show that in a general frame for the soliton solution the energy-momentum tensor becomes:

$$T_{\mu\nu} = \frac{4\hbar u_\mu u_\nu}{\ell^2 \cosh^2\left(\frac{\alpha}{\ell}(y - y_0)\right)}$$

where u^μ is the proper velocity (2-velocity in this case due to the single spatial dimension) of the soliton.

6.7 Relativistic Ideal Continuum Mechanics

Suppose we have a material consisting of N identical relativistic particles. By theorem 4.8, we can (and do) choose the microscopic action of the particles to be invariant under the connected Poincare group. Let $\mathcal{U}$ be the thermodynamic internal energy per particle in the center of momentum frame. Then, let $\mathcal{L}_0$ be the value of a single particle's Lagrangian in its center of momentum frame and consider for a moment all of the particles to have the same velocity. Then, the total Lagrangian in the center of momentum (COM) frame would be:

$$\mathcal{L}_{\text{COM}} = N\mathcal{L}_0. \quad (6.7.1)$$

Suppose we now Lorentz boost to a frame so that now all the particles are moving at velocity $\dot{\vec{x}}$. Then, due to the Lorentz invariance of the action:

$$S = S_{\text{COM}} \implies \int \mathcal{L} dt = \int \mathcal{L}_{\text{COM}} d\tau \implies \mathcal{L} = \mathcal{L}_{\text{COM}} \frac{d\tau}{dt} \quad (6.7.2)$$

where we identified that the proper time element $d\tau = dt_{\text{COM}}$. Then, using the definition of the proper time:

$$\mathcal{L} = N\mathcal{L}_0 \sqrt{1 - |\dot{\vec{x}}|^2}. \quad (6.7.3)$$

From here using the Legendre transformation the energy of the system is immediately:

$$E = \frac{\partial \mathcal{L}}{\partial \dot{\vec{x}}} \cdot \dot{\vec{x}} - \mathcal{L} = -\frac{N\mathcal{L}_0}{\sqrt{1 - |\dot{\vec{x}}|^2}}. \quad (6.7.4)$$

In the center of momentum frame, necessarily $E = N\mathcal{U}$. Therefore:

$$E_{\text{COM}} = N\mathcal{U} = -N\mathcal{L}_0 \implies \mathcal{L}_0 = -\mathcal{U}. \quad (6.7.5)$$

Thus:

$$\mathcal{L}_{\text{COM}} = -N\mathcal{U}. \quad (6.7.6)$$

If we now consider a density of particles with center of momentum frame number density n with a locally well-defined velocity field, then it immediately follows that the Lagrangian density is:

$$\mathcal{L} = -n\mathcal{U}. \quad (6.7.7)$$

The right hand side is automatically Lorentz invariant, so this Lagrangian density is Lorentz invariant as well.

Based on the above analysis, (6.7.7) is the appropriate Lagrangian density for any relativistic material which locally has a well defined velocity field and thus it is what we use for relativistic ideal continuum mechanics. Here by ideal we mean that no dissipative effects have been included. Such effects will change the microscopic velocity distribution and cause a difference between the Eckart and Landau velocities in general, interfering with the idea of a well defined velocity field. Our ability to apply the single particle analysis to the multi-particle averaging without fluctuations requires that q^μ is 0. Because no dissipative effects are included, the entropy field $s(X)$ satisfies:

$$\frac{d}{dt}s(X) = \frac{\partial s}{\partial t} + v^a \frac{\partial s}{\partial x^a} = 0. \quad (6.7.8)$$

Therefore:

$$\frac{\partial}{\partial \lambda}s(X) = \frac{\partial z^\mu}{\partial \lambda} \frac{\partial s}{\partial x^\mu} = \sqrt{-\frac{\partial z^\nu}{\partial \lambda} \frac{\partial z_\nu}{\partial \lambda}} u^0 \left(\frac{\partial s}{\partial t} + v^a \frac{\partial s}{\partial x^a} \right) = 0 \quad (6.7.9)$$

$$\implies s(X) = s_0(\vec{\alpha}(X)) \quad (6.7.10)$$

for some function $s_0(\vec{\alpha}(X))$.

Just as with the nonrelativistic case, for a general ideal material $\mathcal{U}$ can depend on the invariants of the stretch tensor. To understand how to do this, we need the appropriate relativistic definition of the stretch tensor. Because distances are not Lorentz invariant, to properly define the stretch tensor we need to consider the stretching of proper distances under deformations of the body. To do so, we can consider distances measured locally in the body's instantaneous local rest frame. The label distance is by definition:

$$ds_0^2 = \delta_{ab} d\alpha^a d\alpha^b = \delta_{ab} \frac{\partial \alpha^a}{\partial x^\mu} \frac{\partial \alpha^b}{\partial x^\nu} dx^\mu dx^\nu. \quad (6.7.11)$$

In the body's instantaneous local rest frame, $\frac{\partial \alpha^a}{\partial x^0} = 0$ and so:

$$ds_0^2 \stackrel{IRF}{=} \delta_{ab} \frac{\partial \alpha^a}{\partial x^c} \frac{\partial \alpha^b}{\partial x^d} dx^c dx^d. \quad (6.7.12)$$

Therefore, we have that in the rest frame the stretch tensor is given by:

$$C_{00} = 0, \quad C_{0a} = C_{a0} = 0, \quad C_{ab} = \delta_{cd} \frac{\partial \alpha^c}{\partial x^a} \frac{\partial \alpha^d}{\partial x^b}. \quad (6.7.13)$$

This can be written as:

$$C_{\mu\nu} = (\delta_\mu^\rho + u^\rho u_\mu)(\delta_\nu^\sigma + u^\sigma u_\nu) \delta_{ab} \frac{\partial \alpha^a}{\partial x^\rho} \frac{\partial \alpha^b}{\partial x^\sigma}. \quad (6.7.14)$$

Because everything in the above expression transforms appropriately as a tensor, it is true in all reference frames. Thus, the above serves as the appropriate relativistic generalization of the stretch tensor. Just as with the nonrelativistic case, there are 3 nontrivial invariants that can be made out of the stretch tensor and 1 of them is unnecessary as it is determined by the number density n . So, we define:

$$C^{(1)} = \eta^{\mu\nu} C_{\mu\nu}, \quad C^{(2)} = C^{\mu\nu} C_{\mu\nu}. \quad (6.7.15)$$

One can quickly see that in the local instantaneous rest frame these reproduce the nonrelativistic quantities for which we used the same symbols. As well, the determinant of the spatial part C_{ab} in the rest frame is related to the number density in the same way as the nonrelativistic case.

Altogether, these results give us that for an ideal material:

Theorem 6.10: Passive Relativistic Ideal Continuum Mechanics

The action for a relativistic ideal material in the passive formulation is:

$$S[\vec{\alpha}] = \int (-n\mathcal{U}(n, C^{(1)}, C^{(2)}, s_0(\vec{\alpha}))) + qJ^\mu A_\mu d^4x \quad (6.7.16)$$

where q is the charge per particle, $\mathcal{U}$ is the thermodynamic internal energy in the local instantaneous rest frame, J^μ is the number current density given by:

$$J^\mu(X) = -\frac{n_0(\vec{\alpha})}{6} \epsilon_{abc} \epsilon^{\mu\nu\rho\sigma} \frac{\partial \alpha^a}{\partial x^\nu} \frac{\partial \alpha^b}{\partial x^\rho} \frac{\partial \alpha^c}{\partial x^\sigma} \quad (6.7.17)$$

where $n_0(\vec{\alpha})$ is number density of the material in a given default configuration, $s_0(\vec{\alpha})$ is the entropy per particle, $n(X)$ is the rest frame number density given by:

$$n = \sqrt{-J^\mu J_\mu}, \quad (6.7.18)$$

the Eckart velocity u^μ is given by:

$$u^\mu = \frac{J^\mu}{n}, \quad (6.7.19)$$

the stretch tensor is given by:

$$C_{\mu\nu} = (\delta_\mu^\rho + u^\rho u_\mu)(\delta_\nu^\sigma + u^\sigma u_\nu) \delta_{ab} \frac{\partial \alpha^a}{\partial x^\rho} \frac{\partial \alpha^b}{\partial x^\sigma}. \quad (6.7.20)$$

and the stretch tensor invariants are given by:

$$C^{(1)} = \eta^{\mu\nu} C_{\mu\nu}, \quad C^{(2)} = C^{\mu\nu} C_{\mu\nu}. \quad (6.7.21)$$

We can also express our action in active coordinates (in terms of the covariant position fields) by using that:

$$d^4x = \det \left(\frac{\partial z}{\partial(\lambda, \alpha)} \right) d^3\vec{\alpha} d\lambda. \quad (6.7.22)$$

In order to express the action in these coordinates, it would be more convenient to find an appropriate active expression for the invariants of the stretch tensor or for an equivalent set of quantities so that we don't have to rely on the matrix inverse $\frac{\partial \alpha}{\partial x}$ (as in active coordinates $\frac{\partial z}{\partial \alpha}$ is much more easily available). This is easily done by noting that the invariants of matrix can be related to the invariants of its inverse, and so let us define the inverse stretch tensor so that in the rest frame:

$$G^{00} = 0, \quad G^{0a} = G^{a0} = 0, \quad G^{ab} = \delta^{cd} \frac{\partial z^a}{\partial \alpha^c} \frac{\partial z^b}{\partial \alpha^d}. \quad (6.7.23)$$

In the rest frame then the spatial part of G^{ab} is the matrix inverse of C_{ab} . In a general frame this can be written:

$$G^{\mu\nu} = (\delta_\rho^\mu + u^\mu u_\rho)(\delta_\sigma^\nu + u^\nu u_\sigma) \delta^{ab} \frac{\partial z^\rho}{\partial \alpha^a} \frac{\partial z^\sigma}{\partial \alpha^b}. \quad (6.7.24)$$

And, the three nontrivial invariants that can be made out of $G^{\mu\nu}$ contain equivalent information to those that can be made out of $C_{\mu\nu}$ and can be parameterized by the number density n and $G^{(1)}$ and $G^{(2)}$ defined by:

$$G^{(1)} = \eta_{\mu\nu} G^{\mu\nu}, \quad G^{(2)} = G^{\mu\nu} G_{\mu\nu}. \quad (6.7.25)$$

Thus, in active coordinates:

Theorem 6.11: Active Relativistic Ideal Continuum Mechanics

The action for a relativistic ideal material in the active formulation is:

$$S[Z] = \int \left(-\mathcal{U}(n, G^{(1)}, G^{(2)}, s_0) \sqrt{-\frac{\partial z^\mu}{\partial \lambda} \frac{\partial z_\mu}{\partial \lambda}} + q A_\mu \frac{\partial z^\mu}{\partial \lambda} \right) n_0(\vec{\alpha}) d^3 \vec{\alpha} d\lambda \quad (6.7.26)$$

where q is the charge per particle, $\mathcal{U}$ is the thermodynamic internal energy in the local instantaneous rest frame, $n_0(\vec{\alpha})$ is number density of the material in a given default configuration, $s_0(\vec{\alpha})$ is the entropy per particle, $n(X)$ is the rest frame number density given by:

$$n = \frac{n_0}{\det \left(\frac{\partial z}{\partial(\lambda, \vec{\alpha})} \right)} \sqrt{-\frac{\partial z^\mu}{\partial \lambda} \frac{\partial z_\mu}{\partial \lambda}}, \quad (6.7.27)$$

the Eckart velocity u^μ is given by:

$$u^\mu = \frac{\frac{\partial z^\mu}{\partial \lambda}}{\sqrt{-\frac{\partial z^\nu}{\partial \lambda} \frac{\partial z_\nu}{\partial \lambda}}}, \quad (6.7.28)$$

the inverse stretch tensor is given by:

$$G^{\mu\nu} = (\delta_\rho^\mu + u^\mu u_\rho)(\delta_\sigma^\nu + u^\nu u_\sigma) \delta^{ab} \frac{\partial z^\rho}{\partial \alpha^a} \frac{\partial z^\sigma}{\partial \alpha^b}. \quad (6.7.29)$$

and the stretch tensor invariants are given by:

$$G^{(1)} = \eta_{\mu\nu} G^{\mu\nu}, \quad G^{(2)} = G^{\mu\nu} G_{\mu\nu}. \quad (6.7.30)$$

Exercises

Problem 6.17: ★ Relativistic Perfect Fluids. Consider a relativistic ideal continuum mechanical system with a thermodynamic internal energy per particle that depends only on the stretch tensor through the number density so that $\mathcal{U} = \mathcal{U}(n, s)$.

- (a) Show using either the active formulation or the passive formulation of the action that the equation of motion for the fluid becomes:

$$\partial_\nu ((p + n\mathcal{U})u^\mu u^\nu + p\eta^{\mu\nu}) = qn\mathcal{F}_{\mu\nu}u^\nu$$

where $p = n^2 \frac{\partial \mathcal{U}}{\partial n}$ is the thermodynamic pressure of the fluid.

- (b) Show that the energy-momentum tensor of the perfect fluid is:

$$T^{\mu\nu} = (p + n\mathcal{U})u^\mu u^\nu + p\eta^{\mu\nu}.$$

- (c) Assume that the field strength $\mathcal{F}_{\mu\nu}$ satisfies Maxwell's equations with the source current due to the fluid. Show that the combined system satisfies conservation of energy and momentum:

$$\partial_\nu T_{\text{total}}^{\mu\nu} = 0$$

with the combined energy-momentum tensor:

$$T_{\text{total}}^{\mu\nu} = (p + n\mathcal{U})u^\mu u^\nu + p\eta^{\mu\nu} - \mathcal{F}^\mu{}_\rho \mathcal{F}^{\rho\nu} - \frac{1}{4} \eta^{\mu\nu} \mathcal{F}^{\rho\sigma} \mathcal{F}_{\rho\sigma}.$$

Explain using what we have previously found about the electromagnetic energy-momentum tensor why this result is what you should have expected.

Problem 6.18: Relativistic Perfect Gas. Consider a relativistic perfect fluid so that the microscopic Hamiltonian for each particle is simply $\mathcal{H} = \sqrt{|\vec{p}|^2 + m^2}$.

- (a) Using the result of problem 5.43 show that the entropy per particle is:

$$s = 2 + \ln \left(\frac{m^2 T}{2\pi^2 \hbar^3 n} K_2 \left(\frac{m}{T} \right) \right) - \frac{m}{T} \frac{K'_2 \left(\frac{m}{T} \right)}{K_2 \left(\frac{m}{T} \right)}$$

that the pressure is:

$$p = nT$$

and that the internal energy per particle is:

$$\mathcal{U} = T - m \frac{K'_2 \left(\frac{m}{T} \right)}{K_2 \left(\frac{m}{T} \right)}.$$

- (b) The entropy formula is prohibitively complicated so that inverting it by hand is impossible. Instead, we can find an equation relating the temperature to the number density using that the entropy is constant. In particular, show that for a function $A(\vec{\alpha})$:

$$n = A(\vec{\alpha}(X)) T K_2 \left(\frac{m}{T} \right) e^{-\frac{m}{T} \frac{K'_2 \left(\frac{m}{T} \right)}{K_2 \left(\frac{m}{T} \right)}}.$$

Show that this combined with the found constitutive relations for p and $\mathcal{U}$ in terms of n and T and the equation of motion found for the relativistic perfect fluid completes the system of equations of motion for the relativistic perfect gas (these equations together are enough to determine the full time evolution of the system in principle). While explicitly inverting the entropy formula in terms of elementary functions is impossible, it is also rarely needed. Even when the gas is moving relativistically (so that u^a is large), in most real physical scenarios the temperature of the gas is low enough (compared to mc^2) that one can essentially use the nonrelativistic expression for the free energy.

6.8 Relativistic Dissipative Continuum Mechanics

Let us now consider perturbations of ideal continuum mechanics, so that Π, q, d are not assumed to be 0. Here our analysis will closely follow chapter 6 of [95]. It is useful to define some notation for making equations as simple as possible. Define the field $\theta(X)$ as the divergence of the velocity field:

$$\theta = \partial_\mu u^\mu. \quad (6.8.1)$$

For a generic field $\phi(X)$, define $\dot{\phi}$ to mean the derivative of ϕ in the direction of the velocity:

$$\dot{\phi}(X) = u^\mu \partial_\mu \phi. \quad (6.8.2)$$

In the instantaneous local rest frame of the matter $\dot{\phi}$ coincides with $\partial_t \phi(t, \vec{x})$. For a generic field $\phi_{\nu_1 \dots \nu_n}$ which is allowed to be a tensor field, define the projected derivative $\mathcal{D}_\mu \phi_{\nu_1 \dots \nu_n}$ by projecting the derivative and all of the components of ϕ into the spatial directions in the local rest frame:

$$\mathcal{D}_\mu \phi_{\nu_1 \dots \nu_n} = \perp^\rho_\mu \perp^{\sigma_1}_{\nu_1} \dots \perp^{\sigma_n}_{\nu_n} \partial_\rho \phi_{\sigma_1 \dots \sigma_n}. \quad (6.8.3)$$

This object has the advantage that it gives 0 when any index is contracted with u^μ . Finally, for a rank-2 tensor $\phi_{\mu\nu}$ we define $\langle \phi_{\mu\nu} \rangle$ to mean the symmetric traceless spatial part of $\phi_{\mu\nu}$:

$$\langle \phi_{\mu\nu} \rangle = \left(\frac{1}{2} \perp^\rho_\mu \perp^\sigma_\nu + \frac{1}{2} \perp^\rho_\nu \perp^\sigma_\mu - \frac{1}{3} \perp^{\rho\sigma} \perp_{\mu\nu} \right) \phi_{\rho\sigma}. \quad (6.8.4)$$

This quantity is useful because $\sigma^{\mu\nu}$ is symmetric and traceless and so $\sigma^{\mu\nu} \phi_{\mu\nu} = \sigma^{\mu\nu} \langle \phi_{\mu\nu} \rangle$ for all $\phi_{\mu\nu}$.

Beginning with (6.6.72) (recalling $\varepsilon = n\mathcal{U}$) applying some labor to put everything into the additional notation defined above, we find that:

$$\partial_\nu T^{\mu\nu} = u^\mu (\dot{\varepsilon} + (\varepsilon + P)\theta + \mathcal{D}_\nu q^\nu + q^\nu \dot{u}_\nu - \sigma^{\alpha\beta} \langle \mathcal{D}_\alpha u_\beta \rangle) \quad (6.8.5)$$

$$+ (\varepsilon + P)\dot{u}^\mu + \dot{q}^\mu + \theta q^\mu + q^\nu \mathcal{D}_\nu u^\mu + \mathcal{D}^\mu P - \mathcal{D}_\nu \sigma^{\mu\nu} - \sigma^{\mu\nu} \dot{u}_\nu. \quad (6.8.6)$$

Contracting this with u_μ and using (6.6.58) gives:

$$\dot{\varepsilon} + (\varepsilon + P)\theta + \mathcal{D}_\mu q^\mu + 2q^\mu \dot{u}_\mu - \sigma^{\mu\nu} \langle \mathcal{D}_\mu u_\nu \rangle = \Phi. \quad (6.8.7)$$

Alternatively contracting with $\perp^\rho_\mu$ gives:

$$(\varepsilon + P)\dot{u}^\mu + \perp^\mu_\nu \dot{q}^\nu + \theta q^\mu + q^\nu \mathcal{D}_\nu u^\mu + \mathcal{D}^\mu P - \mathcal{D}_\nu \sigma^{\mu\nu} - \sigma^{\mu\nu} \dot{u}_\nu = \mathfrak{f}^\mu. \quad (6.8.8)$$

Equation (6.8.7) then gives the covariant form of energy conservation while (6.8.8) gives the covariant form of momentum conservation. Using that $\varepsilon = n\mathcal{U}$ and the continuity equation for n gives:

$$\dot{\varepsilon} = -\varepsilon\theta + n\dot{\mathcal{U}}. \quad (6.8.9)$$

The thermodynamic internal energy will be a function of the entropy per particle s , the number density n , and the stretch tensor $G^{\mu\nu}$. Then:

$$\dot{\mathcal{U}} = \frac{\partial \mathcal{U}}{\partial s} \dot{s} + \frac{\partial \mathcal{U}}{\partial n} \dot{n} + \frac{\partial \mathcal{U}}{\partial G^{\mu\nu}} \dot{G}^{\mu\nu} = T\dot{s} - p\theta + \frac{\partial \mathcal{U}}{\partial G^{\mu\nu}} \dot{G}^{\mu\nu} \quad (6.8.10)$$

where we have recalled the definition of the temperature T and the thermodynamic pressure p and used the continuity equation for n . The evolution of the stretch tensor cancels against its contribution to the ideal stress $\sigma_{\text{ideal}}^{\mu\nu}$ (as that is what precisely is meant by the ideal part of the stress) when returned to the energy equation. Therefore, returning this to (6.8.7) gives:

$$nT\dot{s} = \Phi - \Pi\theta - \mathcal{D}_\mu q^\mu - 2q^\mu \dot{u}_\mu + d^{\mu\nu} \langle \mathcal{D}_\mu u_\nu \rangle. \quad (6.8.11)$$

At this point we will begin attempting to model the non-ideal variables Π, q, d . Each matter element in the material will have some entropy from averaging over internal degrees of freedom in that matter element. In a particular frame, we define J_s^0 as the entropy density in that frame. As matter moves in space, there will be some flux of entropy across any given surface, due to both the transfer of particles and the change of matter element entropies during interactions. Therefore, there will be some spatial current density. J_s^a of entropy. Because entropy is Lorentz invariant (it is defined as a phase space integral of an integrand involving only the phase space density and both the phase space density and the phase space measure are Lorentz invariant as a Lorentz transformation is a canonical transformation), the entropy current density $J_s^\mu = (J_s^0, J_s^a)$ is a proper 4-vector. Letting s be the equilibrium entropy per particle, for an ideal material where we can identify the local velocity of each particle with the velocity field, the entropy current density is then simply proportional to the number current density so that $J_s^\mu = s n u^\mu$. For non-ideal matter, instead

the entropy current will differ and so take the form:

$$J_s^\mu = snu^\mu + \frac{R^\mu}{T} \quad (6.8.12)$$

for some vector R^μ . The factor of temperature has been added for convenience. This equation essentially has no content as for any given J_s^μ one can define R^μ to be whatever makes this equation true. Our modeling comes in trying to identify an explicit formula for R^μ . So, we will try form a reasonable constitutive relation for R^μ using the principles of effective theory.

Let S_E be the entropy density in the matter's local instantaneous rest frame:

$$S_E = -u_\mu J_s^\mu = sn - \frac{u_\mu R^\mu}{T}. \quad (6.8.13)$$

Local thermodynamic equilibrium will occur when S_E is maximized. Because the non-ideal quantities represent deviations from local thermodynamic equilibrium (as the ideal action is perfectly capable of describing the quasidynamic case), S_E must be maximized when Π, q, d vanish. Further, as J_s^0 is the entropy density in a given frame of reference, the entropy $S[\mathbb{M}]$ in a volume $\mathbb{M}$ is given by:

$$S[\mathbb{M}] = \int_{\mathbb{M}} J_s^0 d\mathbb{S}. \quad (6.8.14)$$

Then, the rate of entropy production $\Gamma[\mathbb{M}]$ in the region $\mathbb{M}$, defined by the rate of change of entropy in $\mathbb{M}$ plus the net flux of entropy out of $\mathbb{M}$, is given by:

$$\Gamma[\mathbb{M}] = \frac{dS[\mathbb{M}]}{dt} + \int_{\partial\mathbb{M}} \vec{J}_s \cdot d\vec{\mathbb{A}} = \int_{\mathbb{M}} \partial_\mu J_s^\mu d\mathbb{S}. \quad (6.8.15)$$

Hence, $\partial_\mu J_s^\mu$ measures the local rate of entropy production per unit volume. Due to the second law of thermodynamics, because we are persistently averaging over local degrees of freedom and insensitive to all developing cross particle correlations, the local entropy production due to being out of thermodynamic equilibrium must be positive. Because we allow for a heat transfer density Φ to our matter, which automatically causes an entropy production density of $\frac{\Phi}{T}$, this means we must have:

$$\partial_\mu J_s^\mu \geq \frac{\Phi}{T} \quad (6.8.16)$$

with equality only occurring in local thermodynamic equilibrium (when Π, q, d vanish).

Let us now explicitly try to develop a constitutive relation for R^μ . It represents deviation from thermodynamic equilibrium and so must be some function of the dissipative fluxes Π, q, d (and the equilibrium ideal quantities). Through the second order in the dissipative fluxes, the most generic Lorentz covariant expression for R^μ is:

$$R^\mu = f_0 \Pi u^\mu + f_1 q^\mu + \alpha_0 \Pi q^\mu - \alpha_1 d^{\mu\nu} q_\nu - \frac{1}{2} (\beta_0 \Pi^2 + \beta_1 q_\nu q^\nu + \beta_2 d^{\alpha\beta} d_{\alpha\beta}) u^\mu \quad (6.8.17)$$

for some scalar functions $f_0, f_1, \alpha_0, \alpha_1, \beta_0, \beta_1, \beta_2$ of only the equilibrium quantities. Here we have excluded the possibility of derivatives of dissipative fluxes as a modeling assumption, but they could be included in principle. With this formula for R^μ , the resulting rest frame entropy density is:

$$S_E = sn + \frac{f_0}{T} \Pi - \frac{1}{2T} (\beta_0 \Pi^2 + \beta_1 q_\nu q^\nu + \beta_2 d^{\alpha\beta} d_{\alpha\beta}). \quad (6.8.18)$$

In order for the equilibrium state $\Pi = 0, q = 0, d = 0$ to be stable, it must be the maximum of this function and so requires that the derivative of S_E with respect to each of these fluxes vanishes in equilibrium and that S_E is concave down at that point:

$$f_0 = 0, \quad \beta_0 \geq 0, \quad \beta_1 \geq 0, \quad \beta_2 \geq 0. \quad (6.8.19)$$

q^μ is intended to represent the heat current density, and so in the rest frame to lowest order in the thermodynamic fluxes, $J_s^a = \frac{q^a}{T}$ in the rest frame of the matter. This requires:

$$f_1 = 1. \quad (6.8.20)$$

Now let us compute the entropy production rate determined by R^μ . Directly differentiating:

$$\begin{aligned} T \partial_\mu J_s^\mu &= nT \dot{s} + \partial_\mu q^\mu - q^\mu \partial_\mu \ln T + T \partial_\mu \left(\frac{\alpha_0}{T} \right) \Pi q^\mu + \alpha_0 q^\mu \partial_\mu \Pi + \alpha_0 \Pi \partial_\mu q^\mu \\ &\quad - T \partial_\mu \left(\frac{\alpha_1}{T} \right) d^{\mu\nu} q_\nu - \alpha_1 \partial_\nu d^{\mu\nu} q_\mu - \alpha_1 d^{\mu\nu} \langle \partial_\mu q_\nu \rangle - T \partial_\mu \left(\frac{\beta_0 u^\mu}{2T} \right) \Pi^2 - \beta_0 \Pi \dot{\Pi} \end{aligned}$$

$$-T\partial_\mu \left(\frac{\beta_1 u^\mu}{2T} \right) q_\nu q^\nu - \beta_1 q_\nu \dot{q}^\nu - T\partial_\mu \left(\frac{\beta_2 u^\mu}{2T} \right) d^{\alpha\beta} d_{\alpha\beta} - \beta_2 d^{\mu\nu} \dot{d}_{\mu\nu}. \quad (6.8.21)$$

Now using (6.8.11), doing a bit of algebra and organization, we find:

$$\begin{aligned} T\partial_\mu J_s^\mu &= \Phi - \Pi \left(\theta - \gamma_0 T \mathcal{D}_\mu \left(\frac{\alpha_0}{T} \right) q^\mu - \alpha_0 \mathcal{D}_\mu q^\mu - \gamma_1 \alpha_0 q^\mu \dot{u}_\mu + T\partial_\mu \left(\frac{\beta_0 u^\mu}{2T} \right) \Pi + \beta_0 \dot{\Pi} \right) \\ &\quad - q^\mu \left(\dot{u}_\mu + \mathcal{D}_\mu \ln T - (1 - \gamma_0) T \mathcal{D}_\mu \left(\frac{\alpha_0}{T} \right) \Pi - \alpha_0 \mathcal{D}_\mu \Pi - (1 - \gamma_1) \alpha_0 \Pi \dot{u}_\mu \right. \\ &\quad \left. + (1 - \gamma_2) T \mathcal{D}^\nu \left(\frac{\alpha_1}{T} \right) d_{\mu\nu} + \alpha_1 \mathcal{D}^\nu d_{\mu\nu} + (1 - \gamma_3) \alpha_1 d_{\mu\nu} \dot{u}^\nu + T\partial_\nu \left(\frac{\beta_1 u^\nu}{2T} \right) q_\mu + \beta_1 \dot{q}_\mu \right) \\ &\quad - d^{\mu\nu} \left\langle -\mathcal{D}_\mu u_\nu + \gamma_2 T \mathcal{D}_\mu \left(\frac{\alpha_1}{T} \right) q_\nu + \gamma_3 \alpha_1 q_\mu \dot{u}_\nu + \alpha_1 \mathcal{D}_\mu q_\nu + T\partial_\rho \left(\frac{\beta_2 u^\rho}{2T} \right) d_{\mu\nu} + \beta_2 \dot{d}_{\mu\nu} \right\rangle \end{aligned} \quad (6.8.22)$$

where the functions $\gamma_0, \gamma_1, \gamma_2, \gamma_3$ are completely arbitrary functions of the equilibrium quantities due to the nonuniqueness of the way we have organized this equation. In order to guarantee that the entropy production satisfies (6.8.16) for all field configurations, we need each independent term here to be nonnegative. Therefore, keeping to the lowest order effective theory that makes this true, we require that for some choice of the γ coefficients and for some functions κ, μ, ζ of the equilibrium quantities:

$$\Pi = -\zeta \left(\theta - \gamma_0 T \mathcal{D}_\mu \left(\frac{\alpha_0}{T} \right) q^\mu - \alpha_0 \mathcal{D}_\mu q^\mu - \gamma_1 \alpha_0 q^\mu \dot{u}_\mu + T\partial_\mu \left(\frac{\beta_0 u^\mu}{2T} \right) \Pi + \beta_0 \dot{\Pi} \right) \quad (6.8.23)$$

$$\begin{aligned} q_\mu &= -\kappa \left(\dot{u}_\mu + \mathcal{D}_\mu \ln T - (1 - \gamma_0) T \mathcal{D}_\mu \left(\frac{\alpha_0}{T} \right) \Pi - \alpha_0 \mathcal{D}_\mu \Pi - (1 - \gamma_1) \alpha_0 \Pi \dot{u}_\mu \right. \\ &\quad \left. + (1 - \gamma_2) T \mathcal{D}^\nu \left(\frac{\alpha_1}{T} \right) d_{\mu\nu} + \alpha_1 \mathcal{D}^\nu d_{\mu\nu} + (1 - \gamma_3) \alpha_1 d_{\mu\nu} \dot{u}^\nu + T\partial_\nu \left(\frac{\beta_1 u^\nu}{2T} \right) q_\mu + \beta_1 \dot{q}_\mu \right) \end{aligned} \quad (6.8.24)$$

$$d_{\mu\nu} = -2\mu \left(-\langle \mathcal{D}_\mu u_\nu \rangle + \gamma_2 T \langle \mathcal{D}_\mu \left(\frac{\alpha_1}{T} \right) q_\nu \rangle + \gamma_3 \alpha_1 \langle q_\mu \dot{u}_\nu \rangle + \alpha_1 \langle \mathcal{D}_\mu q_\nu \rangle + T\partial_\rho \left(\frac{\beta_2 u^\rho}{2T} \right) d_{\mu\nu} + \beta_2 \dot{d}_{\mu\nu} \right). \quad (6.8.25)$$

The coefficients ζ, κ, μ are the relativistic analogs of the bulk viscosity, thermal conductivity, and dynamic viscosity (which is why we have retained the same notation for them). Notice that each of these contains a linearly independent use of the convective time derivative of one of dissipative fluxes so that this constitutive relations serve to give equations of motion for the dissipative fluxes. In the limit that the β coefficients are taken to 0 the resulting equations of motion give diffusive behavior for the velocity field and causality is lost. However, for a range of finite α, β, γ coefficients and positive ζ, κ, μ these equations of motion are causal. They are not automatically causal for all values of these coefficients and detailed analytical study is needed to determine precise constraints. The basic ideas for how to do so are given in chapter 6 of [95], which also gives more technical sources for even more detailed analysis. Note that with these constitutive relations the entropy production becomes:

$$T\partial_\mu J_s^\mu = \Phi + \frac{\Pi^2}{\zeta} + \frac{q^\mu q_\mu}{\kappa} + \frac{d^{\alpha\beta} d_{\alpha\beta}}{2\mu} \geq \Phi \quad (6.8.26)$$

precisely as desired.

The equations of motion (6.8.23)-(6.8.25) determine the evolution of the dissipative fluxes Π, q, d . The number density continuity equation and the energy-momentum tensor transport equations expressed in similar notation are:

$$\dot{n} + n\theta = 0 \quad (6.8.27)$$

$$nT\dot{s} = \Phi - \Pi\theta - \mathcal{D}_\mu q^\mu - 2q^\mu \dot{u}_\mu + d^{\mu\nu} \langle \mathcal{D}_\mu u_\nu \rangle \quad (6.8.28)$$

$$(n\mathcal{U} + p + \Pi)\dot{u}^\mu + \perp^\mu{}_\nu \dot{q}^\nu + \theta q^\mu + q^\nu \mathcal{D}_\nu u^\mu + \mathcal{D}^\mu p + \mathcal{D}^\mu \Pi - \mathcal{D}_\nu \sigma_{\text{ideal}}^{\mu\nu} - \mathcal{D}_\nu d^{\mu\nu} - \sigma_{\text{ideal}}^{\mu\nu} \dot{u}_\nu - d^{\mu\nu} \dot{u}_\nu = \mathfrak{f}^\mu. \quad (6.8.29)$$

Therefore, (6.8.23)-(6.8.25) and (6.8.27)-(6.8.29) provide the full set of equations of motion for relativistic dissipative fluid mechanics at lowest order in effective field theory. These equations of motion are effectively the relativistic generalization of the Navier-Stokes equations and are known as the Israel-Stewart equations of motion.

6.9 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 6.13: Noncirculating flow, the Hamilton-Jacobi Equation, and the Schrödinger equation** shows a sequence of important simplifications of fluid mechanics and hints at the Schrödinger equation, which we will soon find to be an equation of extremely fundamental importance.
- **Problem 6.17: Relativistic Perfect Fluids** computes the equations of motion and energy-momentum tensor for a perfect fluid which provides good practice using the full energy-momentum tensor.

In this chapter we developed the theory of continuum mechanics for both nonrelativistic and relativistic systems. This theory allows us to describe the macroscopic averaged behavior of systems contain many constituents. This required us to consider the matter as a network of interacting local thermodynamic systems. Doing so has given us the tools to make specific predictions for the macroscopic behavior of many different states of matter, even without a precise understanding of the microscopic details of that matter (due to the power of effective theory methods).

In section 6.1, we introduced the degrees of freedom necessary to describe continuum mechanical systems and described both the Lagrangian/active picture and Eulerian/passive picture of those degrees of freedom. In section 6.2 we used symmetry principles to derive the nonrelativistic transport equations which describe the flow of matter, energy, and momentum in the nonrelativistic theory. We also considered the flow of angular momentum, but doing so simply led to having a symmetric stress tensor. In section 6.3 we took a more microscopic approach and analyzed nonrelativistic kinetic theory. We used the microscopic equations of motion of a system of particles and a specific averaging procedure to provide an alternate derivation of the nonrelativistic transport equations. In doing so, we derived exact specific microscopic expressions for all of the quantities appearing in the transport equations. These microscopic expressions can be useful when comparing the results of solving continuum mechanical equations of motion with the results of a many particle simulation. In section 6.4 we developed constitutive relations for many basic states of matter using a combination of microscopic kinetic theory considerations and effective theory methods. Doing so led us to the Euler equations, the Navier-Stokes equations, the Cauchy-Green equations, and the equations of magnetohydrodynamics (MHD). In section 6.5 we found have to give an action principle including dissipative effects for nonrelativistic continuum mechanics in both the active and passive coordinates. In section 6.6 we essentially repeated the symmetry based analysis of section 6.2 for relativistic continuum mechanics and in doing so established the symmetric energy-momentum tensor and its equation of motion as the objects of study for the relativistic transport equations. In section 6.7 we showed the action based description of ideal relativistic continuum mechanics. Finally, in section 6.8 we briefly described how to extend relativistic continuum mechanics to include dissipative effects using the Israel-Stewart formalism.

This chapter is very far from a complete treatment of even basic topics in continuum mechanics or kinetic theory. Because continuum mechanics describes so many types of materials it is an extremely broad collection of fields with deep phenomenology to each. For some basic references, [62] is a classic reference on fluid mechanics, [101] is a great modern work, [109] is my personal favorite, and [95] is helpful for learning relativistic dissipative continuum mechanics. Additionally, [31] is a helpful introduction to variational methods for fluid mechanics and [49] (the original paper for Israel-Stewart theory) is quite clear. The sources I have listed overemphasize fluids relative to other states of matter. This is a simple reflection on what I have read most, and not on the complexity or activity of research on the other states of matter. For example, plasma physics is an extremely deep, technical, and active discipline of research. However, introductory material excepted it is beyond my personal expertise.

Chapter 7

General Relativity

Where there is matter, there is geometry.

– Johannes Kepler [64]

Then there occurred to me the happiest thought of my life, in the following form. The gravitational field has only a relative existence in a way similar to the electric field generated by magnetoelectric induction. Because for an observer falling freely from the roof of a house there exists, at least in his immediate surroundings, no gravitational field. Indeed, if the observer drops some bodies then these remain relative to him in a state of rest or uniform motion, independent of their particular chemical or physical nature.

– Albert Einstein [54]

In chapter 4 we struggled to identify a replacement for Newton’s gravity compatible with special relativity. Doing so is the object of this chapter. The resulting theory, general relativity, is Einstein’s most towering intellectual accomplishment. The theory is significantly more technical than all the physics that came before it. It is the pinnacle of classical theoretical physics. Let us begin.

7.1 Diffeomorphism Symmetry

7.1.1 What Does Gravity Interact With?

Let us recap what we learned in section 4.7. In Newton’s theory of gravity, the gravitational scalar potential is coupled to the mass density. The gauge invariance of Newton’s theory forces mass to be conserved. However, experimentally at high energies mass is not conserved. As well, experimentally light is bent by gravitational fields, but electromagnetic waves are massless and so in Newton’s theory do not interact with gravity at all. Therefore, mass cannot be the correct quantity for interacting with gravity. In special relativity, energy conservation replaces Newton’s mass conservation, because in the nonrelativistic limit the energy conservation of special relativity reproduces both nonrelativistic mass conservation and nonrelativistic energy conservation. So, we should not search for a way to couple whatever fields carry gravity to mass, but instead for a way to couple them to energy. However, unlike mass, energy is not Lorentz invariant. Instead energy is part of the energy-momentum 4-vector, and so the only Poincare symmetric way to couple gravity to energy is to also couple it to momentum.

Because we believe in locality, whatever theory couples gravity to energy and momentum must do so locally. Locally, energy and momentum are given by densities which are components of the energy-momentum tensor $T^\mu{}_\nu$. Thus, locally gravity must couple to the full energy-momentum tensor. That is, $T^\mu{}_\nu$ must be the “external force” on whatever fields carry the gravitational interaction, so that they will have some equation of motion functions $E^\mu{}_\nu$ which are 0 when those fields are free (not interacting with any other energy or momentum) but which in general have:

$$E^\mu{}_\nu = T^\mu{}_\nu. \tag{7.1.1}$$

This is precisely analogous to how in electromagnetism the equation of motion function for the vector potential $\partial_\nu \mathcal{F}^{\mu\nu}$ is set to 0 when it is free but is set to J^μ , the current it couples to, when interacting. Essentially, (7.1.1) simply says that the energy-momentum tensor is the conserved current that is the source of the gravitational interaction.

The energy-momentum tensor must be divergence-free in order to have local energy-momentum conservation. Energy-momentum conservation is not an independent dynamic rule, but a derived fact from Noether's theorem. This means that the time derivatives of T^0_ν for each ν are determined by the spatial derivatives of T^a_ν for all physical states, and so T^0_ν does not have an independent equation of motion and does not represent any independent degrees of freedom. This is precisely like how the charge density J^0 has its time evolution completely determined by the spatial part of the current density J^a in electromagnetism. Because of this, $T^0_\nu - E^0_\nu = 0$ is not an independent equation in (7.1.1) and is exactly a gravitational analog of Gauss' law in electromagnetism. Just as Gauss' law $\rho + \nabla \cdot \vec{P}_A = 0$ is a constraint on the phase space of physically allowed states of electromagnetism, $T^0_\nu - E^0_\nu = 0$ is such a constraint in gravity.

In electromagnetism, the phase space of dynamically independent physical degrees of freedom only couples to the spatial part of the current density, not J^0 . However, there is no gauge invariant way to construct this phase space covariantly, because what counts as the charge density vs the current density is itself not covariant. (This does not mean the theory is not covariant, just that this way of expressing the theory is not covariant.) Because of this, Gauss' law is included in electromagnetism for the purpose of making the action manifestly covariant. But, because it is added in such a way that charge is conserved automatically, the constraint is first class (as it must weakly Poisson commute with the full Hamiltonian to be preserved dynamically). The Lagrange multiplier associated to Gauss' law adds the unphysical degree of freedom A_0 to electromagnetism and the first class constraint is the generator all of the gauge transformations of the unphysical degrees of freedom of the theory, by the logic of section 4.6.

Similarly, in gravity the phase space of dynamically independent physical degrees of freedom only couples to T^a_ν , not T^0_μ . However, there is no covariant way to construct this phase space for the same reason as electromagnetism. So, we include the gravitational Gauss' laws $T^0_\nu - E^0_\nu = 0$ for the purposes of making the action of the theory manifestly covariant. Because these constraints will be added in a way that conserves energy-momentum automatically, these constraints are first class for the same reason. Then, the Lagrange multiplier associated to these constraints will be some added unphysical gravitational degrees of freedom and the first class constraints will act as the generators of gauge transformations of those degrees of freedom.

The most general linear combination of the constraints imposed by energy-momentum conservation is:

$$C[f] = \int_{\mathbb{S}} f^\nu(t, \vec{x}) (T^0_\nu - E^0_\nu) d\mathbb{S} \quad (7.1.2)$$

for some vector field with components f^μ . Because of our understanding of phase space constraints from theorem 2.16, this quantity $C[f]$ generates the gauge transformations of gravity with gauge functions $f^\nu(t, \vec{x})$. We can tell what this generator does geometrically by thinking about what it affects a point particle. By construction of the energy-momentum tensor, $-T^0_0$ is the energy density and T^0_a is the linear momentum density. For a point particle, the energy density is simply the particle's Hamiltonian $\mathcal{H}$ times a Dirac delta at the location of the particle $\vec{z}(t)$:

$$T^0_0(t, \vec{x}) = -\mathcal{H}(t, \vec{z}, \vec{p}) \delta(\vec{x} - \vec{z}(t)) \quad (7.1.3)$$

and the linear momentum density is similarly the particle's momentum times the same Dirac delta:

$$T^0_a(t, \vec{x}) = p_a(t) \delta(\vec{x} - \vec{z}(t)). \quad (7.1.4)$$

Therefore, for gravity interacting with a point particle:

$$C[f] = -f^0(t, \vec{z}) \mathcal{H}(t, \vec{z}, \vec{p}) + f^a(t, \vec{z}) p_a(t) - \int_{\mathbb{S}} f^\nu(t, \vec{x}) E^0_\nu d\mathbb{S}. \quad (7.1.5)$$

By comparing to Noether's theorem version 1 (theorem 1.9), this is exactly the formula for the generator of a canonical transformation in which:

$$\mathcal{D}t = f^0(t, \vec{z}), \quad \mathcal{D}z^a = f^a(t, \vec{z}). \quad (7.1.6)$$

(The piece proportional to the equation of motion functions E^μ_ν does not contribute to the canonical transformations of the point particle because by definition those are the equations of motion functions corresponding to a free gravitational field and so have no dependence on the degrees of freedom of the external source produced by the particle.)

Equation (7.1.6) is a spacetime translation. However, it is unlike the spacetime translations we have

considered previously. Previously, when we considered spacetime translations they were always by a globally constant amount (shifting all times or positions by the same amount). (7.1.6) is a spacetime translation where every point in time and space is allowed to be translated differently. That is, (7.1.6) gives a **local spacetime translation**. Such a transformation is called a **gauge diffeomorphism**. These transformations must be the gauge transformations of gravity in order for it to couple to the locally conserved energy-momentum tensor. Therefore, **gravity is a gauge theory where the gauge transformations are gauge diffeomorphisms**¹

7.1.2 What is a Diffeomorphism?

To get a solid handle on what gauge diffeomorphisms are, we first need to develop a couple of tools. We call the set of all points in spacetime the spacetime manifold $\mathbb{T}$. We will make more precise what exactly a manifold is next subsection, but for now we should understand it as a set of points for which there is a meaningful notion of differentiation. Let $X \in \mathbb{T}$ be an event in spacetime. We represent that event by coordinates x^μ , which means we have some function $x^\mu(X)$ which takes a point and spits out the a list of real numbers which are the coordinates of the point in our coordinate system. The number of real numbers it takes to specify a point in the manifold is called the dimension of the manifold, which for the physical world is 4 (1 time direction and 3 spatial directions). This map needs to be smooth and smoothly invertible, at least locally, in order for this to be a good coordinate system so that each value of x^μ corresponds to a distinct point X and so that nearby points X and X' have nearby coordinates.

Let $\xi^\mu(X)$ be a vector field performing a gauge diffeomorphism. Then, equation (7.1.6) can then be written covariantly as:

$$\mathcal{D}x^\mu = \xi^\mu(x). \quad (7.1.7)$$

We can view this as a differential equation defining the motion of a point in coordinates. Consider a curve $x'^\mu(\varepsilon)$ which begins at $\varepsilon = 0$ at the coordinates x^μ and which satisfies at each ε :

$$\frac{dx'^\mu}{d\varepsilon} = \xi^\mu(x'). \quad (7.1.8)$$

Then, the solution to this differential equation will give some function of the form:

$$x'^\mu(\varepsilon) = U_\xi^\mu(\varepsilon, x), \quad U_\xi^\mu(0, x) = x^\mu \quad (7.1.9)$$

where $U_\xi^\mu(\varepsilon, x)$ depends smoothly on ε . The function U_ξ is really just T from (1.3.1) and ξ is just f from (1.3.3) where we see that the **gauge diffeomorphism provides a continuous transformation of spacetime coordinates**. The solution curves $x'^\mu(\varepsilon)$ are called the integral curves or streamlines of ξ^μ or the flow generated by ξ^μ . It is useful to define the transformation $x'^\mu(x) = U_\xi(1, x)$ ². Because x is related to X invertibly and smoothly and x is related to x' invertibly and smoothly, x' is related to X invertibly and smoothly by function composition:

$$x'^\mu(X) = x'^\mu(x(X)). \quad (7.1.10)$$

Thus, $x'^\mu(X)$ is another good coordinate system! Because we require gauge diffeomorphism symmetry and said transformation turns the coordinate system x^μ into x'^μ , both coordinate systems must be equally good for physics (we must have symmetry under this change of coordinates).

The set of smooth invertible (with smooth inverse) coordinate transformations $x'^\mu = x'^\mu(x)$ on a given manifold is called the set of **diffeomorphisms** on that manifold³. Gauge diffeomorphisms are a subset of all diffeomorphisms. In particular, gauge diffeomorphisms are those coordinate transformations that can be formed by limits of compositions of transformations produced by flows of the form of (7.1.7). The group of gauge diffeomorphisms is the full set of diffeomorphisms which are continuously connected to the identity

¹A very technically minded reader will note that really gravity is only a gauge theory where the gauge transformations are small diffeomorphisms, meaning diffeomorphisms which limit to the identity transformation sufficiently far away. This is because if one wants the constraint generators to converge as integrals, the integrands must decay sufficiently quickly at large distances. The argument given here only concerns what happens at finite volumes, and the theory of large diffeomorphisms which act nontrivially arbitrarily far away is very interesting and difficult. Whenever we say diffeomorphism symmetry, we always mean symmetry under small gauge diffeomorphisms as in order to discuss what large diffeomorphisms are considered symmetries one has to specify what boundary conditions are required.

²In general one needs to take some care in what vector fields are allowed when evolving all the way out to $\varepsilon = 1$. In 1 dimension for example, the vector field $\xi(x) = x^2$ causes the equation $\frac{dx}{d\varepsilon} = x^2$ to blow up to infinity at finite ε and so does not represent any physically reasonable coordinate transformation. We should really only consider vector fields which are smooth and die off sufficiently quickly that these blow ups do not occur.

³Mathematicians generally consider diffeomorphisms as a map between two different manifolds, but physicists typically use diffeomorphisms as being restricted to maps from a manifold to itself.

transformation (meaning all smooth invertible transformations $x'^\mu = F^\mu(x)$ for which there exists a function $G^\mu(\varepsilon, x)$ depending smoothly on ε so that $G^\mu(1, x) = F^\mu(x)$ and $G^\mu(0, x) = x^\mu$). Therefore, what we have been calling gauge diffeomorphisms we could also call connected diffeomorphisms. There are diffeomorphisms which are not connected to the identity and we do not have to require symmetry under them (time reversal, parity for example). Because we only have to have symmetry under connected diffeomorphisms, one should in principle say that we demand only connected diffeomorphism or gauge diffeomorphisms symmetry. However, we will always just say diffeomorphism symmetry and we will always just mean symmetry under gauge diffeomorphisms. We will generically refer to gauge diffeomorphisms as *diffs*.

Because the coordinate systems x'^μ and x^μ must be equally good for doing physics, the laws of physics (our equations of motion) take no particularly special privileged form in either coordinates. Therefore, **diffeomorphism symmetry requires that there is no privileged natural coordinate system for physics.**

7.1.3 General Coordinate Transformations

To understand exactly what are the physical consequences of diffeomorphism symmetry and what it means to have no privileged coordinate system, we need to first understand the transformation properties of quantities which may appear in our theory under a diffeomorphism. In the previous chapters, we always based our calculations on Cartesian coordinates, but now we need to understand general coordinate transformations. Because general coordinate transformations can do so much, it is best to understand our theory as much as possible in a way which is coordinate invariant, so that what exactly is required by diff symmetry is clearly singled out. Doing this requires learning a little bit of differential geometry.

At each event $X(x)$ in the **spacetime manifold**, there are many possible directions one could move toward another point in spacetime. The space of displacements $dX(x)$, meaning the vector space of all possible displacement vectors at the point $X \in \mathbb{T}$ which keep one in the manifold (and so lie tangent to it), is called the **tangent space** of $\mathbb{T}$ at X , written $T_X(\mathbb{T})$. Suppose we move from $X(x)$ a small amount to a very nearby point in a way so that only one of our coordinates changes. Suppose it changes by an amount dx^μ . Then, the resulting vector dX from that displacement defines the **coordinate basis vector** $\vec{e}_\mu(X)$ by $dX = \vec{e}_\mu dx^\mu$. Under a general small movement of position to a nearby point, all of the coordinates are allowed to change, each by an amount dx^μ , and by the linearity of displacements, the generic displacement vector is:

$$dX = dx^\mu \vec{e}_\mu. \quad (7.1.11)$$

Using the ordinary chain rule, under a change of coordinates $x'^\mu = x'^\mu(x)$, the coordinate displacements transform by:

$$dx'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} dx^\nu. \quad (7.1.12)$$

Now that we are considering general coordinate transformations, not just translations and Lorentz transformations, (7.1.12) is the definition of the transformation property for quantities which properly transform with an upper index. (As always, a quantity is written with an upper index if it transforms the same way as coordinate displacements.) Similarly, using the chain rule, under a change of coordinates the coordinate partial derivatives transform by:

$$\partial'_\mu = \frac{\partial x^\nu}{\partial x'^\mu} \partial_\nu. \quad (7.1.13)$$

Here we have defined the matrix of derivatives $\frac{\partial x^\nu}{\partial x'^\mu}$ as the matrix of derivatives of the inverse transformation $x^\nu(x')$:

$$x^\mu(x'(x)) = x^\mu. \quad (7.1.14)$$

By differentiating with respect to x^ν :

$$\frac{\partial x^\mu}{\partial x'^\rho} \frac{\partial x'^\rho}{\partial x^\nu} = \delta^\mu_\nu. \quad (7.1.15)$$

Therefore, equivalently, $\frac{\partial x^\nu}{\partial x'^\mu}$ is the matrix inverse of $\frac{\partial x'^\mu}{\partial x^\nu}$. As always, the coordinate partial derivatives transform under the inverse transformation property of the coordinate displacements and that inverse transformation property is the defining property for quantities which are written properly with a lower index.

Because the displacement vector dX is a purely geometric object, it does not change under a coordinate transformation (which just changes how that object is expressed), we can use (7.1.11) to determine how the coordinate basis vectors transform:

$$dX = dx^\mu \vec{e}_\mu(x) = dx'^\mu \vec{e}'_\mu(x') \quad (7.1.16)$$

$$\implies dx'^\mu \frac{\partial x^\nu}{\partial x'^\mu} \vec{e}_\nu(x) = dx'^\mu \vec{e}'_\mu(x') \quad (7.1.17)$$

$$\implies \boxed{\vec{e}'_\mu(x') = \frac{\partial x^\nu}{\partial x'^\mu} \vec{e}_\nu(x)} \quad (7.1.18)$$

where this follows because these are true for all possible coordinate displacements dx^μ .

A generic vector field $\xi(X)$ will be some linear combination of our basis vectors $\vec{e}_\mu$. The tangent space at X , $T_X(\mathbb{T})$, is a vector space spanned by $\vec{e}_\mu(X)$. This is true for each X in $\mathbb{T}$, and so the tangent spaces form a family of vector spaces (the set consisting of elements $T_X(\mathbb{T})$ for each $X \in \mathbb{T}$). That set of all tangent spaces of $\mathbb{T}$ is called the tangent bundle $T(\mathbb{T})$. Because $\xi(X)$ for each X is a linear combination of $\vec{e}_\mu(X)$, it is for each X an element of $T_X(\mathbb{T})$. So, formally, a vector field $\xi(X)$ is a map from the manifold $\mathbb{T}$ to that manifold's tangent bundle $T(\mathbb{T})$ so that for each X it is specifically a map into the tangent space at X , $T_X(\mathbb{T})$. We can write a generic vector field in components and coordinates:

$$\xi(X) = \xi^\mu(x) \vec{e}_\mu(x) \quad (7.1.19)$$

and as physicists tend to be, we are sometimes reckless in calling the components $\xi^\mu(x)$ the vector field rather than the actual geometric object $\xi(X)$, whose definition does not depend on our coordinates. Because the vector field $\xi(X)$ is a geometric object independent of any coordinates, it does not transform when coordinates are changed. With this, we can determine the coordinate transformation property of the components $\xi^\mu(x)$:

$$\xi(X) = \xi^\mu(x) \vec{e}_\mu(x) = \xi'^\mu(x') \vec{e}'_\mu(x') \quad (7.1.20)$$

$$\implies \xi^\mu(x) \frac{\partial x'^\nu}{\partial x^\mu} \vec{e}'_\nu = \xi'^\mu \vec{e}'_\mu \quad (7.1.21)$$

$$\implies \xi'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} \xi^\nu. \quad (7.1.22)$$

Thus the components of a generic vector field transform exactly like the components of a coordinate displacement vector, as expected.

In order to have causality structure, we need to have a notion of proper time/proper length between events. In Minkowskian coordinates, the proper time was given by $d\tau^2 = -\eta_{\mu\nu} dx^\mu dx^\nu$. When we first developed index notation, we found that the coordinate independent expression for the proper time is:

$$d\tau^2 = -dX \cdot dX \quad (7.1.23)$$

where the dot product $\cdot$ is a pseudo-inner product in the sense that it is symmetric, bilinear, and nondegenerate. Expressed in terms of the coordinate basis vectors:

$$d\tau^2 = -\vec{e}_\mu \cdot \vec{e}_\nu dx^\mu dx^\nu. \quad (7.1.24)$$

So, it is useful to define the **metric tensor** as the symmetric rank-2 tensor whose components are these pseudo-inner products:

$$\boxed{g_{\mu\nu}(x) \stackrel{\text{def}}{=} \vec{e}_\mu(x) \cdot \vec{e}_\nu(x)} \implies \boxed{g_{\mu\nu}(x) = g_{\nu\mu}(x)}. \quad (7.1.25)$$

The pseudo-inner product of any two vectors ξ and ψ with components ξ^μ and ψ^μ then becomes:

$$\boxed{\xi \cdot \psi = g_{\mu\nu} \xi^\mu \psi^\nu} \quad (7.1.26)$$

and the proper time becomes:

$$\boxed{d\tau^2 = -g_{\mu\nu} dx^\mu dx^\nu}. \quad (7.1.27)$$

Because the proper time element, expressed in a given coordinate system, determines the metric tensor and vice versa, some sources will confusingly also call the expression for the proper time element the metric. We will not do this. We will either call $-g_{\mu\nu} dx^\mu dx^\nu$ the proper time element or the line element.

From the definition of the metric tensor, under a coordinate transformation:

$$g'_{\mu\nu}(x') = \vec{e}'_\mu(x') \cdot \vec{e}'_\nu(x') = \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial x^\sigma}{\partial x'^\nu} \vec{e}_\rho(x) \cdot \vec{e}_\sigma(x) \quad (7.1.28)$$

$$\implies \boxed{g'_{\mu\nu}(x') = \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial x^\sigma}{\partial x'^\nu} g_{\rho\sigma}(x)}. \quad (7.1.29)$$

Because we want to have a notion of timelike, lightlike, and spacelike displacements with there only being 1 time direction in any given frame, $g_{\mu\nu}$ viewed as a matrix must be invertible (so that there are no displacement directions which contribute nothing to the proper time), have exactly one negative eigenvalue (as that gives the timelike direction), and have the rest of its eigenvalues be positive (as those give the spacelike directions). Suppose that at a particular point X_0 of interest with coordinates x_0^μ in some particular initial coordinate system x^μ which is written without primes, the components of the metric tensor take the values $g_{\mu\nu}(x_0)$. Then under a general coordinate transformation to a new coordinate system $x'^\mu(x)$, the transformed metric tensor at the same point is given by:

$$g'_{\mu\nu}(x'_0) = \frac{\partial x^\rho(x_0)}{\partial x'^\mu} \frac{\partial x^\sigma(x_0)}{\partial x'^\nu} g_{\rho\sigma}(x_0). \quad (7.1.30)$$

We can define the matrix g as the 4x4 matrix with components $g_{\rho\sigma}(x_0)$, the matrix J as the 4x4 matrix with components $\frac{\partial x^\rho(x_0)}{\partial x'^\mu}$, and the matrix g' as the 4x4 matrix with components $g'_{\mu\nu}(x'_0)$. Then, this equation can be written as the matrix equation:

$$g' = JgJ^T. \quad (7.1.31)$$

The matrix J is necessarily invertible so that the coordinate transformation is invertible but otherwise, because we are allowed to make any coordinate transformation which is connected to the identity, by choosing the appropriate coordinate transformation, J can be any invertible matrix that is connected to the identity matrix. By construction, g is a real symmetric 4x4 matrix and therefore can be diagonalized by some rotation matrix R . Because of our previous conditions on g , one of its eigenvalues is negative and the other three are positive. Therefore, there exists a matrix R so that:

$$RgR^T = \begin{pmatrix} -a^2 & 0 & 0 & 0 \\ 0 & b^2 & 0 & 0 \\ 0 & 0 & c^2 & 0 \\ 0 & 0 & 0 & d^2 \end{pmatrix} \quad (7.1.32)$$

for some positive real numbers a, b, c, d . Define then the matrix D :

$$D = \begin{pmatrix} \frac{1}{a} & 0 & 0 & 0 \\ 0 & \frac{1}{b} & 0 & 0 \\ 0 & 0 & \frac{1}{c} & 0 \\ 0 & 0 & 0 & \frac{1}{d} \end{pmatrix}. \quad (7.1.33)$$

This is a dilation matrix that scales the eigenvectors of g each by a corresponding factor. Automatically then:

$$DRgR^T D^T = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \eta. \quad (7.1.34)$$

The matrix R is continuously connected to the identity by considering the limit of its rotation angle being taken to 0. The matrix D is continuously connected to the identity by considering the limit of its diagonal elements toward 1. Therefore, DR is connected to the identity and so it is possible to perform a diffeomorphism so that at the coordinates x_0^μ , the matrix $J = DR$. By doing so, in the new coordinates x'^μ at the point X_0 , the metric tensor will be sent to the Minkowski metric:

$$g'_{\mu\nu}(x'_0) = \eta_{\mu\nu}. \quad (7.1.35)$$

It is possible to do this at a single point X_0 for any causal metric tensor as described. Thus, we say that **a spacetime manifold is locally like Minkowski space**. It would be a separate physical claim to require that our metric tensor could be transformed to $\eta_{\mu\nu}$ everywhere all at once, which would then make spacetime exactly Minkowski space.

The ingredients we have described so far culminate in the idea of a Lorentzian manifold, also called a pseudo-Riemannian manifold. A **Lorentzian manifold** is a set of points $\mathbb{T}$ which is smooth enough to allow differentiation, equipped with a tangent bundle $T(\mathbb{T})$ of vector spaces ($T_X(\mathbb{T})$ for each $X \in \mathbb{T}$), and equipped with a metric tensor $g_{\mu\nu}(X)$ which defines a pseudo-inner product on vectors in $T_X(\mathbb{T})$ and that can at any individual point X be transformed by coordinate transformation into the Minkowski metric $\eta_{\mu\nu}$.

Because we know how to define a vector field on a manifold, we can use that definition to define tensor

fields on the manifold. A tensor field $\Phi(X)$ of rank N on the spacetime $\mathbb{T}$ is a map from points in spacetime to the N fold tensor product of the tangent bundle $T(\mathbb{T})$ with itself, so that for each X , $\Phi(X)$ is an element of the N fold tensor product of the tangent space $T_X(\mathbb{T})$ at X . Because the coordinate basis vectors $\vec{e}_\mu(X)$ form a basis for the tangent space $T_X(\mathbb{T})$, the tensor products $\vec{e}_{\mu_1}(X) \otimes \dots \otimes \vec{e}_{\mu_N}(X)$ form a basis for the N fold tensor product of the tangent space with itself. Hence, in coordinates and components a generic tensor field of rank N takes the form:

$$\Phi(X) = \phi^{\mu_1 \dots \mu_N}(x) \vec{e}_{\mu_1(x)} \otimes \dots \otimes \vec{e}_{\mu_N(x)}. \quad (7.1.36)$$

You probably can predict the transformation properties of the components $\phi^{\mu_1 \dots \mu_N}(x)$ from what we have already discussed. In particular, because $\Phi(X)$ is a geometrical object:

$$\Phi(X) = \phi^{\mu_1 \dots \mu_N}(x) \vec{e}_{\mu_1(x)} \otimes \dots \otimes \vec{e}_{\mu_N(x)} = \phi'^{\mu_1 \dots \mu_N}(x') \vec{e}'_{\mu_1(x')} \otimes \dots \otimes \vec{e}'_{\mu_N(x')} \quad (7.1.37)$$

$$\implies \phi'^{\mu_1 \dots \mu_N}(x') = \frac{\partial x'^{\mu_1}}{\partial x^{\nu_1}} \dots \frac{\partial x'^{\mu_N}}{\partial x^{\nu_N}} \phi^{\nu_1 \dots \nu_N}(x). \quad (7.1.38)$$

Just like when we first introduced covariant notation, indices can be lowered and raised using the metric tensor. It is possible at a single point to transform the metric tensor at that point to the Minkowski metric, which has determinant -1 . Every invertible coordinate transformation necessarily has an invertible matrix of partial derivatives $\frac{\partial x'^\mu}{\partial x^\nu}$, thus that matrix has nonzero determinant. By the transformation property of the metric tensor and the fact that the determinant of a matrix product is the product of determinants:

$$\det g' = \det \left(\frac{\partial x}{\partial x'} \right)^2 \det g. \quad (7.1.39)$$

Because the determinant of the Minkowski metric is negative and the coordinate transformation determinant is nonzero and so squares to a positive number, the determinant of the metric tensor is negative at every point in spacetime. Because the determinant of the metric tensor is negative, and thus nonzero, the metric tensor is invertible as a matrix. Define the inverse metric tensor $g^{\mu\nu}(x)$ as that matrix inverse:

$$g^{\mu\rho}(x) g_{\rho\nu}(x) = \delta^\mu_\nu. \quad (7.1.40)$$

If $\xi^\mu(x)$ are the components of a vector field, then we define $\xi_\mu(x)$ by:

$$\xi_\mu(x) = g_{\mu\nu}(x) \xi^\nu(x). \quad (7.1.41)$$

Consequently, the components of $\xi_\mu(x)$ transform as:

$$\xi'_\mu(x') = g'_{\mu\nu}(x') \xi'^\nu(x') = \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial x^\sigma}{\partial x'^\nu} g_{\rho\sigma}(x) \frac{\partial x'^\nu}{\partial x^\alpha} \xi^\alpha(x) \quad (7.1.42)$$

$$= \frac{\partial x^\rho}{\partial x'^\mu} \delta^\sigma_\alpha g_{\rho\sigma} \xi^\alpha = \frac{\partial x^\rho}{\partial x'^\mu} g_{\rho\sigma} \xi^\sigma \quad (7.1.43)$$

$$= \frac{\partial x^\nu}{\partial x'^\mu} \xi_\nu(x). \quad (7.1.44)$$

Therefore, the components $\xi_\mu(x)$ transform correctly for an object with a lower index. Similarly, if instead we had assumed $\xi_\mu(x)$ transforms correctly for a lower index object, then $g^{\mu\nu} \xi_\nu(x)$ transforms correctly for an upper index object (this is quick to see using what we have already shown and that $g^{\mu\nu}$ is the matrix inverse of $g_{\mu\nu}$). So, $g^{\mu\nu}$ raises tensor indices and $g_{\mu\nu}$ lowers tensor indices exactly as desired.

Because the tangent space $T_X(\mathbb{T})$ is a vector space at X , it is possible to consider the space of linear maps from the tangent space to the real numbers, which is known as its dual vector space. The dual vector space to the tangent space is called the **cotangent space** $T_X^*(\mathbb{T})$, where the star does not indicate any kind of complex conjugation. The collection of cotangent spaces of a manifold is called its cotangent bundle $T^*(\mathbb{T})$. If ξ^μ are the components of a vector field and ψ_μ are the lowered components of another vector field, then the contraction $\psi_\mu \xi^\mu$ is automatically coordinate invariant:

$$\xi'^\mu(x') \psi_\mu(x') = \frac{\partial x'^\mu}{\partial x^\nu} \xi^\nu(x) \frac{\partial x^\rho}{\partial x'^\mu} \psi_\rho(x) = \delta^\rho_\nu \xi^\nu(x) \psi_\rho(x) = \xi^\mu(x) \psi_\mu(x). \quad (7.1.45)$$

As well, any linear combination of the components $\xi^\mu(x)$ to the real numbers can be written in the form $\xi^\mu(x) \psi_\mu(x)$ for some coefficients $\psi_\mu(x)$ and so while vectors in the tangent space have components with an upper index $\xi^\mu(x)$, vectors in the cotangent space have components with a lower index $\psi_\mu(x)$. Because we have access to a metric tensor which can raise and lower indices at will, the distinction between the tangent space and cotangent space is incidental, and we will generally just think about every tensor field using the tangent space.

When contracting the indices of tensorial quantities, the result is a tensor of appropriately reduced rank. Suppose $\Phi(X)$ is a rank N tensor. Then, we could define a new tensor $\Psi(X)$ of rank $N - 2$ which is formed from contracting two indices of $\Phi(X)$:

$$\Phi(X) = \phi^{\mu_1 \dots \mu_N}(x) \vec{e}_{\mu_1} \otimes \dots \otimes \vec{e}_{\mu_N} \quad (7.1.46)$$

$$\Psi(X) = \phi^{\mu_1 \dots \mu_{N-2} \nu} \vec{e}_{\mu_1} \otimes \dots \otimes \vec{e}_{\mu_{N-2}} = \psi^{\mu_1 \dots \mu_{N-2}} \vec{e}_{\mu_1} \otimes \dots \otimes \vec{e}_{\mu_{N-2}}. \quad (7.1.47)$$

Then, the transformation properties of the components of Φ automatically imply that the components of Ψ transform properly as the components of a tensor. This is the generalization of the fact that contracting two vectors gives a scalar. Furthermore, if $\Phi(X)$ is a rank N tensor and $\Psi(X)$ is a completely unrelated rank M tensor, then the tensor product $\Phi(X) \otimes \Psi(X)$ is a rank $M + N$ tensor.

To this point we have always talked about coordinate systems as a set of functions from the manifold to a list of real numbers which is smooth and invertible. In general we need to be slightly more careful. A coordinate **chart** on a manifold $\mathbb{T}$ of dimension d is a function $x(X)$ from an open subset U of $\mathbb{T}$ into an open subset $x(U)$ of $\mathbb{R}^d$ which is smooth and smoothly invertible. Generally, it is not possible to use a single coordinate chart to cover the whole manifold. Instead, typically it takes several (say N) coordinate charts $x_1(X), \dots, x_N(X)$ on corresponding patches $U_1, \dots, U_N$ of $\mathbb{T}$ so that the union of $U_1, \dots, U_N$ covers the whole manifold $\mathbb{T}$ and so that on any region where two different U 's overlap, there is a smooth and smoothly invertible map between their coordinates (those maps are called transition functions). This set of coordinate charts together with their associated patches and transition functions is called an **atlas**. Essentially, a single coordinate chart allows you to map out part of a manifold into coordinates but in general one needs many maps (charts) of different regions (patches) and instructions on how to stitch them together (transition functions) to make a complete picture (the atlas) of the full manifold. When considering a small enough but still finitely large region of interest on a manifold, a single coordinate chart is all one ever needs to discuss. But, when considering large scale and especially global properties, one needs the full atlas.

7.1.4 Lie Derivatives

The previous subsection demonstrated how we can define the tensorial quantities of interest in physics in a coordinate independent way and what the resulting general coordinate transformation properties of the components of those objects are. It is **NOT** a restriction on physics to say that we can cast everything in a coordinate agnostic way. Any theory can be written in a coordinate independent way. For example, the nonrelativistic Lorentz equation of motion $m\ddot{\vec{x}} = q(\vec{E} + \dot{\vec{x}} \times \vec{B})$ is independent whatever of coordinate system is used on space to compute the components of these vectorial quantities. It can be made independent of the choice of time coordinate as well with some additional effort. When an equation is written in a way that does not depend on the special properties of any coordinate system and so is a valid equation in any coordinates, that equation is said to be **generally covariant**. General covariance means that any coordinates could be used, but does not mean that all quantities look the same in all coordinates. General covariance is just a way of writing equations, not a physical assumption.

The physical restriction of diffeomorphism symmetry comes from requiring that the equations of our theory have symmetry under all coordinate transformations connected to the identity. The distinction here is subtle but important. In the Lorentz force equation of motion, if $\vec{E}$ and $\vec{B}$ are fixed background quantities which are not considered dynamical in the theory, then the equation of motion $m\ddot{\vec{x}} = q(\vec{E} + \dot{\vec{x}} \times \vec{B})$ only has rotational symmetry if $\vec{E}$ and $\vec{B}$ are 0. This is because under a rotation, $\vec{E}' = \hat{R}\vec{E}$ and similarly for $\vec{B}$, and so the resulting equation of motion is only the same when viewed as a function of the only dynamical variable $\vec{x}$ if $\vec{E}' = \vec{E}$ and $\vec{B}' = \vec{B}$ for all rotations $\hat{R}$, which is only satisfied by the 0 vector. However, if $\vec{E}$ and $\vec{B}$ are derived from a vector potential which is a field in our theory which gets in own equation, then the equation of motion must be understood as a function of both $\vec{x}$ and the vector potential and will be the same function before and after rotation for any vector potential. When considering symmetries of a physical scenario under coordinate transformation, one has to carefully understand what is a dynamical variable in the action (and so is transformed by the coordinate transformation without having to be unchanged) and what is a background to the variables (and so must remain constant under the transformation to have symmetry).

Suppose we have a theory which has a background scalar field $\phi(x)$. Under coordinate transformation, $\phi(x)$ transforms as:

$$\phi'(x') = \phi(x). \quad (7.1.48)$$

In general the function $\phi'(x)$ will be a different function than $\phi(x)$. However, if the coordinate transformation

is a symmetry of our physical scenario, then because $\phi(x)$ is a part of our physical scenario and not a dynamical variable, the two must be equal. That is, for a symmetry:

$$\phi'(x) = \phi(x). \quad (7.1.49)$$

To be specific, by background quantity in our theory, we mean that $\phi(x)$ appears in the equations of motion for some variable in our action but does not get varied itself to have an equation of motion. Viewed another way, by using that $\phi'(x') = \phi(x)$, this equation equivalently states that $\phi(x') = \phi(x)$.

Suppose $\xi^\mu(x)$ is a vector field which produces a gauge diffeomorphism. The Lie derivative L_ξ of a quantity is defined by how the value of that quantity changes under the flow of that diffeomorphism. For scalar fields, this means:

$$L_\xi \phi \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{\phi(x') - \phi(x)}{\varepsilon}. \quad (7.1.50)$$

The Lie derivative thus measures the extent to which the quantity changes under a diffeomorphism when viewed as a background variable. Thus, to have diff symmetry, **the Lie derivatives of all background variables must be 0 under the symmetries of our theory.**

Using equation (7.1.8):

$$x'^\mu = x^\mu + \varepsilon \xi^\mu(x) + \mathcal{O}(\varepsilon^2) \quad (7.1.51)$$

and so by using the chain rule, the Lie derivative of a scalar field immediately becomes:

$$L_\xi \phi = \xi^\mu \partial_\mu \phi. \quad (7.1.52)$$

Because we must have diffeomorphism symmetry, if $\phi(x)$ is a background quantity, its Lie derivative must vanish for all ξ^μ and so:

$$\xi^\mu \partial_\mu \phi = 0 \quad \forall \quad \xi^\mu \implies \partial_\mu \phi = 0 \implies \phi = \text{uniform constant}. \quad (7.1.53)$$

The only scalar field invariant under all diffeomorphisms is a constant. Therefore, in a diff symmetric theory we cannot have any nontrivial background scalar fields.

Suppose we instead have a theory which has a background tensor field of rank $M + N$ which we express with some components raised and some lowered as $\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x)$. Under coordinate transformation, these components transform as:

$$\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') = \frac{\partial x'^{\mu_1}}{\partial x^{\rho_1}} \dots \frac{\partial x'^{\mu_M}}{\partial x^{\rho_M}} \frac{\partial x^{\sigma_1}}{\partial x'^{\nu_1}} \dots \frac{\partial x^{\sigma_N}}{\partial x'^{\nu_N}} \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N}(x). \quad (7.1.54)$$

If this coordinate transformation is a symmetry of our physical scenario, then because $\phi(x)$ is a part of our physical scenario it must be unchanged. That is, symmetry of our tensor field under the transformation requires:

$$\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x) = \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x). \quad (7.1.55)$$

Equivalently (because the above holds for all x):

$$\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') = \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') \quad (7.1.56)$$

$$\implies \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') - \frac{\partial x'^{\mu_1}}{\partial x^{\rho_1}} \dots \frac{\partial x'^{\mu_M}}{\partial x^{\rho_M}} \frac{\partial x^{\sigma_1}}{\partial x'^{\nu_1}} \dots \frac{\partial x^{\sigma_N}}{\partial x'^{\nu_N}} \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N}(x) = 0. \quad (7.1.57)$$

Therefore, just like for the scalar field, the Lie derivative of a tensor field is defined by how the tensor field intrinsically changes under a diffeomorphism:

$$L_\xi \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') - \frac{\partial x'^{\mu_1}}{\partial x^{\rho_1}} \dots \frac{\partial x'^{\mu_M}}{\partial x^{\rho_M}} \frac{\partial x^{\sigma_1}}{\partial x'^{\nu_1}} \dots \frac{\partial x^{\sigma_N}}{\partial x'^{\nu_N}} \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N}(x)}{\varepsilon}. \quad (7.1.58)$$

This Lie derivative vanishes if and only if the diffeomorphism produced by the flow of ξ^μ is a symmetry of that tensor field.

In order to give a simplified formula for the Lie derivative of a tensor field, we need to study the change of basis matrix of derivatives slightly. By equation (7.1.51):

$$\frac{\partial x'^\mu}{\partial x^\nu} = \delta^\mu_\nu + \varepsilon \partial_\nu \xi^\mu + \mathcal{O}(\varepsilon^2). \quad (7.1.59)$$

In order to get a similar formula for the inverse matrix we use that in the $\varepsilon \rightarrow 0$ limit the transformation

becomes the identity:

$$\left. \frac{\partial x'^\mu}{\partial x^\nu} \right|_{\varepsilon=0} = \delta_\nu^\mu \implies \left. \frac{\partial x^\mu}{\partial x'^\nu} \right|_{\varepsilon=0} = \delta_\nu^\mu. \quad (7.1.60)$$

Therefore, for some matrix $J^\mu{}_\nu(x)$ (independent of ε):

$$\frac{\partial x^\mu}{\partial x'^\nu} = \delta_\nu^\mu + \varepsilon J^\mu{}_\nu(x) + \mathcal{O}(\varepsilon^2). \quad (7.1.61)$$

Then, inputting this into the matrix inverse condition:

$$\frac{\partial x'^\mu}{\partial x^\rho} \frac{\partial x^\rho}{\partial x'^\nu} = \delta_\nu^\mu \implies (\delta_\rho^\mu + \varepsilon \partial_\rho \xi^\mu + \mathcal{O}(\varepsilon^2)) (\delta_\nu^\rho + \varepsilon J^\rho{}_\nu + \mathcal{O}(\varepsilon^2)) = \delta_\nu^\mu \quad (7.1.62)$$

$$\delta_\nu^\mu + \varepsilon \partial_\nu \xi^\mu + \varepsilon J^\mu{}_\nu + \mathcal{O}(\varepsilon^2) = \delta_\nu^\mu \quad (7.1.63)$$

$$\implies J^\mu{}_\nu = -\partial_\nu \xi^\mu \quad (7.1.64)$$

$$\implies \frac{\partial x^\mu}{\partial x'^\nu} = \delta_\nu^\mu - \varepsilon \partial_\nu \xi^\mu + \mathcal{O}(\varepsilon^2). \quad (7.1.65)$$

Using this and expanding the definition in (7.1.58) to first order in ε , we find that simplifying gives precisely:

$$\boxed{L_\xi \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_N} = \xi^\rho \partial_\rho \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_N} - \phi^{\rho \mu_2 \dots \mu_M}{}_{\nu_1 \dots \nu_N} \partial_\rho \xi^{\mu_1} - \dots - \phi^{\mu_1 \dots \mu_{M-1} \rho}{}_{\nu_1 \dots \nu_N} \partial_\rho \xi^{\mu_M} + \phi^{\mu_1 \dots \mu_M}{}_{\rho \nu_2 \dots \nu_N} \partial_{\nu_1} \xi^\rho + \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_{N-1} \rho} \partial_{\nu_N} \xi^\rho.} \quad (7.1.66)$$

You should note that the Lie derivative defined here coincides exactly with the Lie bracket of vector fields derived in section 1.3 when the tensor field considered is simply a vector field. In particular, for a vector field ψ^μ :

$$L_\xi \psi^\mu = \xi^\nu \partial_\nu \psi^\mu - \psi^\nu \partial_\nu \xi^\mu = [\hat{\xi}, \hat{\psi}]^\mu = (\hat{\psi} \angle \hat{\xi})^\mu \quad (7.1.67)$$

where $\hat{\xi} = \xi^\mu \partial_\mu$ and $\hat{\psi} = \psi^\mu \partial_\mu$ are the differential operators which perform diffeomorphisms of the coordinates by ξ^μ and ψ^μ respectively.

If a tensor field ϕ is to be symmetric under all gauge diffeomorphisms, this Lie derivative must vanish for all choices of ξ^μ . At any individual x_0 , it is possible to define a smooth vector field so that $\xi^\mu(x_0)$ is non zero but all of the partial derivatives $\partial_\nu \xi^\mu(x_0)$ are 0. Therefore, if the Lie derivative is to vanish for all ξ , each component of the term proportional to ξ^μ must vanish separately at each point:

$$\partial_\rho \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_N} = 0 \implies \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_N} = \text{uniform constant}. \quad (7.1.68)$$

Thus, a tensor field symmetric under all diffeomorphisms must be uniformly constant. Further, at any individual x_0 , it is possible to define a smooth vector field so that $\xi^\mu(x_0)$ is 0 and exactly one arbitrary entry in the matrix of partial derivatives $\partial_\rho \xi^\sigma(x_0)$ is nonzero. Therefore, the terms multiplying each such component must vanish separately and so we have:

$$-\phi^{\rho \mu_2 \dots \mu_M}{}_{\nu_1 \dots \nu_N} \delta_\sigma^{\mu_1} - \dots - \phi^{\mu_1 \dots \mu_{M-1} \rho}{}_{\nu_1 \dots \nu_N} \delta_\sigma^{\mu_M} + \phi^{\mu_1 \dots \mu_M}{}_{\sigma \nu_2 \dots \nu_N} \delta_{\nu_1}^\rho + \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_{N-1} \sigma} \delta_{\nu_N}^\rho = 0. \quad (7.1.69)$$

By contracting this formula with δ_ρ^σ , each of the terms with a minus sign become equal, and each of the terms with a plus sign become equal, giving as a result:

$$(N - M) \phi^{\mu_1 \dots \mu_M}{}_{\nu_1 \dots \nu_N} = 0. \quad (7.1.70)$$

Therefore, for $N \neq M$, the only possible components for a tensor field so that the tensor is symmetric under all diffeomorphisms is for the tensor itself to vanish! In the case $N = M$ this conclusion is modified *slightly*. This is because the Kronecker δ_ν^μ transforms correctly as the components of a tensor with one upper and one lower index. So, constant coefficient sums of products of Kronecker deltas can be used to form genuine tensors which have an equal number of upper and lower indices and such tensors have vanishing Lie derivative under all diffeomorphisms. However, these are all the tensors with that property. As well, these tensors are essentially trivial, as all they do is contract indices. Therefore, **there are no nontrivial tensors which are invariant under all diffeomorphisms**.

Because of this, due to diffeomorphism symmetry, there can be no nontrivial background tensors in our action. None. This is an enormous shift, because until this point, we have always had the Minkowski metric as a background tensor! The Minkowski metric is symmetric under *some* diffeomorphisms (all Poincare transformations) but it is certainly not symmetric under *all* gauge diffeomorphisms, as we require. In fact, because the metric tensor is a tensor written with two lower indices, no metric tensor can be symmetric under all diffeomorphisms. Therefore, **the metric tensor cannot be a background tensor**. We must have a

metric tensor in order to have a notion of proper time, and so in order to both have a metric tensor and diffeomorphism symmetry, **the metric tensor must be a dynamical variable in our theory.**

Replacing the Minkowski metric $\eta_{\mu\nu}$ with a dynamical metric tensor $g_{\mu\nu}(x)$ means the metric now gets an equation of motion by varying the action. This is an enormous discovery. For a dynamical metric, while it is always possible to transform it to the Minkowski metric at a single point, there is no reason to believe that it can be transformed simultaneously to the Minkowski metric everywhere (in fact, requiring us to be able to do so illegally reintroduces the Minkowski metric as a background tensor). Therefore, **by making the metric dynamical, spacetime can no longer be Minkowski space.** Minkowski space is just three dimensional Euclidean space at each time with an orthogonal time direction and a way to measure proper times and distances. We keep the ability to measure proper times and distances, but now our general spacetime manifold will not simply be like Euclidean space with an orthogonal time direction. Instead, with a generic metric, **spacetime is generically a curved manifold.** Making the metric dynamical forces us to consider spacetime as having a dynamical and typically curved geometry! Because spacetime has no fixed background metric and so no fixed background geometry, this discovery is often called the **background independence of general relativity.**

The argument of this section can be summarized in a few steps. Gravity must couple to mass in the nonrelativistic limit to reproduce observations. In the relativistic case this requires that gravity couples to the energy-momentum tensor, because it is the only conserved covariant object from which one may extract the mass density in the nonrelativistic limit. The local conservation laws of the energy-momentum tensor cause some gravitational equations of motion to be degenerate in precisely the same way that local charge conservation causes Gauss' law to be degenerate with the other Maxwell's equations. The degenerate equations of motion are thus first class constraints which generate gauge transformations of the theory. Because energy and momentum generate spacetime translations, the transformations generated by these constraints are local spacetime translations, called gauge diffeomorphisms. Thus, any relativistic theory of gravity must have symmetry under gauge diffeomorphisms. No metric tensor can be symmetric under all gauge diffeomorphisms, and so no metric tensor can be a fixed background quantity in the theory. A metric tensor is necessary to define a notion of proper time, proper distance, or causality, and so we need to keep the metric without it being a background quantity. To have a metric tensor that isn't background, we must make it a dynamical variable in the theory. Because the metric is now dynamical, it may take any generic value as a field. A spacetime manifold with a generic metric tensor is generally geometrically nontrivial, and thus any relativistic theory of gravity must be a theory of curved evolving spacetime.

We are now ready to state the fundamental assumptions of **Einstein Classical Mechanics (ECM).** First, we are still working with the convenient fiction of point-particles when discussing matter (to be corrected in Part II). A moving matter particle will trace out a curve in spacetime (by noting its position at each time), known as the worldline of the particle. Because a massive particle must always be moving slower than light to not introduce causality violations, the 4-velocity of the particle must always be timelike. In components, the 4-velocity is the derivative of the coordinates of the particle with respect to proper time, and so is the tangent vector to the worldline at the particle's location. Because the worldline of the particle everywhere must have a timelike tangent, the worldline of a massive particle is said to be a timelike curve:

Assumption :: ECMI - Matter is point-like

Matter consists of moving points. The points have no internal structure and so a particle's motion is completely specified by a timelike curve in spacetime, called the particle's worldline.

We have discovered that diffeomorphism symmetry is the fundamental gauge symmetry of gravity and so:

Assumption :: ECMII - Diffeomorphism Symmetry

The Universe has symmetry under gauge diffeomorphisms.

From this, we have discovered that spacetime is curved and dynamical, with the geometry captured by the metric tensor and so:

Assumption :: ECMIII - Spacetime is Lorentzian

Spacetime is a Lorentzian manifold and the metric tensor of that manifold is a dynamical variable.

A theory of curved dynamical spacetime is called **general relativity**. One may very reasonably wonder how general relativity could possibly reproduce the more familiar Minkowski spacetime and its global Poincare symmetries (spacetime translations and Lorentz transformations). In order to explain the success of Minkowski space and special relativistic physics, whatever theory we do find for the metric will have to at low energies far enough away from any objects approximately reproduce Minkowskian physics. As well, in order to explain the successful aspects of Newton's gravity, it will have to be able to appropriately reproduce that theory at low speeds. General relativity will succeed in both of these efforts.

Exercises

Problem 7.1: Symmetries of Minkowski Space. Consider Minkowski spacetime. Let ξ^μ be a vector field which is a symmetry of this spacetime. A vector field which generates a symmetry of a spacetime is called a Killing vector of that spacetime.

- (a) Show that the symmetry condition ($L_\xi \eta_{\mu\nu} = 0$) is equivalent to:

$$\partial_\mu \xi_\nu + \partial_\nu \xi_\mu = 0.$$

- (b) Show by taking a derivative of the above condition that $\partial_{\mu\nu} \xi_\rho = 0$. Show further then that the symmetry condition is solved by:

$$\xi^\mu(x) = a^\mu - 2\theta^\mu{}_\nu x^\nu$$

where a^μ is a constant vector and $\theta_{\mu\nu} = -\theta_{\nu\mu}$ is a constant antisymmetric tensor.

- (c) Explain by considering the behavior of ξ^μ as a diffeomorphism how the previous part shows that the symmetries of Minkowski space are precisely Poincare transformations (global spacetime translations and Lorentz transformations). Show that the parameters a^μ correspond to a translation and $\theta^{\alpha\beta}$ correspond to Lorentz transformation parameters.

Problem 7.2: Symmetries of the Electromagnetic field. Consider a generic uniform $\mathcal{F}_{\mu\nu}$ in Minkowski spacetime.

- (a) Let ξ^μ be a symmetry of both Minkowski space and $\mathcal{F}_{\mu\nu}$. Show that for a generic uniform $\mathcal{F}_{\mu\nu}$, the most general such ξ^μ has the form:

$$\xi^\mu(x) = a^\mu$$

for arbitrary constant a^μ .

- (b) Show that for a given a^μ , it is possible to find a vector potential A_μ for the field strength such that A_μ also has strict symmetry under $\xi^\mu = a^\mu$ (in the sense that $L_\xi A_\mu = 0$).
- (c) Show that if A_μ has been constructed as described in the previous part then there must exist a'^μ so that $\xi'^\mu = a'^\mu$ is only a symmetry of A_μ up to a gauge transformation (in the sense that $L_{\xi'} A_\mu = \partial_\mu f$ for some scalar field f). Thus conclude that when considering the symmetries of the electromagnetic field one must allow the vector potential to change by a gauge transformation.

7.2 Differentiation on Manifolds

7.2.1 Connection and Covariant Differentiation

Now that we are working on a spacetime with nontrivial geometry, defining a meaningful notion of differentiation is slightly trickier. A scalar field $\phi(x)$ is a map from the spacetime manifold $\mathbb{T}$ into the real numbers $\mathbb{R}$, and there is no issue defining its derivative:

$$\xi^\mu \partial_\mu \phi(x) = \lim_{\varepsilon \rightarrow 0} \frac{\phi(x + \varepsilon \xi) - \phi(x)}{\varepsilon} \quad (7.2.1)$$

where $x + \varepsilon \xi$ is the list of coordinate values with entries $x^\nu + \varepsilon \xi^\nu$ and ξ^ν are some arbitrary coefficients by which the coordinates are incremented. The transformation property of $\partial_\mu \phi$ is necessarily different from ϕ . Using the chain rule:

$$\partial'_\mu \phi'(x') = \frac{\partial x^\nu}{\partial x'^\mu} \partial_\nu \phi(x) \quad (7.2.2)$$

and so the components of $\partial_\mu \phi$ transform correctly for a lower index object. Automatically, the quantity $g^{\mu\nu} \partial_\nu \phi \vec{e}_\mu$ is a proper vector field.

A vector field $A(x)$ (with components $A^\mu(x)$) is a map from the spacetime manifold $\mathbb{T}$ into the tangent bundle $T(\mathbb{T})$, specifically at each $X \in \mathbb{T}$ giving a vector in the tangent space $T_X(\mathbb{T})$. Each tangent space $T_X(\mathbb{T})$ is a vector space spanned by the coordinate basis vectors at X . However, for $X \neq X'$, the tangent spaces $T_X(\mathbb{T})$ and $T_{X'}(\mathbb{T})$ are two different vector spaces and so there is no preexisting way to take linear combinations of vectors in $T_X(\mathbb{T})$ and $T_{X'}(\mathbb{T})$. This is a problem, because one might suspect that you could define the derivative of $A(x)$ by a difference quotient:

$$\xi^\mu \partial_\mu A(x) \stackrel{?}{=} \lim_{\varepsilon \rightarrow 0} \frac{A(x + \varepsilon \xi) - A(x)}{\varepsilon} \quad (7.2.3)$$

however this numerator involves the difference of two vectors in different vector spaces ($A(x + \varepsilon \xi)$ is a vector in $T_{X(x + \varepsilon \xi)}(\mathbb{T})$ while $A(x)$ is a vector in $T_{X(x)}(\mathbb{T})$) and so is undefined. This may seem like a pedantic point at first, but is in fact a quite significant geometric problem. Consider a curved surface, such as the surface of a sphere. The tangent space T_X on that sphere at some point is (as we defined it) the space of displacement vectors on the manifold at that point, and so is the space of all the vectors one could draw starting at the point X which are tangent to the surface of the sphere (hence the name tangent space). Visually, the tangent space T_X of the surface is the plane that is tangent to the sphere at the point X . The tangent space $T_{X'}$ at a different nearby point X' will be a different plane. While from outside of the sphere (called an extrinsic perspective) one could imagine linear combinations of vectors that are parallel to the sphere at one point with vectors that are parallel at another nearby point, there is absolutely no guarantee that the result of such a linear combination will be tangent to the sphere at either X or X' , and so does not produce a valid displacement. Such a linear combination has no intrinsic description in terms of the sphere itself.

The trouble with these differing tangent spaces is solved by the notion of **parallel transport**. Suppose for two very close points X and X' we had a function that takes a vector $A(x) \in T_X(\mathbb{T})$ and outputs a vector in $T_{X'}(\mathbb{T})$. We write such a function, called a parallel transport map, as $\Upsilon(A, x, x')$. Then, we could use this function to put both terms in the numerator of (7.2.3) in the same vector space, thus allowing us to take a difference between them. The resulting derivative is no longer a literal partial derivative, and so we give it a different name. It is called the **covariant derivative** and it is written as ∇_μ . Therefore, the covariant derivative is defined by:

$$\xi^\mu \nabla_\mu A(x) \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(A(x + \varepsilon \xi), x + \varepsilon \xi, x) - A(x)}{\varepsilon}. \quad (7.2.4)$$

Obviously different choices of the parallel transport map Υ will result in different definitions of the covariant derivative, and so now we turn to the question of what is the most geometrically natural choice of definition. In order for the covariant derivative to be geometrically meaningful, its definition has to be independent of the coordinates used. This is reflected in that the left hand side is linear in the coefficients ξ^μ and so whatever function Υ actually is, it must be so that it reproduces that linearity in ξ^μ in the $\varepsilon \rightarrow 0$ limit. As well, because Υ acts as a map between vector spaces, in order to respect the linearity of those vector spaces it must be linear itself in how it acts on A . That is, we require:

$$\Upsilon(A^\nu \vec{e}_\nu, x, x') = A^\nu \Upsilon(\vec{e}_\nu, x, x') \quad (7.2.5)$$

for all coefficients A^ν . Alternatively, one can see that this is demanded by requiring the covariant derivative

operator ∇_μ itself to be linear ($\nabla_\mu(A + B) = \nabla_\mu A + \nabla_\mu B$).

By using the linearity of parallel transport, we can simplify our derivative definition slightly:

$$\xi^\mu \nabla_\mu A(x) = \lim_{\varepsilon \rightarrow 0} \frac{A^\nu(x + \varepsilon \xi) \Upsilon(\vec{e}_\nu(x + \varepsilon \xi), x + \varepsilon \xi, x) - A^\nu(x) \vec{e}_\nu(x)}{\varepsilon} \quad (7.2.6)$$

$$= \lim_{\varepsilon \rightarrow 0} \left(A^\nu(x + \varepsilon \xi) \frac{\Upsilon(\vec{e}_\nu(x + \varepsilon \xi), x + \varepsilon \xi, x) - \vec{e}_\nu(x)}{\varepsilon} + \frac{A^\nu(x + \varepsilon \xi) - A^\nu(x)}{\varepsilon} \vec{e}_\nu(x) \right) \quad (7.2.7)$$

$$= A^\nu(x) \xi^\mu \nabla_\mu \vec{e}_\nu(x) + \xi^\mu (\partial_\mu A^\nu(x)) \vec{e}_\nu(x). \quad (7.2.8)$$

Therefore, if we know how to take the covariant derivatives of our basis vectors then we know how to take the covariant derivative of any vector field.

Because $\nabla_\mu A(x)$ is given by (the limit of) a difference of two vectors in $T_X(\mathbb{T})$ (up to a scalar multiplier), it is also a vector in $T_X(\mathbb{T})$ (because it is a vector space). Thus, there exist components $\nabla_\mu A^\nu(x)$ so that:

$$\nabla_\mu A(x) = (\nabla_\mu A^\nu) \vec{e}_\nu. \quad (7.2.9)$$

By the identical logic, $\nabla_\mu \vec{e}_\nu$ is a vector in $T_X(\mathbb{T})$ and so can be written as a linear combination of the basis vectors $\vec{e}_\rho$. The coefficients of that linear combination are called the **connection** $\Gamma^\rho_{\nu\mu}(x)$:

$$\boxed{\nabla_\mu \vec{e}_\nu(x) = \Gamma^\rho_{\nu\mu}(x) \vec{e}_\rho(x).} \quad (7.2.10)$$

Then, (7.2.8) written in components gives:

$$\boxed{\nabla_\mu A^\nu = \partial_\mu A^\nu + \Gamma^\nu_{\rho\mu} A^\rho.} \quad (7.2.11)$$

The connection coefficients $\Gamma^\rho_{\nu\mu}$ are named so because through relating the covariant derivatives of basis vectors to the basis vectors themselves, they tell us how to “connect” nearby tangent spaces by parallel transport. In fact, through solving a differential equation, the connection can be used to fully recover the parallel transport map.

Suppose we have a path through the manifold $X(\lambda)$ parameterized by a parameter λ , written in coordinates as $x^\mu(\lambda)$. Suppose we have a vector $A(0)$ in the tangent space at $X(0)$ which we want to parallel transport along the curve so that $A(\lambda)$ is the parallel transported vector the tangent space $T_{X(\lambda)}(\mathbb{T})$. From $X(\lambda)$ we could transport that vector to the nearby point $X(\lambda + \varepsilon)$ using Υ to define a new vector $A'_\varepsilon(\lambda)$:

$$A'_\varepsilon(\lambda) = \Upsilon(A(\lambda), x(\lambda), x(\lambda + \varepsilon)). \quad (7.2.12)$$

We could then parallel transport this back to $x(\lambda)$. For ε sufficiently small, this is guaranteed to simply undo the original parallel transport and so:

$$\Upsilon(A'_\varepsilon(\lambda), x(\lambda + \varepsilon), x(\lambda)) = A(\lambda). \quad (7.2.13)$$

This can be rewritten suggestively as:

$$\frac{\Upsilon(A'_\varepsilon(\lambda), x(\lambda + \varepsilon), x(\lambda)) - A(\lambda)}{\varepsilon} = 0. \quad (7.2.14)$$

We now define a family of vectors $A(\lambda)$ parameterized by λ so that at each λ the vector $A(\lambda)$ is parallel transported along the curve $x(\lambda)$. That is, for ε sufficiently small, we identify $A'_\varepsilon(\lambda) = A(\lambda + \varepsilon)$. Then, in the $\varepsilon \rightarrow 0$ limit:

$$\lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(A(\lambda + \varepsilon), x(\lambda + \varepsilon), x(\lambda)) - A(\lambda)}{\varepsilon} = 0 \quad (7.2.15)$$

$$\implies \frac{dx^\mu}{d\lambda} \nabla_\mu A = 0. \quad (7.2.16)$$

Here we have used that $x^\mu(\lambda + \varepsilon) = x^\mu(\lambda) + \varepsilon \frac{dx^\mu}{d\lambda}(\lambda) + \mathcal{O}(\varepsilon^2)$. This gives a differential equation for how to parallel transport an initial vector $A(0)$ at $X(0)$ along the curve $X(\lambda)$ to other points. Thus, it determines the parallel transport map Υ from the covariant derivative (or equivalently the connection coefficients).

Importantly, the connection is **NOT** a tensor and the connection coefficients do not form the components of a tensor. The reason why is clear. For a vector field $A(x)$, $\xi^\mu \nabla_\mu A$ produces another vector field. Thus, the components $\nabla_\mu A^\nu$ do transform correctly as components of a tensor. That is:

$$\nabla'_\mu A'^\nu(x') = \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial x'^\nu}{\partial x^\sigma} \nabla_\rho A^\sigma(x) \quad (7.2.17)$$

under a coordinate transformation. The partial derivatives $\partial_\mu A^\nu$ do **NOT** transform correctly as the

components of a tensor. Specifically:

$$\partial'_\mu A'^\nu(x') = \frac{\partial x^\rho}{\partial x'^\mu} \partial_\rho \left(\frac{\partial x'^\nu}{\partial x^\sigma} A^\sigma \right) = \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial x'^\nu}{\partial x^\sigma} \partial_\rho A^\sigma + \frac{\partial x^\rho}{\partial x'^\mu} \frac{\partial^2 x'^\nu}{\partial x^\rho \partial x^\sigma} A^\sigma. \quad (7.2.18)$$

The connection coefficients transform however they must so that (7.2.11) is true (as that equation is equivalent to their definition in (7.2.10)). Therefore, they cannot be the components of a tensor as they are the difference between the components of a tensor and a matrix of coefficients which are not the coefficients of a tensor:

$$\Gamma'^\rho{}_{\mu\nu} A'^\mu = \nabla'_\nu A'^\rho - \partial'_\nu A'^\rho = \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\sigma} \nabla_\mu A^\sigma - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\sigma} \partial_\mu A^\sigma - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\mu \partial x^\sigma} A^\sigma \quad (7.2.19)$$

$$= \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\sigma} (\partial_\mu A^\sigma + \Gamma^\sigma{}_{\gamma\mu} A^\gamma) - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\sigma} \partial_\mu A^\sigma - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\mu \partial x^\sigma} A^\sigma \quad (7.2.20)$$

$$= \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\sigma} \Gamma^\sigma{}_{\gamma\mu} A^\gamma - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\mu \partial x^\sigma} A^\sigma. \quad (7.2.21)$$

Because this holds for all A^μ , we have:

$$\Gamma'^\rho{}_{\mu\nu} \frac{\partial x'^\mu}{\partial x^\sigma} = \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial x'^\rho}{\partial x^\gamma} \Gamma^\gamma{}_{\sigma\mu} - \frac{\partial x^\mu}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\mu \partial x^\sigma}. \quad (7.2.22)$$

Inverting the derivative matrix then gives:

$$\Gamma'^\rho{}_{\mu\nu}(x') = \frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \Gamma^\gamma{}_{\alpha\beta}(x) - \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} \quad (7.2.23)$$

which is not the correct transformation property for the components of a tensor of any rank, as expected. The connection coefficients are nontensorial precisely to cancel the nontensorial aspect of the the partial derivatives of vector field components, so that the covariant derivatives of vector field components *are* tensorial. Because the connection coefficients are not tensorial we will never raise or lower the indices of the connection coefficients using the metric. The indices of the connection coefficients will be permanently fixed in their positions so that we are never tricked into misunderstanding their transformation properties.

There are further geometric conditions that a reasonable parallel transport map should satisfy, and consequent conditions on the connection coefficients. The pseudo-inner product of two vectors using the metric is a coordinate invariant real number, and so should be unaffected by parallel transport. That is, we require for two vector fields $A(x)$, $B(x)$ that:

$$\Upsilon(A(x), x, x') \cdot \Upsilon(B(x), x, x') = A(x) \cdot B(x). \quad (7.2.24)$$

This property is known as the **metricity** or metric compatibility of parallel transport. Geometrically, because the pseudo-inner product of vectors is used to determine angles and lengths, metricity requires that the angles between vectors and lengths of vectors be preserved by parallel transport. Returning to the sphere as a visual example, between two nearby points on that sphere one can imagine the shortest arc that connects them. If a vector is drawn tangent to the sphere at one point, that vector could be scooted along the arc (the meaning of transport in parallel transport) in such a way that its angle relative to the arc's tangent is constant (the meaning of parallel in parallel transport) during the scooting, until it arrives at the other point. This then gives a full parallel transport map, plainly satisfying linearity and metricity, with a clear geometric picture. Alternatively, from a physical perspective, the pseudo-inner product is used to determine proper times and proper lengths, and so any physically reasonable notion of parallel transport should preserve those physical properties and thus be metric compatible.

Let us see what metricity requires of the connection coefficients. For brevity, let $x'^\mu = x^\mu + \varepsilon \xi^\mu$ for some coefficients ξ^μ . Because the metricity condition holds for all x and x' sufficiently close to each other, it also holds for renaming x to x' and x' to x (as such points still remain the same sufficiently close distance from each other after relabeling). Then, in components, metricity requires:

$$g_{\mu\nu}(x) \Upsilon^\mu(A(x'), x', x) \Upsilon^\nu(B(x'), x', x) = g_{\mu\nu}(x') A^\mu(x') B^\nu(x'). \quad (7.2.25)$$

For brevity, write A' to mean $A(x')$, B' to mean $B(x')$, and g' to mean $g(x')$. Unprimed quantities then are all evaluated at x . Then, with some slight algebra, this equation may be rearranged to:

$$\begin{aligned} g_{\mu\nu} A^\mu \frac{\Upsilon^\nu(B', x', x) - B^\nu}{\varepsilon} + g_{\mu\nu} \frac{\Upsilon^\mu(A', x', x) - A^\mu}{\varepsilon} B^\nu \\ + \varepsilon g_{\mu\nu} \frac{\Upsilon^\mu(A', x', x) - A^\mu}{\varepsilon} \frac{\Upsilon^\nu(B', x', x) - B^\nu}{\varepsilon} - \frac{g'_{\mu\nu} A'^\mu B'^\nu - g_{\mu\nu} A^\mu B^\nu}{\varepsilon} = 0. \end{aligned} \quad (7.2.26)$$

Each of these terms now has a simple $\varepsilon \rightarrow 0$ limit. Taking the $\varepsilon \rightarrow 0$ limit of this equation gives:

$$g_{\mu\nu}A^\mu\xi^\rho\nabla_\rho B^\nu + g_{\mu\nu}\xi^\rho(\nabla_\rho A^\mu)B^\nu + 0 - \xi^\rho\partial_\rho(g_{\mu\nu}A^\mu B^\nu) = 0. \quad (7.2.27)$$

Because this equation is true for all coefficients ξ^ρ , we have:

$$A^\mu B^\nu\partial_\rho g_{\mu\nu} + g_{\mu\nu}B^\nu\partial_\rho A^\mu + g_{\mu\nu}A^\mu\partial_\rho B^\nu = g_{\mu\nu}A^\mu\nabla_\rho B^\nu + g_{\mu\nu}B^\nu\nabla_\rho A^\mu. \quad (7.2.28)$$

Now using (7.2.11) on the right hand side and simplifying we have:

$$A^\mu B^\nu(g_{\mu\sigma}\Gamma^\sigma_{\nu\rho} + g_{\nu\sigma}\Gamma^\sigma_{\mu\rho} - \partial_\rho g_{\mu\nu}) = 0. \quad (7.2.29)$$

Because this holds for all A^μ and B^ν , due to metricity, the connection coefficients must satisfy:

$$\boxed{g_{\mu\sigma}\Gamma^\sigma_{\nu\rho} + g_{\nu\sigma}\Gamma^\sigma_{\mu\rho} = \partial_\rho g_{\mu\nu}.} \quad (7.2.30)$$

The **torsion** $T^\rho_{\mu\nu}$ of a connection is defined by the combination:

$$T^\rho_{\mu\nu} = -T^\rho_{\nu\mu} = \frac{\Gamma^\rho_{\mu\nu} - \Gamma^\rho_{\nu\mu}}{2}. \quad (7.2.31)$$

Using the torsion it is possible to interchange the lower indices of the connection coefficients:

$$\Gamma^\rho_{\mu\nu} = \Gamma^\rho_{\nu\mu} + 2T^\rho_{\mu\nu}. \quad (7.2.32)$$

Using the transformation property of the connection coefficients, we can see that the torsion is genuinely a tensor:

$$T'^\rho_{\mu\nu} = \frac{\Gamma'^\rho_{\mu\nu} - \Gamma'^\rho_{\nu\mu}}{2} \quad (7.2.33)$$

$$= \frac{1}{2} \left(\frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \Gamma^\gamma_{\alpha\beta} - \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} \right) - \frac{1}{2} \left(\frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \Gamma^\gamma_{\beta\alpha} - \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} \right) \quad (7.2.34)$$

$$= \frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\Gamma^\gamma_{\alpha\beta} - \Gamma^\gamma_{\beta\alpha}}{2} \quad (7.2.35)$$

$$= \frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} T^\gamma_{\alpha\beta}. \quad (7.2.36)$$

Because the torsion tensor is genuinely tensorial, we will raise and lower its indices with the metric tensor as usual.

Through iterative use and reuse of the metricity conditions and the definition of torsion, we can find a nice expression for the connection coefficients. In particular:

$$g_{\rho\sigma}\Gamma^\rho_{\mu\nu} = \partial_\nu g_{\sigma\mu} - g_{\mu\rho}\Gamma^\rho_{\sigma\nu} = \partial_\nu g_{\sigma\mu} - g_{\mu\rho}(\Gamma^\rho_{\nu\sigma} + 2T^\rho_{\nu\sigma}) \quad (7.2.37)$$

$$= \partial_\nu g_{\sigma\mu} + 2T_{\mu\nu\sigma} - g_{\mu\rho}\Gamma^\rho_{\nu\sigma} = \partial_\nu g_{\sigma\mu} + 2T_{\mu\nu\sigma} - \partial_\sigma g_{\mu\nu} + g_{\nu\rho}\Gamma^\rho_{\mu\sigma} \quad (7.2.38)$$

$$= \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu} + 2T_{\mu\nu\sigma} + 2T_{\nu\mu\sigma} + g_{\nu\rho}\Gamma^\rho_{\sigma\mu} \quad (7.2.39)$$

$$= \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu} + 2T_{\mu\nu\sigma} + 2T_{\nu\mu\sigma} + \partial_\mu g_{\sigma\nu} - g_{\rho\sigma}\Gamma^\rho_{\nu\mu} \quad (7.2.40)$$

$$= \partial_\mu g_{\sigma\nu} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu} + 2T_{\mu\nu\sigma} + 2T_{\nu\mu\sigma} - g_{\rho\sigma}\Gamma^\rho_{\mu\nu} - 2T_{\sigma\nu\mu}. \quad (7.2.41)$$

We can move the second factor of $g_{\rho\sigma}\Gamma^\rho_{\mu\nu}$ to the left hand side and use the inverse metric to arrive at:

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2}g^{\rho\sigma}(\partial_\mu g_{\sigma\nu} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu}) + T^\rho_{\mu\nu} + T_{\mu\nu}{}^\rho + T_{\nu\mu}{}^\rho. \quad (7.2.42)$$

If the torsion tensor for our connection vanishes (such a connection is called **torsion free**) we see that there is a unique possible resulting connection. That connection is known as the **Levi-Civita connection**, and its given solely in terms of the metric tensors and its first derivatives. The connection coefficients of the Levi-Civita connection are called the **Christoffel symbols**. This gives us:

Theorem 7.1: Levi-Civita Theorem

The unique metric compatible torsion free connection on a Lorentzian manifold is the Levi-Civita connection, which has connection coefficients given by the Christoffel symbols:

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2}g^{\rho\sigma}(\partial_\mu g_{\sigma\nu} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu}). \quad (7.2.43)$$

There is a natural geometric reason to privilege a torsion free connection. A generic smooth manifold

can be viewed extrinsically as being embedded in a higher dimensional flat space. For example, the surface of a sphere is a curved 2-dimensional manifold but can be imagined as living in a completely flat 3-dimensional Euclidean space. Let $\mathbb{M}$ be a flat manifold into which we have embedded the spacetime manifold $\mathbb{T}$. Let $\vec{z}$ be used to indicate a point in $\mathbb{M}$. In a flat manifold, a point can be identified with a vector (the vector that points from the origin to that point) and the tangent space at each point in the manifold is the same vector space. So, it is possible on a flat manifold to take the ordinary partial derivatives of vectors in a sensible way. Let x^μ be coordinates for $\mathbb{T}$ so that $\vec{z}(x)$ gives not just a generic point in $\mathbb{M}$ but specifically a point in $\mathbb{T}$ for each x^μ . Then, the coordinate basis vectors for $\mathbb{T}$ can be defined precisely by the usual difference quotient used to define coordinate basis vectors in a flat space:

$$\vec{e}_\mu = \frac{\partial \vec{z}}{\partial x^\mu}. \quad (7.2.44)$$

This definition gives just the vector based at the point $\vec{z}(x)$ which points in the direction of $\vec{z}(x')$ where x' is changed from x only in the μ direction and only by a very small positive amount. Consequently, due to the equivalence of mixed partials:

$$\partial_\nu \vec{e}_\mu = \frac{\partial^2 \vec{z}}{\partial x^\mu \partial x^\nu} = \partial_\mu \vec{e}_\nu. \quad (7.2.45)$$

The vector $\partial_\nu \vec{e}_\mu$ will generally not be tangent to the surface of $\mathbb{T}$. However, we can define the projection of that vector onto the tangent space of $\mathbb{T}$ at $\vec{z}(x)$. This projected piece then gives the rate of change of $\vec{e}_\mu$ in the ν direction parallel to the surface of $\mathbb{T}$. We take this as the geometric definition of the covariant derivative. That is:

$$\partial_\nu \vec{e}_\mu = \nabla_\nu \vec{e}_\mu + \vec{n}_{\mu\nu} \quad (7.2.46)$$

where $\vec{n}_{\mu\nu}$ is a vector orthogonal to the surface of $\mathbb{T}$ (this way $\nabla_\nu \vec{e}_\mu$ captures the full part of $\partial_\nu \vec{e}_\mu$ which is tangential to the surface of $\mathbb{T}$). The pseudo-inner product of both sides with $\vec{e}_\rho$ then gives:

$$\vec{e}_\rho \cdot \partial_\nu \vec{e}_\mu = \vec{e}_\rho \cdot \nabla_\nu \vec{e}_\mu \quad (7.2.47)$$

(because $\vec{e}_\rho$ is tangential to $\mathbb{T}$ and $\vec{n}_{\mu\nu}$ is orthogonal to it). Then, using the definition of the connection coefficients in (7.2.10), we find:

$$\Gamma^\rho_{\mu\nu} = g^{\rho\sigma} \vec{e}_\sigma \cdot \partial_\nu \vec{e}_\mu. \quad (7.2.48)$$

Due to (7.2.45) the right hand side is symmetric in interchanging μ and ν . Thus the left hand side is as well, and consequently the connection is torsion free. Therefore, if one imagines the connection as arising from the tangential projection of ordinary differentiation between points in a flat embedding space, the connection is automatically torsion free.

The flat space embedding argument is a compelling geometrical argument why when studying a geometrical surface one would take a torsion free connection. I find it a compelling argument why we should expect general relativity to be torsion free, but it is a bit metaphysical use motivation based on imagining spacetime embedded in some higher dimensional flat space. So, it is important to also have a good intrinsic argument why a torsion free connection is reasonable. By the Levi-Civita theorem, on any Lorentzian manifold one can construct a metric compatible and torsion free connection out of the metric and its first partial derivatives. Therefore, there is nothing assumed physically in using such a connection. The physical assumption comes in saying that this is the relevant connection, meaning that no other dynamical degrees of freedom need be considered in the theory. The metric degrees of freedom are all that are required by diffeomorphism symmetry. Of course further degrees of freedom (such as an independent torsion tensor) can be added to the theory as extra fields, but that is precisely what they would be, extra. One can always take the Levi-Civita connection to be defined as the connection of interest, and reinterpret the torsion (if it is present) as just some extra field in the theory which gets its own equations of motion in the action. As usual, we consider first the simplest possible theory consistent with our symmetries, which means considering the minimal degrees of freedom necessary. In this case, that means considering the metric as our dynamical quantity, and excluding the torsion. If experiment found torsion to be necessary, we would add it. So far, all gravitational experiments are consistent with vanishing torsion.

Because there are good geometric and physical reasons to prefer a torsion free connection, beginning now we will always set the torsion tensor to be 0. Consequently, the connection coefficients will always be given by the Christoffel symbols as in theorem 7.1.

From the definition of the covariant derivative and the requirement that the components $\nabla_\mu A^\nu$ transform

properly as a tensor, it is straightforward to define $\nabla_\mu A_\nu$ by the usual index lowering:

$$\nabla_\mu A_\nu = g_{\nu\rho} \nabla_\mu A^\rho. \quad (7.2.49)$$

Then, using metricity of the connection:

$$\nabla_\mu A_\nu = g_{\nu\rho} (\partial_\mu A^\rho + \Gamma^\rho_{\sigma\mu} A^\sigma) = \partial_\mu (g_{\nu\rho} A^\rho) - A^\rho \partial_\mu g_{\nu\rho} + \Gamma^\rho_{\sigma\mu} A^\sigma \quad (7.2.50)$$

$$= \partial_\mu A_\nu - A^\rho (g_{\nu\sigma} \Gamma^\sigma_{\rho\mu} + g_{\rho\sigma} \Gamma^\sigma_{\nu\mu}) + \Gamma^\rho_{\sigma\mu} A^\sigma. \quad (7.2.51)$$

Finishing simplification gives:

$$\boxed{\nabla_\mu A_\nu = \partial_\mu A_\nu - \Gamma^\rho_{\nu\mu} A_\rho.} \quad (7.2.52)$$

Now that we understand how to covariantly differentiate vector fields, we can immediately covariantly differentiate tensor fields. If $\Phi(x)$ is a tensor field written with some combination of raised and lowered components $\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x)$, then we can continue to simply use (7.2.4) to define the covariant derivative of the tensor field, where the parallel transport map is defined to distribute over vectors in a tensor product:

$$\Upsilon(\vec{e}_{\mu_1} \otimes \dots \otimes \vec{e}_{\mu_N}, x, x') = \Upsilon(\vec{e}_{\mu_1}, x, x') \otimes \dots \otimes \Upsilon(\vec{e}_{\mu_N}, x, x'). \quad (7.2.53)$$

This condition is necessary for the parallel transport of a tensor product to be both independent of the basis used for constructing the tensor product and for the parallel transport of a contraction of tensor to be given by the contraction of the parallel transported tensors (which is just metric compatibility extended to tensors). Then:

$$\xi^\mu \nabla_\mu \Phi = \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(\Phi(x + \varepsilon \xi), x + \varepsilon \xi, x) - \Phi(x)}{\varepsilon}. \quad (7.2.54)$$

The result of this definition, when propagated down to the components of Φ , naturally reproduces a factor of the connection coefficients for each index of Φ , with the upper indices behavior exactly like upper index vectors and lower indices behaving exactly like lower index vectors. The result then is:

$$\boxed{\begin{aligned} \nabla_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} &= \partial_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} + \Gamma^{\mu_1}_{\sigma\rho} \phi^{\sigma \mu_2 \dots \mu_M}_{\nu_1 \dots \nu_N} + \dots + \Gamma^{\mu_M}_{\sigma\rho} \phi^{\mu_1 \dots \mu_{M-1} \sigma}_{\nu_1 \dots \nu_N} \\ &\quad - \Gamma^\sigma_{\nu_1 \rho} \phi^{\mu_1 \dots \mu_M}_{\sigma \nu_2 \dots \nu_N} - \dots - \Gamma^\sigma_{\nu_N \rho} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_{N-1} \sigma}. \end{aligned}} \quad (7.2.55)$$

Warning: Partial derivatives commute with each other. Covariant derivatives do not! Do not interchange the order of covariant differentiation. For now, if doing such a thing would be necessary, use the definition of the covariant derivative in terms of partial derivatives and connection coefficients to see what extra terms are necessary to safely do so. Later, we will develop a more efficient formula for commutator of covariant derivatives.

Equation (7.2.55) is a bit obnoxious in how many symbols it takes to communicate a highly ordered idea. In order to make it more digestible and repeatably writable, it is useful to introduce an operator known as **DeWitt's index shuffling operator** $\hat{G}^\alpha_\beta$. The index shuffling operator is defined to be a linear operator which acts on tensor components as:

$$\boxed{\begin{aligned} \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} &= \delta^{\mu_1}_\beta \phi^{\alpha \mu_2 \dots \mu_M}_{\nu_1 \dots \nu_N} + \dots + \delta^{\mu_M}_\beta \phi^{\mu_1 \dots \mu_{M-1} \alpha}_{\nu_1 \dots \nu_N} \\ &\quad - \delta^\alpha_{\nu_1} \phi^{\mu_1 \dots \mu_M}_{\beta \nu_2 \dots \nu_N} - \dots - \delta^\alpha_{\nu_N} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_{N-1} \beta}. \end{aligned}} \quad (7.2.56)$$

Acting the index shuffler on the components of a tensor produces the components of a new tensor with one more upper and one more lower index. Then, the covariant derivative of a tensor can be written simply as:

$$\boxed{\nabla_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} = \partial_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} + \Gamma^\beta_{\alpha\rho} \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}.} \quad (7.2.57)$$

The index shuffler is also useful for other purposes. For example, recalling the Lie derivative of a tensor field from equation (7.1.66), we can express that result much more simply as:

$$L_\xi \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} = \xi^\rho \partial_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} - \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}. \quad (7.2.58)$$

The partial derivatives appearing here can be rewritten in terms of covariant derivatives and connection coefficients. Doing so and using that the connection is torsion free gives:

$$\boxed{L_\xi \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} = \xi^\rho \nabla_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} - \nabla_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}.} \quad (7.2.59)$$

Now we can plainly see that the Lie derivative of a tensor is in fact a tensor, as everything on the right hand side transforms correctly for the components of a tensor.

The index shuffler also appears nicely in the transformation property of a tensor field under a change of

coordinates. Consider a coordinate change of the form (7.1.51) for a tensor (thus transforming by (7.1.54)) and use (7.1.59) and (7.1.65). Doing so gives:

$$\begin{aligned} \phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') &= \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x) + \varepsilon \partial_\alpha \xi^\beta \phi^{\alpha \mu_2 \dots \mu_M}_{\nu_1 \dots \nu_N} + \dots + \varepsilon \partial_\alpha \xi^\beta \phi^{\mu_1 \dots \mu_{M-1} \alpha}_{\nu_1 \dots \nu_N} \\ &\quad - \varepsilon \partial_\alpha \xi^\beta \phi^{\mu_1 \dots \mu_M}_{\beta \nu_2 \dots \nu_N} - \dots - \varepsilon \partial_\alpha \xi^\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_{N-1} \beta} + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (7.2.60)$$

This is horrendous, but can be repackaged very nicely using the index shuffler:

$$\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') = \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x) + \varepsilon \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} + \mathcal{O}(\varepsilon^2). \quad (7.2.61)$$

Viewed as a field transformation then, a coordinate change acts as:

$$\left. \frac{\partial}{\partial \varepsilon} \phi'^a(\varepsilon, x, \phi) \right|_{\varepsilon=0} = \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^a \quad (7.2.62)$$

where a is used as a “compound index”, meaning just the list of whatever tensor indices ϕ^a should have. This expression is not covariant because the ε derivative here involves a difference quotient between field values at different points (x' versus x). When considering field transformations, the covariant object is:

$$\mathcal{D}\phi^a = \left. \frac{\partial}{\partial \varepsilon} \Upsilon^a(\phi'(\varepsilon, x, \phi), x', x) \right|_{\varepsilon=0} \quad (7.2.63)$$

which just simply performs the parallel transport back to x necessary to prevent subtracting tensor values at different points. The additional pieces contributed by that parallel transport simply replace the partial derivatives of ξ^μ by covariant derivatives so that:

$$\boxed{\mathcal{D}\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} = \nabla_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}}. \quad (7.2.64)$$

Using this and (7.1.7), the Lie derivative can also be repackaged nicely as:

$$L_\xi \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} = \mathcal{D}x^\rho \nabla_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} - \mathcal{D}\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}. \quad (7.2.65)$$

Recalling that $\mathcal{D}\phi$ gives the change per unit ε of $\phi'(x')$ relative to $\phi(x)$, we can also define the rate of change of ϕ at fixed x by:

$$\mathcal{D}\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}|_x = \lim_{\varepsilon \rightarrow 0} \frac{\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x) - \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x)}{\varepsilon} \quad (7.2.66)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x' - \varepsilon \xi) - \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x)}{\varepsilon} \quad (7.2.67)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{\phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') - \varepsilon \xi^\rho \partial_\rho \phi'^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x') - \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}(x)}{\varepsilon} \quad (7.2.68)$$

$$= \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} - \xi^\rho \partial_\rho \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \quad (7.2.69)$$

$$= -L_\xi \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}. \quad (7.2.70)$$

Therefore one other way of understanding the Lie derivative of a tensor field is as the negative rate of change of the field under a coordinate transformation at fixed position.

It is important to note that one cannot pass factors of the metric past the index shuffler, and so needs to be careful when raising and lowering its indices. In particular, consider the difference between lowering the index of a vector field before and after being acted upon by the index shuffler:

$$g_{\mu\nu} \hat{G}^\alpha_\beta A^\nu - \hat{G}^\alpha_\beta (g_{\mu\nu} A^\nu) = g_{\mu\beta} A^\alpha + \delta_\mu^\alpha A_\beta \neq 0. \quad (7.2.71)$$

So, be careful! Do not accidentally assume these are the same. Because the metric does not commute with the index shuffler, it also doesn't commute with the Lie derivative in general, and so $L_\xi A_\mu$ is not the same thing as $g_{\mu\nu} L_\xi A^\nu$.

The index shuffler satisfies a product rule which is very useful for calculations. Consider the shuffle of the product of two tensors:

$$\begin{aligned} \hat{G}^\alpha_\beta (\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) &= \delta^\mu_\beta \phi^{\alpha \mu_2 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \dots + \delta^\mu_\beta \phi^{\mu_1 \dots \mu_{M-1} \alpha}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} \\ &\quad + \delta^\rho_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\alpha \rho_2 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \dots + \delta^\rho_\beta \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_{K-1} \alpha}_{\sigma_1 \dots \sigma_L} \\ &\quad - \delta^\alpha_{\nu_1} \phi^{\mu_1 \dots \mu_M}_{\beta \nu_2 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} - \dots - \delta^\alpha_{\nu_N} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_{N-1} \beta} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} \\ &\quad - \delta^\alpha_{\sigma_1} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\beta \sigma_2 \dots \sigma_L} - \dots - \delta^\alpha_{\sigma_L} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_{L-1} \beta} \\ &= \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} (\delta^\mu_\beta \phi^{\alpha \mu_2 \dots \mu_M}_{\nu_1 \dots \nu_N} + \dots + \delta^\mu_\beta \phi^{\mu_1 \dots \mu_{M-1} \alpha}_{\nu_1 \dots \nu_N} \end{aligned} \quad (7.2.72)$$

$$\begin{aligned}
& -\delta_{\nu_1}^{\alpha} \phi^{\mu_1 \dots \mu_M}_{\beta \nu_2 \dots \nu_N} - \dots - \delta_{\nu_N}^{\alpha} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_{N-1} \beta}) \\
& + \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} (\delta_{\beta}^{\rho_1} \psi^{\alpha \rho_2 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \dots + \delta_{\beta}^{\rho_K} \psi^{\rho_1 \dots \rho_{K-1} \alpha}_{\sigma_1 \dots \sigma_L} \\
& - \delta_{\sigma_1}^{\alpha} \psi^{\rho_1 \dots \rho_K}_{\beta \sigma_2 \dots \sigma_L} - \dots - \delta_{\sigma_L}^{\alpha} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_{L-1} \beta}).
\end{aligned} \tag{7.2.73}$$

This last equation simply reproduces the structure of the index shuffler, giving:

$$\boxed{\hat{G}^{\alpha}_{\beta}(\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) = (\hat{G}^{\alpha}_{\beta} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}) \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \hat{G}^{\alpha}_{\beta} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}} \tag{7.2.74}$$

which is exactly like how the product rule acts for differentiation. In fact, returning this to the definition of the covariant derivative:

$$\begin{aligned}
\nabla_{\gamma}(\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) &= \partial_{\gamma}(\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) + \Gamma^{\beta}_{\alpha \gamma} \hat{G}^{\alpha}_{\beta}(\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) \\
&= \partial_{\gamma} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \partial_{\gamma} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} \\
&\quad + \Gamma^{\beta}_{\alpha \gamma} (\hat{G}^{\alpha}_{\beta} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}) \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \Gamma^{\beta}_{\alpha \gamma} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \hat{G}^{\alpha}_{\beta} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}.
\end{aligned} \tag{7.2.75}$$

Collecting terms gives that the covariant derivative does in fact satisfy the product rule:

$$\boxed{\nabla_{\gamma}(\phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}) = (\nabla_{\gamma} \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N}) \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L} + \phi^{\mu_1 \dots \mu_M}_{\nu_1 \dots \nu_N} \nabla_{\gamma} \psi^{\rho_1 \dots \rho_K}_{\sigma_1 \dots \sigma_L}.} \tag{7.2.76}$$

Using the covariant derivative, the metricity of the connection can be expressed more nicely. The covariant derivative of the metric tensor gives:

$$\nabla_{\rho} g_{\mu\nu} = \partial_{\rho} g_{\mu\nu} - \Gamma^{\sigma}_{\mu\rho} g_{\sigma\nu} - \Gamma^{\sigma}_{\nu\rho} g_{\mu\sigma} = 0 \tag{7.2.77}$$

by using (7.2.30). Therefore, the metricity of the connection is equivalent to:

$$\boxed{\nabla_{\rho} g_{\mu\nu} = 0.} \tag{7.2.78}$$

So, one can safely commute the metric with the covariant derivative because the term which would be produced from doing so due to the product rule is 0 due to metricity.

Sometimes the metric of a given physical scenario will have a symmetry, just as sometimes the vector potential may have a symmetry (such as an axial rotation symmetry and translation symmetry of a vector potential producing a uniform constant electric field). By the logic of the previous section, if ξ^{μ} generates a change of coordinates which is a symmetry of our physical scenario, then $L_{\xi} g_{\mu\nu} = 0$. Such a vector field is called a **Killing vector field** for our metric. Generically, a metric has no Killing vectors, but in some particularly simple physical scenarios there may be several present. For a generic vector field ξ^{μ} , using (7.2.59) and (7.2.78):

$$L_{\xi} g_{\mu\nu} = \xi^{\rho} \nabla_{\rho} g_{\mu\nu} - \nabla_{\alpha} \xi^{\beta} (-\delta^{\alpha}_{\mu} g_{\beta\nu} - \delta^{\alpha}_{\nu} g_{\mu\beta}) = \nabla_{\mu} \xi_{\nu} + \nabla_{\nu} \xi_{\mu}. \tag{7.2.79}$$

Thus, if ξ^{μ} is a Killing vector field of the metric we have:

$$\boxed{\nabla_{\mu} \xi_{\nu} + \nabla_{\nu} \xi_{\mu} = 0} \tag{7.2.80}$$

which is known as Killing's equation.

7.2.2 Geodesic Equation

In a flat space, such as Minkowski space, it is possible to consider a straight line between two events. In a curved space, the naive version of the idea of a straight line doesn't make sense. For example, to connect two points on a sphere, one necessarily has to move in a curved path (when viewed extrinsically) because the sphere itself is curved. However, there is a natural generalization of the notion of a straight line. In a flat space, the straight line between two points is shortest path connecting those points, in other words, the path connecting the points with stationary arclength. Thus, the straightest path between two points on a differentiable manifold is defined as the path with stationary arclength. Such a path is called a **geodesic**. Consider a path through spacetime which begins at a point $x^{\mu}(0)$ and ends at a point $x^{\mu}(1)$, between which it is parameterized by $x^{\mu}(\lambda)$. The proper time element along this path is then given by (7.1.27):

$$d\tau^2 = -g_{\mu\nu}(x(\lambda)) dx^{\mu}(\lambda) dx^{\nu}(\lambda). \tag{7.2.81}$$

In general, we may consider a path which is timelike (and so $d\tau^2 > 0$), spacelike (and so $ds^2 = -d\tau^2 > 0$), or lightlike (and so $d\tau^2 = 0$). In either the timelike or spacelike case, we define the proper interval dI by:

$$dI = \sqrt{|g_{\mu\nu}(x(\lambda))dx^\mu(\lambda)dx^\nu(\lambda)|}. \quad (7.2.82)$$

The lightlike case can be treated as the limit in which the spacelike and timelike agree. The total interval along the path is then given by:

$$I[x] = \int_0^1 \sqrt{\left| g_{\mu\nu}(x(\lambda)) \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda} \right|} d\lambda. \quad (7.2.83)$$

The geodesic between $x^\mu(0)$ and $x^\mu(1)$ then is the curve connecting those points which makes $I[x]$ stationary. We will assume that the curve is either everywhere timelike or everywhere spacelike. For a timelike or spacelike geodesic this is automatic, and then is automatically true in a small neighborhood of such a geodesic and so is valid in the variational principle about geodesics. Let $\sigma = -1$ if the curve is timelike and $\sigma = 1$ if the curve is spacelike. Then, the proper interval integral is of the form of an action functional, written as the integral of the “Lagrangian”:

$$\mathcal{L}(x, \dot{x}) = \sqrt{\sigma g_{\mu\nu} \dot{x}^\mu \dot{x}^\nu} \quad (7.2.84)$$

where we are using $\dot{x}^\mu = \frac{dx^\mu}{d\lambda}$ as a shorthand. The requirement that the geodesic make I stationary means the functional derivative of I must vanish when evaluated on the geodesic. Familiarly:

$$\frac{\delta I}{\delta x^\mu(\lambda)} = \frac{\partial \mathcal{L}}{\partial x^\mu} - \frac{d}{d\lambda} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}^\mu} \right) \quad (7.2.85)$$

and in particular for (7.2.84):

$$\frac{\partial \mathcal{L}}{\partial x^\mu} = \frac{\sigma}{2\mathcal{L}} \partial_\mu g_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda}, \quad \frac{\partial \mathcal{L}}{\partial \dot{x}^\mu} = \frac{\sigma}{\mathcal{L}} g_{\mu\nu} \frac{dx^\nu}{d\lambda}. \quad (7.2.86)$$

Then:

$$\frac{\delta I}{\delta x^\mu(\lambda)} = \frac{\sigma}{2\mathcal{L}} \partial_\mu g_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} - \frac{d}{d\lambda} \left(\frac{\sigma}{\mathcal{L}} g_{\mu\nu} \frac{dx^\nu}{d\lambda} \right) \quad (7.2.87)$$

$$= \frac{\sigma}{2\mathcal{L}} \partial_\mu g_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} - \frac{\sigma}{\mathcal{L}} \frac{d}{d\lambda} (g_{\mu\nu}) \frac{dx^\nu}{d\lambda} - \frac{\sigma}{\mathcal{L}} g_{\mu\nu} \frac{d^2 x^\nu}{d\lambda^2} + \frac{\sigma}{\mathcal{L}^2} g_{\mu\nu} \frac{dx^\nu}{d\lambda} \frac{d\mathcal{L}}{d\lambda} \quad (7.2.88)$$

$$= \frac{\sigma}{2\mathcal{L}} \partial_\mu g_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} - \frac{\sigma}{\mathcal{L}} \partial_\rho g_{\mu\nu} \frac{dx^\rho}{d\lambda} \frac{dx^\nu}{d\lambda} - \frac{\sigma}{\mathcal{L}} g_{\mu\nu} \frac{d^2 x^\nu}{d\lambda^2} + \frac{\sigma}{\mathcal{L}^2} g_{\mu\nu} \frac{dx^\nu}{d\lambda} \frac{d\mathcal{L}}{d\lambda} \quad (7.2.89)$$

$$= -\frac{\sigma}{\mathcal{L}} g_{\mu\nu} \left(\frac{d^2 x^\nu}{d\lambda^2} + \frac{1}{2} g^{\nu\gamma} (\partial_\rho g_{\gamma\sigma} + \partial_\sigma g_{\gamma\rho} - \partial_\gamma g_{\rho\sigma}) \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} - \frac{1}{\mathcal{L}} \frac{dx^\nu}{d\lambda} \frac{d\mathcal{L}}{d\lambda} \right) \quad (7.2.90)$$

$$= -\frac{\sigma}{\mathcal{L}} g_{\mu\nu} \left(\frac{d^2 x^\nu}{d\lambda^2} + \Gamma^\nu_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} - \frac{1}{\mathcal{L}} \frac{dx^\nu}{d\lambda} \frac{d\mathcal{L}}{d\lambda} \right). \quad (7.2.91)$$

Requiring that the path $x^\mu(\lambda)$ makes the proper interval stationary then gives:

$$\frac{\delta I}{\delta x^\mu(\lambda)} \stackrel{!}{=} 0 \implies \frac{d^2 x^\mu}{d\lambda^2} + \Gamma^\mu_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} = \frac{1}{\mathcal{L}} \frac{dx^\mu}{d\lambda} \frac{d\mathcal{L}}{d\lambda}. \quad (7.2.92)$$

So far the path parameter λ has been completely arbitrary. From this equation of motion it is not possible to determine $\frac{d\mathcal{L}}{d\lambda}$, and this is because the parameter λ has not been fully specified. In fact, $\frac{d\mathcal{L}}{d\lambda}$ is completely arbitrary as a function. Under a reparameterization $\lambda' = \lambda'(\lambda)$ by a smooth increasing function, we have:

$$\mathcal{L}' = \sqrt{\sigma g_{\mu\nu} \frac{dx^\mu}{d\lambda'} \frac{dx^\nu}{d\lambda'}} = \frac{d\lambda}{d\lambda'} \sqrt{\sigma g_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} = \frac{d\lambda}{d\lambda'} \mathcal{L}. \quad (7.2.93)$$

Thus, by changing the definition of λ , we can change $\mathcal{L}$ by an arbitrarily λ -dependent positive multiplier. The most natural class of parameters are **affine parameters**. A parameter λ for a geodesic $x^\mu(\lambda)$ is called affine if:

$$\frac{d}{d\lambda} \sqrt{\sigma g_{\mu\nu}(x) \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} = 0. \quad (7.2.94)$$

We would then call the path $x^\mu(\lambda)$ an affinely parameterized geodesic. Being affinely parameterized is not a geometric property of the geodesic, it is a property of how we express the path of the geodesic as a function.

For an affinely parameterized geodesic then, (7.2.92) becomes:

$$\boxed{\frac{d^2 x^\mu}{d\lambda^2} + \Gamma^\mu_{\rho\sigma}(x(\lambda)) \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} = 0.} \quad (7.2.95)$$

This is known as the **geodesic equation**. When working with a geodesic, we will invariably choose to parameterize it affinely. Note that this equation as written is insensitive to σ , and so both spacelike and timelike geodesics satisfy the geodesic equation. Spacelike and timelike geodesics are only distinguished in the eventual sign of $g_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}$ determined by their boundary conditions. In the limit that the two coincide, we have that lightlike geodesics also satisfy the geodesic equation but with $g_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda} = 0$.

The geodesic equation can be written nicely in a covariant form. The λ velocity $\frac{dx^\mu}{d\lambda}$ components plainly form the components of a 4-vector in $T_{X(\lambda)}(\mathbb{T})$ as they transform correctly as a tensor under a change of coordinates using the chain rule:

$$\frac{dx'^\mu}{d\lambda} = \frac{\partial x'^\mu}{\partial x^\nu}(x(\lambda)) \frac{dx^\nu}{d\lambda}. \quad (7.2.96)$$

The covariant derivative of a tensor field Φ in the direction of the 4-velocity is given by:

$$\frac{dx^\nu}{d\lambda} \nabla_\nu \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N} = \frac{dx^\nu}{d\lambda} \partial_\nu \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N} + \frac{dx^\nu}{d\lambda} \Gamma^\beta_{\alpha\nu} \hat{G}^\alpha_\beta \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N} \quad (7.2.97)$$

$$= \left(\frac{d}{d\lambda} + \frac{dx^\nu}{d\lambda} \Gamma^\beta_{\alpha\nu}(x(\lambda)) \hat{G}^\alpha_\beta \right) \phi^{\rho_1 \dots \rho_M}_{\nu_1 \dots \nu_N}. \quad (7.2.98)$$

It is useful then to define the covariant total λ derivative so that it agrees with this directional derivative on tensor fields:

$$\frac{D}{D\lambda} \stackrel{\text{def}}{=} \frac{d}{d\lambda} + \frac{dx^\nu}{d\lambda} \Gamma^\beta_{\alpha\nu}(x(\lambda)) \hat{G}^\alpha_\beta \quad (7.2.99)$$

$$\Rightarrow \frac{dx^\nu}{d\lambda} \nabla_\nu \phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N}(x(\lambda)) = \frac{D\phi^{\rho_1 \dots \rho_M}_{\sigma_1 \dots \sigma_N}}{D\lambda}. \quad (7.2.100)$$

With the understanding that the coordinates x^μ are to be treated as a list of scalar functions, the covariant λ derivative and ordinary λ derivative of the coordinates agree:

$$\frac{Dx^\mu}{D\lambda} = \frac{dx^\mu}{d\lambda}. \quad (7.2.101)$$

Then, the geodesic equation can be rewritten as:

$$\boxed{\frac{D^2 x^\mu}{D\lambda^2} = 0.} \quad (7.2.102)$$

In this way, the geodesic equation essentially just states that the path has a vanishing covariant acceleration!

7.2.3 Local Inertial Frames

We found in equation (7.1.35) that on a Lorentzian manifold it is always possible to pick coordinates so that the metric tensor at a particular point of interest in those coordinates is simply the Minkowskian metric. Because of this, a Lorentzian manifold is said to be locally like Minkowski space. We can go further. Let X_0 be a particular point of interest and suppose we are already using a coordinate system x^μ so that:

$$g_{\mu\nu}(x_0) = \eta_{\mu\nu}. \quad (7.2.103)$$

Then, suppose we define a new coordinate system x'^μ as some generic smooth function of x^μ which is to agree with our unprimed coordinate system at lowest order near X_0 . That is:

$$x'^\mu = x^\mu + \frac{1}{2} M^\mu_{\rho\sigma} (x^\rho - x_0^\rho)(x^\sigma - x_0^\sigma) + \mathcal{O}(x - x_0)^3 \quad (7.2.104)$$

for some constants $M^\mu_{\rho\sigma}$ which we can see are given by:

$$M^\mu_{\rho\sigma} = M^\mu_{\sigma\rho} = \frac{\partial^2 x'^\mu}{\partial x^\rho \partial x^\sigma}(x_0). \quad (7.2.105)$$

Returning this to the transformation property for the connection coefficients in (7.2.23) gives:

$$\Gamma'^\mu_{\rho\sigma}(x_0) = \Gamma^\mu_{\rho\sigma}(x_0) - M^\mu_{\rho\sigma}. \quad (7.2.106)$$

Thus, by choosing the coefficients:

$$M^\mu{}_{\rho\sigma} = \Gamma^\mu{}_{\rho\sigma}(x_0) \quad (7.2.107)$$

which is always possible for a torsion free connection, we immediately have that:

$$\Gamma^\mu{}_{\rho\sigma}(x_0) = 0. \quad (7.2.108)$$

Thus, it is always possible to choose coordinates so that the metric tensor at a particular point of interest is the Minkowski metric AND so that the connection coefficients at that particular point of interest vanish. Such a coordinate system is called a **local inertial frame** at the point of interest. Due to the metricity condition, once the connection vanishes at a point, it automatically follows that the first derivatives of the metric $\partial_\rho g_{\mu\nu}$ all vanish at that point.

Geometrically, at a point of interest, a local inertial frame coordinate system at that point behaves most like the usual Cartesian coordinates on flat space. Because the metric at X_0 is simply the Minkowski metric, the coordinate displacements at X_0 can be thought of as ordinary special relativistic coordinate displacements. As well, because the connection coefficients vanish at X_0 , the geodesic equation at X_0 simply becomes $\frac{d^2 x^\mu}{d\lambda^2} = 0$. If the local inertial frame could be extended, this would simply integrate to the equation of a straight line. Because the local inertial frame can only be defined locally, instead it says that geodesics are locally like straight lines when viewed in that coordinate system.

We will often use the abbreviation LIRF for local inertial reference frame. In a LIRF at X_0 , the covariant derivative simply becomes the partial derivative (because all the connection coefficients vanish, as they do in Minkowski space), and all pseudo-inner products can be computed using the Minkowski metric. A LIRF then gives us a direct comparison point between general relativity and special relativity. In order for a general relativistic theory to reproduce our special relativistic theories, in a LIRF the quantities in the general relativistic theory must equal the special relativistic quantities up to terms which are negligible when special relativity is valid. Suppose we have a special relativistic action which we wish to upgrade to a general relativistic action. In a LIRF, the metric $g_{\mu\nu}$ simply becomes $\eta_{\mu\nu}$ and so every factor of the $\eta_{\mu\nu}$ in the special relativistic action ought to be replaced by $g_{\mu\nu}$ in the general relativistic theory. Similarly, in a LIRF, the covariant derivative ∇_μ simply becomes ∂_μ and so every factor of the partial derivative in the special relativistic action ought to be replaced by ∇_μ in the general relativistic theory. Making only these replacements (and any others strictly necessary to produce a match between general relativity in a LIRF and special relativity) is called making the **minimal replacement**. Additional terms that are small for nearly Minkowskian spacetimes may be added to the action beyond these minimal ones if experiment so demands. Often, the minimal replacement is experimentally correct, and on a case-by-case basis there are geometric and theoretical reasons why we might expect this. Once a general relativistic theory has been constructed in a LIRF in a coordinate invariant form, due to that coordinate invariance, the theory is then valid in all coordinate systems.

You may naturally think that because we can, at a point, make the metric Minkowskian and all its first derivatives vanish, perhaps we can go further and make its second, third, and so on derivatives vanish. This is not so. To see this, let us consider the next order of the general smooth coordinate transformation given in (7.2.104). Suppose at X_0 we have already chosen coordinates so that we are in a LIRF. Then, we can still take:

$$x'^\mu = x^\mu + \frac{1}{6} N^\mu{}_{\alpha\beta\gamma} (x^\alpha - x_0^\alpha)(x^\beta - x_0^\beta)(x^\gamma - x_0^\gamma) + \mathcal{O}(x - x_0)^4. \quad (7.2.109)$$

This transformation will preserve the LIRF conditions. However, it will change the first derivatives of the connection. The coefficients $N^\mu{}_{\alpha\beta\gamma}$ are determined by:

$$N^\mu{}_{\alpha\beta\gamma} = \frac{\partial^3 x'^\mu}{\partial x^\alpha \partial x^\beta \partial x^\gamma}(x_0) \quad (7.2.110)$$

and so these coefficients are necessarily fully symmetric in interchanging any pair of α, β, γ .

Differentiating (7.2.23) gives:

$$\begin{aligned} \partial'_\sigma \Gamma^\rho{}_{\mu\nu}(x') &= \frac{\partial x^\lambda}{\partial x'^\sigma} \partial_\lambda \left(\frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \right) \Gamma^\gamma{}_{\alpha\beta}(x) + \frac{\partial x'^\rho}{\partial x^\gamma} \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial x^\lambda}{\partial x'^\sigma} \partial_\lambda \Gamma^\gamma{}_{\alpha\beta}(x) \\ &\quad - \frac{\partial x^\lambda}{\partial x'^\sigma} \partial_\lambda \left(\frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} \right) \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} - \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial^2 x'^\rho}{\partial x^\alpha \partial x^\beta} \frac{\partial x^\lambda}{\partial x'^\sigma} \frac{\partial^3 x'^\rho}{\partial x^\alpha \partial x^\beta \partial x^\lambda}. \end{aligned} \quad (7.2.111)$$

Evaluating this at X_0 using (7.2.109) and the LIRF conditions gives:

$$\partial'_\sigma \Gamma'^\rho{}_{\mu\nu}(x_0) = \partial_\sigma \Gamma^\rho{}_{\mu\nu}(x_0) - N^\rho{}_{\sigma\mu\nu}. \quad (7.2.112)$$

Immediately then:

$$\partial'_\sigma \Gamma'^\rho{}_{\mu\nu}(x_0) - \partial'_\nu \Gamma'^\rho{}_{\mu\sigma}(x_0) = \partial_\sigma \Gamma^\rho{}_{\mu\nu}(x_0) - \partial_\nu \Gamma^\rho{}_{\mu\sigma}(x_0) \quad (7.2.113)$$

due to the index symmetries of $N^\rho{}_{\sigma\mu\nu}$. Thus, this anti-symmetric combination of derivatives of the connection cannot generically be made 0 at a point of interest in a LIRF. The first derivatives of the connection are related to the second derivatives of the metric, and so the second derivatives of the metric contain some information that cannot be erased by a change of coordinates. This gives them a good chance of representing something geometrically meaningful and coordinate invariant. This is our first hint at the precise meaning of curvature of a manifold, which we will cover in depth later in the chapter.

Exercises

Problem 7.3: Connection on a Sphere. Consider a sphere of radius R embedded in 3 dimensional Euclidean space. Use spherical coordinates (r, θ, φ) for the Euclidean space and define the sphere by $|\vec{x}| = R$.

- (a) Explain that (θ, φ) provide coordinates on the sphere. Show that the coordinate basis vectors (expressed in Cartesian components) on the sphere are:

$$\vec{e}_\theta = \frac{\partial \vec{x}}{\partial \theta} = (R \cos \theta \cos \varphi, R \cos \theta \sin \varphi, -R \sin \theta), \quad \vec{e}_\varphi = \frac{\partial \vec{x}}{\partial \varphi} = (-R \sin \theta \sin \varphi, R \sin \theta \cos \varphi, 0).$$

- (b) Show that the metric on the sphere is:

$$g_{\theta\theta} = R^2, \quad g_{\theta\varphi} = 0, \quad g_{\varphi\varphi} = R^2 \sin^2 \theta.$$

- (c) Show that (using the natural connection induced by the embedding Euclidean space) the connection coefficients on the sphere are:

$$\begin{aligned} \Gamma^\theta{}_{\theta\theta} &= 0, & \Gamma^\theta{}_{\theta\varphi} &= 0, & \Gamma^\theta{}_{\varphi\varphi} &= -\sin \theta \cos \theta, \\ \Gamma^\varphi{}_{\theta\theta} &= 0, & \Gamma^\varphi{}_{\theta\varphi} &= \frac{\cos \theta}{\sin \theta}, & \Gamma^\varphi{}_{\varphi\varphi} &= 0. \end{aligned}$$

- (d) Consider geodesics on the sphere. Show, either by directly using the geodesic equation of motion or by varying the arclength functional explicitly in terms of the metric, that the geodesics of the sphere satisfy:

$$\frac{d^2\theta}{ds^2} - \sin \theta \cos \theta \left(\frac{d\varphi}{ds} \right)^2 = 0, \quad \frac{d}{ds} \left(\sin^2 \theta \frac{d\varphi}{ds} \right) = 0$$

where s is the arclength parameter of the geodesic. Show, using the rotational symmetry of the sphere, that without loss of generality we can take the geodesic to begin at $\theta = 0, \varphi = 0$ and to end at $\theta = \alpha, \varphi = 0$ for some value of α . Show that with this definition the geodesic is given by:

$$\theta(s) = \frac{s}{R}, \quad \varphi(s) = 0.$$

Explain geometrically that this means that geodesics on the sphere are given by “great circles” or in other words circles of radius equal to the radius of the sphere.

- (e) Suppose ξ_μ is a Killing vector field for the sphere. Show that it must satisfy:

$$\partial_\theta \xi_\theta = 0, \quad \partial_\theta \xi_\varphi + \partial_\varphi \xi_\theta = 2 \frac{\cos \theta}{\sin \theta} \xi_\varphi, \quad \partial_\varphi \xi_\varphi = -\sin \theta \cos \theta \xi_\theta.$$

Solve these conditions to show that the most general Killing vector $\vec{\xi}$ on the sphere is given by:

$$\vec{\xi} = \alpha_x \vec{\xi}_x + \alpha_y \vec{\xi}_y + \alpha_z \vec{\xi}_z$$

where $\alpha_x, \alpha_y, \alpha_z$ are arbitrary coefficients and $\vec{\xi}_x, \vec{\xi}_y, \vec{\xi}_z$ are vectors which generate rotations about the x, y, z directions. Show that those vectors are given explicitly on the sphere by:

$$\vec{\xi}_x = -\sin \varphi \vec{e}_\theta - \frac{\cos \theta}{\sin \theta} \cos \varphi \vec{e}_\varphi, \quad \vec{\xi}_y = \cos \varphi \vec{e}_\theta - \frac{\cos \theta}{\sin \theta} \sin \varphi \vec{e}_\varphi, \quad \vec{\xi}_z = \vec{e}_\varphi.$$

7.3 General Relativistic Particle

Let us now generalize the theory of a point particle to the case of motion on a generic Lorentzian manifold. In (4.9.63) we found that a special relativistic point particle interacting with electromagnetism has covariant action given by:

$$S = \int_{\lambda_0}^{\lambda_f} \left(-m \frac{d\tau}{d\lambda} + q A_\mu \frac{dx^\mu}{d\lambda} \right) d\lambda \quad (7.3.1)$$

where the particle's worldline $x^\mu(\lambda)$ is expressed in terms of an arbitrary parameter λ . As written, this action is already comprised purely of coordinate invariant combinations and so in a general metric, this action can be written as:

$$S = \int_{\lambda_0}^{\lambda_f} \left(-m \sqrt{-g_{\mu\nu}(x) \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} + q A_\mu \frac{dx^\mu}{d\lambda} \right) d\lambda. \quad (7.3.2)$$

This action is the integral of the λ -Lagrangian:

$$\mathcal{L}_\lambda = -m \sqrt{-g_{\mu\nu}(x) \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} + q A_\mu \frac{dx^\mu}{d\lambda}. \quad (7.3.3)$$

From this we can find the resulting equations of motion using the Euler-Lagrange equations:

$$\frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} = \left(\frac{m}{2} \partial_\mu g_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} + q \partial_\mu A_\nu \frac{dx^\nu}{d\lambda} \right) \frac{d\tau}{d\lambda}, \quad \frac{\partial \mathcal{L}_\lambda}{\partial \frac{dx^\mu}{d\lambda}} = m g_{\mu\nu} \frac{dx^\nu}{d\lambda} + q A_\mu. \quad (7.3.4)$$

$$\Rightarrow \frac{\delta S}{\delta x^\mu(\lambda)} = \frac{\partial \mathcal{L}_\lambda}{\partial x^\mu} - \frac{d}{d\lambda} \frac{\partial \mathcal{L}_\lambda}{\partial \frac{dx^\mu}{d\lambda}} \quad (7.3.5)$$

$$= g_{\mu\nu} \left(q \mathcal{F}^\nu{}_\rho \frac{dx^\rho}{d\lambda} - m \frac{d^2 x^\nu}{d\lambda^2} - m \Gamma^\nu{}_{\rho\sigma} \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} \right) \frac{d\tau}{d\lambda} \quad (7.3.6)$$

$$\stackrel{!}{=} 0. \quad (7.3.7)$$

Thus, we arrive at the covariant equation of motion:

$$m \frac{D^2 x^\mu}{D\tau^2} = q \mathcal{F}^\mu{}_\nu \frac{Dx^\nu}{D\tau} \quad (7.3.8)$$

where we have recalled the definition of the covariant parameter derivative from (7.2.99) and parameterized the path in terms of the proper time τ instead of the arbitrary parameter λ . In the case the particle is uncharged or the electromagnetic field vanishes, this simply reduces to the geodesic equation for a timelike curve. Thus, **massive particles solely under the influence of gravity follow timelike geodesics**. We also used the familiar definition of the field strength $\mathcal{F}_{\mu\nu}$ in terms of partial derivatives of the vector potential, however importantly the connection coefficients cancel out regardless of whether partial derivatives or covariant derivatives are used to defined $\mathcal{F}_{\mu\nu}$:

$$\mathcal{F}_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu = \partial_\mu A_\nu - \partial_\nu A_\mu. \quad (7.3.9)$$

In a local inertial rest frame, the connection coefficients vanish. Thus, for a particle solely under the influence of gravity, it is possible to instantaneously go to a coordinate system in which the coordinate acceleration of the particle is 0. This is the precise meaning of the Einstein quote at the start of the chapter. Locally and instantaneously, there is a reference frame in which there is no gravitational effect. Gravity only has a relative existence in the sense that different frames move differently. While one frame can be made to not move, this can only be done one frame at a time. Two geodesics which start nearby moving initially in parallel will not generically remain in parallel at later times, and so two particles falling such geodesics will experience inarguable motion relative to each other.

From the derivative of the λ -Lagrangian with respect to $\frac{dx^\mu}{d\lambda}$, we can identify that the conjugate momentum p_μ to x^μ is:

$$p_\mu = \frac{\partial \mathcal{L}_\lambda}{\partial \frac{dx^\mu}{d\lambda}} = m \frac{Dx_\mu}{D\tau} + q A_\mu. \quad (7.3.10)$$

If a particular physical scenario as experienced by the particle (and thus the metric and the vector potential it experiences) has symmetry under a diffeomorphism generated by a vector field ξ^μ , then by Noether's theorem

the corresponding conserved generator is:

$$G = \xi^\mu p_\mu - \mathcal{D}f = m\xi_\mu \frac{Dx^\mu}{D\tau} + q\xi^\mu A_\mu - \mathcal{D}f. \quad (7.3.11)$$

where f is the surface term added to the action under the transformation. It is insightful to look at the total derivative of this generator:

$$\frac{dG}{d\tau} = m \frac{D\xi_\mu}{D\tau} \frac{Dx^\mu}{D\tau} + m\xi_\mu \frac{D^2x^\mu}{D\tau^2} + q \frac{D\xi^\mu}{D\tau} A_\mu + q\xi^\mu \frac{DA_\mu}{D\tau} - \frac{D\mathcal{D}f}{D\tau} \quad (7.3.12)$$

$$= m \frac{Dx^\mu}{D\tau} \frac{Dx^\nu}{D\tau} \nabla_\nu \xi_\mu + q\xi_\mu \mathcal{F}^\mu{}_\nu \frac{Dx^\nu}{D\tau} + q \frac{Dx^\nu}{D\tau} \nabla_\nu \xi^\mu A_\mu + q \frac{Dx^\nu}{D\tau} \xi^\mu \nabla_\nu A_\mu - \frac{Dx^\nu}{D\tau} \nabla_\nu \mathcal{D}f \quad (7.3.13)$$

$$= \frac{m}{2} \frac{Dx^\mu}{D\tau} \frac{Dx^\nu}{D\tau} (\nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu) + q \frac{Dx^\nu}{D\tau} (\xi^\mu \nabla_\mu A_\nu + \nabla_\nu \xi^\mu A_\mu - \nabla_\nu \mathcal{D}f) \quad (7.3.14)$$

$$= \frac{m}{2} \frac{Dx^\mu}{D\tau} \frac{Dx^\nu}{D\tau} L_\xi g_{\mu\nu} + q \frac{Dx^\mu}{D\tau} \left(L_\xi A_\mu - \frac{1}{q} \nabla_\mu \mathcal{D}f \right). \quad (7.3.15)$$

If the transformation generated by ξ^μ is a symmetry of the physical scenario, it must leave the metric tensor unchanged and only change the vector potential by a gauge transformation. Thus:

$$L_\xi g_{\mu\nu} = 0, \quad L_\xi A_\mu = \nabla_\mu \frac{\mathcal{D}f}{q} \quad (7.3.16)$$

where this last condition serves to define the scalar function $\mathcal{D}f$. For scalar functions, the covariant and partial derivatives coincide and so the gauge transformation may be represented by the addition of either $\partial_\mu f$ or $\nabla_\mu f$ to the metric. With these symmetry conditions, we have automatically that the generator is in fact conserved:

$$\frac{dG}{d\tau} = 0. \quad (7.3.17)$$

Thus, if the metric has a Killing vector which is also a symmetry of the electromagnetic field then the generator of diffeomorphisms corresponding to that Killing vector for a particle in motion under that metric and electromagnetic field is conserved.

In order to define a Hamiltonian formulation for our particle's motion, we need to specify a time direction. To be precise, due to general covariance, we may identify any timelike coordinate x^0 with coordinate time (a timelike coordinate is one which has negative coefficient on its squared displacement in the proper time). For a given choice of timelike coordinate x^0 , there is a hypersurface $\Sigma(t)$ of all points in spacetime which have the value of $x^0 = t$. Because this is a surface at fixed time, it will be spacelike (meaning any two points on it are spacelike separated). Such a hypersurface is called a time slice or Cauchy slice. Because each event in spacetime occurs at one and only one time, each X exists in one and only one $\Sigma(t)$. Thus, the one parameter family of all $\Sigma(t)$ together cover all of spacetime. This covering is called a timelike foliation of spacetime. On the surface $\Sigma(t)$ and so at points for which $x^0 = t$, the remaining coordinates x^a are all free and all displacements are spacelike. So, the proper length element becomes:

$$ds^2 = -d\tau^2 = g_{ab} dx^a dx^b \quad (7.3.18)$$

on $\Sigma(t)$. We can therefore think of the hypersurface $\Sigma(t)$ as a manifold with a positive-definite metric (which is called a Riemannian manifold) γ_{ab} given by:

$$\gamma_{ab}(t, x) = g_{ab}(t, x). \quad (7.3.19)$$

When treating $\Sigma(t)$ as a manifold, we will use γ^{ab} to mean the inverse matrix to γ_{ab} as a 3x3 matrix and refer to γ_{ab} as the (spatial) metric. The other components of the full metric (g_{00} and g_{0a}) get alternate names as well when working in this "3+1" decomposition (3+1 refers to the explicit decomposition into three spatial directions and one time direction). The **shift vector** is a vector field defined to have components:

$$N_a(t, x) = g_{0a}(t, x). \quad (7.3.20)$$

It is a genuine vector field with respect to redefinitions of the spatial coordinates. We will use the metric on $\Sigma(t)$ to define index raising and lowering as well as the inner product so that:

$$N^a = \gamma^{ab} N_b, \quad N^2 = N^a N_a. \quad (7.3.21)$$

The **lapse function** L is defined so that $L \geq 0$ and:

$$g_{00} = -L^2 + N^2. \quad (7.3.22)$$

The inverse full metric $g^{\mu\nu}$ can be expressed nicely using the inverse matrix condition:

$$g^{\mu\rho}g_{\rho\nu} = \delta_\nu^\mu. \quad (7.3.23)$$

The $0a$ components of which give:

$$g^{00}N_a + g^{0b}\gamma_{ab} = 0 \implies g^{0a} = -g^{00}N^a. \quad (7.3.24)$$

As well, the 00 component gives:

$$-g^{00}(L^2 - N^2) + g^{0a}N_a = 1 \quad (7.3.25)$$

$$\implies g^{00} = -\frac{1}{L^2}, \quad g^{0a} = \frac{N^a}{L^2}. \quad (7.3.26)$$

Then, the ab components give:

$$\frac{N^aN_b}{L^2} + g^{ac}\gamma_{cb} = \delta_b^a \implies g^{ab} = \gamma^{ab} - \frac{N^aN^b}{L^2}. \quad (7.3.27)$$

The $a0$ components give no new information.

Let the vector $\vec{n}(t, x)$ be the unit vector field which is orthogonal to the surface of $\Sigma(t)$ and which is future oriented (meaning has positive timelike component). This vector has the interpretation as the direction in which time passes but one does not move spatially at all. This does not mean that displacements in the direction of $\vec{n}$ have $dx^a = 0$. This is because the spacelike coordinates x^a may have definitions which involve moving in a time dependent way as viewed with x^0 as the time coordinate. By definition, $\vec{n}$ must be orthogonal to every vector in the tangent space of Σ . Because being on Σ fixed x^0 but leaves the remaining coordinates free, the tangent space of Σ is spanned by the coordinate vectors $\vec{e}_a$. Thus:

$$\vec{n} = n^\mu \vec{e}_\mu = n^0 \vec{e}_0 + n^a \vec{e}_a, \quad (7.3.28)$$

$$\vec{n} \cdot \vec{e}_a = n^0 g_{0a} + n^b g_{ab} \stackrel{!}{=} 0 \implies n^a = -n^0 N^a \implies \vec{n} = n^0 (\vec{e}_0 - N^a \vec{e}_a). \quad (7.3.29)$$

Because $\vec{n}$ is normalized, timelike, and future oriented, we must have:

$$\vec{n} \cdot \vec{n} = -L^2(n^0)^2 \stackrel{!}{=} -1 \implies n^0 = \frac{1}{L} \implies \vec{n} = \frac{1}{L} (\vec{e}_0 - N^a \vec{e}_a). \quad (7.3.30)$$

Consider then a displacement of position in the direction of $\vec{n}$. That is, suppose:

$$dX = A\vec{n} \quad (7.3.31)$$

for a positive constant A . Then:

$$dx^a = -N^a dt. \quad (7.3.32)$$

This gives us the interpretation of the shift vector. The shift vector is negative the coordinate velocity $\frac{dx^a}{dt}$ at which one must move to exit Σ normally. In essence, the shift vector measures the rate at which points of fixed spatial coordinates are shifted between the different time slices. When leaving the surface of Σ normally, the resulting proper time element is:

$$d\tau^2 = -g_{\mu\nu}dx^\mu dx^\nu = -g_{00}dt^2 - 2g_{0a}dtdx^a - g_{ab}dx^a dx^b \quad (7.3.33)$$

$$= L^2 dt^2 - N^2 dt^2 + 2N_a N^a dt^2 - \gamma_{ab}N^a N^b dt^2 = L^2 dt^2 \quad (7.3.34)$$

$$\implies d\tau = Ldt. \quad (7.3.35)$$

This gives us the interpretation of the lapse function. The lapse function measures the rate at which proper time passes per coordinate time moving normally to Σ .

By rewriting the metric in terms of the lapse function, shift vector, and spatial metric, the action for our relativistic particle becomes:

$$S = \int_{t_0}^{t_f} \left(-mL \sqrt{1 - \frac{\gamma_{ab}(\dot{x}^a + N^a)(\dot{x}^b + N^b)}{L^2}} + qA_a \dot{x}^a - q\phi \right) dt \quad (7.3.36)$$

where $\phi = -A_0$ is the electromagnetic “scalar” (with respect to rotations) potential. Thus, the Lagrangian is:

$$\mathcal{L} = -mL \sqrt{1 - \frac{\gamma_{ab}(\dot{x}^a + N^a)(\dot{x}^b + N^b)}{L^2}} + qA_a \dot{x}^a - q\phi. \quad (7.3.37)$$

This gives the conjugate momentum:

$$p_a = \frac{\partial \mathcal{L}}{\partial \dot{x}^a} = \frac{m\gamma_{ab}(\dot{x}^b + N^b)}{\sqrt{L^2 - \gamma_{cd}(\dot{x}^c + N^c)(\dot{x}^d + N^d)}} + qA_a. \quad (7.3.38)$$

By subtracting the vector potential contribution and taking the spatial vector magnitude of both sides we find:

$$\gamma^{ab}(p_a - qA_a)(p_b - qA_b) = \frac{m^2\gamma_{ab}(\dot{x}^a + N^a)(\dot{x}^b + N^b)}{L^2 - \gamma_{cd}(\dot{x}^c + N^c)(\dot{x}^d + N^d)} \quad (7.3.39)$$

$$\implies \gamma_{ab}(\dot{x}^a + N^a)(\dot{x}^b + N^b) = \frac{L^2\gamma^{ab}(p_a - qA_a)(p_b - qA_b)}{m^2 + \gamma^{cd}(p_c - qA_c)(p_d - qA_d)}. \quad (7.3.40)$$

With this, we can use the Legendre transformation to find the Hamiltonian for our particle:

$$\mathcal{H} = p_a\dot{x}^a - \mathcal{L} = L\sqrt{m^2 + \gamma^{ab}(p_a - qA_a)(p_b - qA_b)} - N^a(p_a - qA_a) + q\phi. \quad (7.3.41)$$

Hamilton's equations applied to this Hamiltonian produce equivalent equations of motion to (7.3.8), however they will be in a form which is not manifestly covariant (in the sense that their transformation properties will be unobvious).

The Hamiltonian perspective of our particle is useful for understanding its nonrelativistic limit. For performing this analysis it is simplest to consider the absence of electromagnetism (no generality is gained or lost by doing so, just some equations shortened). So, we set $q = 0$. We expect that this Hamiltonian should be able to reproduce the Newtonian scalar potential theory of gravity at low speeds and in weak gravitational fields. There is another condition on reproducing Newtonian mechanics. The Newtonian theory as presented was always done in an “inertial frame”, in the sense that the frame was not accelerating (acceleration being an absolute Galilean boost invariant quantity in the Newtonian theory). Due to this, the particle's linear momentum was proportional to its velocity. Due to the presence of the shift vector, our general relativistic particle's linear momentum is not in the same direction as its velocity in general. We already identified that $-N^a$ is the induced coordinate velocity from moving purely in the direction orthogonal to the “space” part ($\Sigma(t)$) of spacetime. In the nonrelativistic limit this can be identified as a time dependent Galilean boost. Therefore, in general coordinates with time dependent $N^a(t, x(t))$, a particle's coordinate velocity is essentially being measured in an accelerating frame. In a neighborhood of our particle, it is always possible to choose coordinates x^μ so that $g_{0a} = N_a = 0$ (this typically cannot be done globally, but can be guaranteed in an appropriately small finite size neighborhood). So, we only expect Newtonian physics to emerge in coordinates in which near the particle we have set $N_a = 0$. Assuming we have locally set $N_a = 0$, the small gravitational field conditions are that our metric is nearly the Minkowski metric:

$$g_{\mu\nu} = \eta_{\mu\nu} + \delta g_{\mu\nu} \implies L = 1 + \delta L, \quad \gamma^{ab} = \delta^{ab} + \delta\gamma^{ab} \quad (7.3.42)$$

where δL and $\delta\gamma^{ab}$ we will take to be small. The low speed approximation (in Hamiltonian coordinates) is then that $\frac{p_a}{m}$ is small. Returning these conditions to our Hamiltonian we have:

$$\mathcal{H} = (1 + \delta L)\sqrt{m^2 + (\delta^{ab} + \delta\gamma^{ab})p_ap_b} = m + m\delta L + \frac{\delta^{ab}p_ap_b}{2m} + \frac{(\delta L\delta^{ab} + (1 + \delta L)\delta\gamma^{ab})p_ap_b}{2m} + \mathcal{O}(p^4). \quad (7.3.43)$$

The terms containing both a metric fluctuation and two powers of the momentum are suppressed relative to the terms containing only one or the other due to both being small. The leading term m is due to the difference between the relativistic and nonrelativistic definitions of the energy zero-point. Therefore, the leading order nonrelativistic Hamiltonian extracted from this theory is:

$$\mathcal{H}_{\text{Gal}} = \frac{\delta^{ab}p_ap_b}{2m} + m\delta L. \quad (7.3.44)$$

This precisely matches the Hamiltonian of a Galilean particle interacting with a Newtonian gravitational scalar potential ϕ by identifying:

$$\delta L = \phi. \quad (7.3.45)$$

This is of course only half of the matching that needs to be done between general relativity and Newton's gravity. This establishes how the Newtonian potential is extracted from the metric, but we still need to see how whatever equations of motion we find for the metric can reproduce Gauss' law for ϕ in the nonrelativistic limit. The relationship between the lapse function and the Newtonian scalar potential does give a nice interpretative element to gravity. The lapse function measures the rate at which proper time passes per unit coordinate time. Here proper time would be the time experienced by the moving particle and coordinate time would be the time measured by an observer. In Newton's gravity, ϕ is always negative (because the gravitational constant G is positive and mass density is always positive) and so $L < 1$. Consequently, the time

between points of motion as measured by an observer for an object in motion under gravity is always greater than the time experienced by the object itself. This gravitational time dilation can be quite significant, and in fact must actively be accounted for on GPS satellites in order for them to remain precise enough for our uses on Earth. (The clocks on GPS satellites have to be adjusted to stay in sync with Earth clocks.) Perhaps surprisingly at first, this general relativistic time dilation effect in the case of GPS is much larger than the pure special relativistic time dilation (the special relativistic time dilation is due to fact that the satellites have a relative velocity to Earth).

Exercises

Problem 7.4: ★ Aristotle's Force Revisited. This question is credited to John P. Ralston. Let us go back to section 1.1. For our configuration $Q = (x^1, x^2, x^3)$ for a point-mass moving in a generic spacetime we would by equation (1.1.6) write that for some velocity field $v^a(x^0, x^1, x^2, x^3)$:

$$\frac{dx^a}{dx^0} = v^a(x^0, x^1, x^2, x^3)$$

where we have used x^0 as our coordinate time.

- (a) Explain that generically one can introduce a parameter λ for which $\lambda(x^0)$ is an increasing smooth function, so that the equation of motion can be rewritten as:

$$\frac{dx^\mu}{d\lambda} = u^\mu(X)$$

for some vector field u .

- (b) Argue that different particles may respond to spatial/temporal inhomogeneities differently so that the equation of motion can be rewritten:

$$\frac{dx^\mu}{d\lambda} = \frac{U^\mu(X)}{m}$$

for some constant m which indicates the strength with which the particle is affected by the inhomogeneities and $U(X)$ is some vector field external to the particle.

- (c) Explain that any vector field $U(X)$ can be decomposed as:

$$U_\mu(X) = \partial_\mu S(X) - K_\mu(X)$$

for some vector field K and scalar field S . As well, show that S and K are only defined up to modifying them by a scalar function $f(X)$:

$$K'_\mu = K_\mu + \partial_\mu f, \quad S' = S + f.$$

With these show that the equation of motion becomes:

$$\frac{dx^\mu}{d\lambda} = g^{\mu\nu}(\partial_\nu S - K_\nu).$$

- (d) Differentiate the first order equation of motion for x^μ to receive a second order equation of motion. Show, by recalling the definition of the covariant parameter derivative, that it can be put in the form:

$$mg_{\mu\nu} \frac{D^2 x^\mu}{D\lambda^2} = \frac{1}{2m} \nabla_\mu (U^\nu U_\nu) + (\nabla_\mu K_\nu - \nabla_\nu K_\mu) \frac{Dx^\nu}{D\lambda}.$$

- (e) Show that it is possible to define the parameter λ so that $U^\mu U_\mu$ is constant. Show that for such parameters:

$$mg_{\mu\nu} \frac{D^2 x^\mu}{D\lambda^2} = (\nabla_\mu K_\nu - \nabla_\nu K_\mu) \frac{Dx^\nu}{D\lambda}.$$

Compare this equation of motion with (7.3.8) (and so identify that (7.3.8) is trivially true for some potentials once we assume our configuration is given by a point).

- (f) Show that the function S can be determined as:

$$S(X) = S_0 + \int_0^\lambda (-md\tau(\lambda) + K_\mu dx^\mu(\lambda))$$

(for some constant S_0) and with $d\tau$ the proper time element of the body. Show that the variation of S , viewed as a functional of x^μ , is 0 under the equation of motion. Thus conclude (as we had already established) that there is ultimately no content to the use of a stationary action to find equations of motion for this system beyond the assumption that equations of motion exist and that your set of variables is complete.

7.4 Integration on Manifolds

7.4.1 Spacetime Integration

In order to study a field theory on the spacetime manifold, such as electromagnetism in curved spacetime, we first need to understand how to perform integration on our manifold. When we considered Minkowski space, the volume measure $d\mathbb{T} = dt dx dy dz$ was preserved by all of the symmetries of the theory. However, the measure $dx^0 dx^1 dx^2 dx^3$ in general coordinates is not invariant under all coordinate transformations. We can find the appropriate coordinate invariant volume measure by the minimal replacement approach. In a LIRF, we want the volume measure to become $dx^0 dx^1 dx^2 dx^3$, to match our Minkowski space results. Let the coordinates $r^\mu(X)$ be coordinates for a LIRF at the point X_0 . Then, the volume measure $d\mathbb{T}$ at X_0 is given by:

$$d\mathbb{T}(X_0) = dr^0 dr^1 dr^2 dr^3 \quad (7.4.1)$$

where the coordinate displacements are all at X_0 . In general coordinates x^μ , there will be some relation $r^\mu(x)$ which transforms then into the LIRF coordinates. Then, using standard calculus:

$$dr^0 dr^1 dr^2 dr^3 = \left| \det \frac{\partial r}{\partial x} \right| dx^0 dx^1 dx^2 dx^3. \quad (7.4.2)$$

This determinant can be written more nicely by remembering the transformation property of the metric tensor and using that the determinant of a product is the product of determinants. In the LIRF, the metric is simply the Minkowski metric and so:

$$g_{\mu\nu}(X_0) = \frac{\partial r^\rho}{\partial x^\mu}(X_0) \frac{\partial r^\sigma}{\partial x^\nu}(X_0) \eta_{\rho\sigma} \quad (7.4.3)$$

$$\Rightarrow \det g = \left(\det \frac{\partial r}{\partial x} \right)^2 \det \eta = - \left(\det \frac{\partial r}{\partial x} \right)^2 \quad (7.4.4)$$

$$\Rightarrow \left| \det \frac{\partial r}{\partial x} \right| = \sqrt{-\det g}. \quad (7.4.5)$$

Therefore, the coordinate invariant volume measure on spacetime is:

$$d\mathbb{T} = \sqrt{-\det g} d^4 x. \quad (7.4.6)$$

With our volume measure, we can now consider integrations over regions of spacetime. Let $\mathbb{M}$ be a subset of spacetime which is smooth enough for it itself to be a manifold. Then, for a scalar function $f(X)$, we can define the integral:

$$I = \int_{\mathbb{M}} f(X) d\mathbb{T} = \int_{\mathbb{M}} f(x) \sqrt{-\det g} d^4 x. \quad (7.4.7)$$

Then, this integral is in fact a coordinate invariant number. Importantly, the function $f(X)$ must be a scalar function. This integral would not be coordinate invariant if we instead considered the integral of some tensor components, like by replacing $f(X)$ with a component $A^\mu(X)$ of a vector field. Conceptually, such an integral involves addition of vectors in different tangent spaces and so is geometrically meaningless. Computationally, such an integral is not coordinate invariant and because physics is independent of what coordinates we use, is not physically interesting. **Only volume integrals of scalar quantities are geometrically meaningful.** (Here scalars may mean proper scalars or pseudoscalars – which are distinguished by being even or odd under parity). Do not integrate tensor components; the result is garbage.

The Levi-Civita symbol often appears when doing integration (it is used in the construction of the normal vector to a surface in a surface integral, or in the formation of determinants in a volume integral). So, it is important for us to understand its transformation properties. Define the purely numerical Levi-Civita symbol $[\mu\nu\rho\sigma]$ the way we previously defined the Levi-Civita symbol:

$$[0123] = 1, \quad [\mu\nu\rho\sigma] = -[\mu\nu\sigma\rho] = -[\mu\sigma\rho\nu] = -[\sigma\nu\rho\mu]. \quad (7.4.8)$$

This numerical Levi-Civita symbol is written in such an unfamiliar way to emphasize that it is not a covariant object. By this I mean that if one has a tensor which has components given by $[\mu\nu\rho\sigma]$ in one coordinate system, then in another coordinate system the components of that tensor will generally not be $[\mu\nu\rho\sigma]$.

Consider a coordinate transformation $x'(x)$ and the combination:

$$F_{\mu\nu\rho\sigma} = [\alpha\beta\gamma\delta] \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial x^\gamma}{\partial x'^\rho} \frac{\partial x^\delta}{\partial x'^\sigma}. \quad (7.4.9)$$

Automatically, $F_{\mu\nu\rho\sigma}$ is antisymmetric under all index interchanges and so necessarily proportional to $[\mu\nu\rho\sigma]$. That is, for some coefficient:

$$F_{\mu\nu\rho\sigma} = C[\mu\nu\rho\sigma]. \quad (7.4.10)$$

Covariance of the numerical Levi-Civita symbol would only hold if C was equal to 1. This coefficient can be determined by fully contracting both sides with $[\mu\nu\rho\sigma]$ (with summation over μ, ν, ρ, σ implicit):

$$F_{\mu\nu\rho\sigma}[\mu\nu\rho\sigma] = C[\mu\nu\rho\sigma][\mu\nu\rho\sigma] = 24C \quad (7.4.11)$$

$$\implies C = \frac{1}{24} F_{\mu\nu\rho\sigma}[\mu\nu\rho\sigma]. \quad (7.4.12)$$

These equations look gross because the indices don't have conventional happy placements, but this is perfectly well defined numerically (just not covariant). Recall that the determinant of a 4x4 matrix $M_{\mu\nu}$ is defined by:

$$\det M = \frac{1}{24} [\mu\nu\rho\sigma] [\alpha\beta\gamma\delta] M_{\mu\alpha} M_{\nu\beta} M_{\rho\gamma} M_{\sigma\delta}. \quad (7.4.13)$$

Now using the definition of F :

$$C = \frac{1}{24} [\mu\nu\rho\sigma] [\alpha\beta\gamma\delta] \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial x^\gamma}{\partial x'^\rho} \frac{\partial x^\delta}{\partial x'^\sigma} = \det \frac{\partial x}{\partial x'}. \quad (7.4.14)$$

Therefore:

$$\boxed{[\alpha\beta\gamma\delta] \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial x^\gamma}{\partial x'^\rho} \frac{\partial x^\delta}{\partial x'^\sigma} = \det \left(\frac{\partial x}{\partial x'} \right) [\mu\nu\rho\sigma]} \quad (7.4.15)$$

which expresses the extent to which the numerical Levi-Civita symbol fails to be covariant (if it were covariant, then the right hand side would simply be $[\mu\nu\rho\sigma]$).

To find the appropriate covariant generalization of the numerical Levi-Civita symbol, we can again use analysis based on a LIRF. We define the Levi-Civita pseudotensor $\epsilon_{\mu\nu\rho\sigma}$ so that:

$$\epsilon_{\mu\nu\rho\sigma} = [\mu\nu\rho\sigma] \text{ in a LIRF} \quad (7.4.16)$$

and so that $\epsilon_{\mu\nu\rho\sigma}$ is covariant under orientation preserving coordinate transformations:

$$\epsilon_{\mu\nu\rho\sigma}(x') = \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} \frac{\partial x^\gamma}{\partial x'^\rho} \frac{\partial x^\delta}{\partial x'^\sigma} \epsilon_{\alpha\beta\gamma\delta}(x). \quad (7.4.17)$$

A coordinate transformation is said to be orientation preserving if the determinant of its coordinate transformation matrix is positive. Automatically then, in general coordinates:

$$\epsilon_{\mu\nu\rho\sigma} = \frac{\partial r^\alpha}{\partial x^\mu} \frac{\partial r^\beta}{\partial x^\nu} \frac{\partial r^\gamma}{\partial x^\rho} \frac{\partial r^\delta}{\partial x^\sigma} [\alpha\beta\gamma\delta] = \det \left(\frac{\partial r}{\partial x} \right) [\mu\nu\rho\sigma]. \quad (7.4.18)$$

Then, using (7.4.5), we have:

$$\boxed{\epsilon_{\mu\nu\rho\sigma} = [\mu\nu\rho\sigma] \sqrt{-\det g}} \quad (7.4.19)$$

It can now be seen why this is only a proper tensor for orientation preserving coordinate transformations as only for such transformations does this definition satisfy (7.4.18), due to the sign of the coordinate transformation determinant appearing. Because of this the covariant Levi-Civita symbol $\epsilon_{\mu\nu\rho\sigma}$ is called a **pseudotensor**, as its components transform like a tensor under an orientation preserving coordinate transformation and negative of like that of a tensor under orientation reversing coordinate transformations.

Because $\epsilon_{\mu\nu\rho\sigma}$ is now a covariantly defined object, we will raise and lower its indices using the metric tensor and contractions of quantities with it will give appropriately covariant tensors or pseudotensors of reduced rank. There is a nice corresponding expression to (7.4.19) for the fully raised Levi-Civita pseudotensor:

$$\epsilon^{\mu\nu\rho\sigma} = g^{\mu\alpha} g^{\nu\beta} g^{\rho\gamma} g^{\sigma\delta} \epsilon_{\alpha\beta\gamma\delta}. \quad (7.4.20)$$

This expression is automatically antisymmetric in all its indices and thus proportional to $[\mu\nu\rho\sigma]$ for some coefficient D :

$$\epsilon^{\mu\nu\rho\sigma} = D[\mu\nu\rho\sigma]. \quad (7.4.21)$$

Contracting both sides fully with $[\mu\nu\rho\sigma]$, using the definition of $\epsilon_{\alpha\beta\gamma\delta}$, and using that the determinant of a

matrix inverse is the reciprocal of the determinant:

$$[\mu\nu\rho\sigma]g^{\mu\alpha}g^{\nu\beta}g^{\rho\gamma}g^{\sigma\delta}[\alpha\beta\gamma\delta]\sqrt{-\det g} = D[\mu\nu\rho\sigma][\mu\nu\rho\sigma] \quad (7.4.22)$$

$$\implies 24 \frac{1}{\det g} \sqrt{-\det g} = 24D \implies D = \frac{-1}{\sqrt{-\det g}} \quad (7.4.23)$$

$$\implies \boxed{\epsilon^{\mu\nu\rho\sigma} = -\frac{[\mu\nu\rho\sigma]}{\sqrt{-\det g}}}. \quad (7.4.24)$$

7.4.2 Surface Integration

Much of this and the next subsection are based on [88]. Now let us study how to perform surface integrals in spacetime in a covariant way. The volume integration considered before was over a 4-dimensional subregion of spacetime. This is the appropriate type of integration experienced by the Lagrangian density when forming the action, but we also like to consider quantities such as the total energy or total electric charge of our system, which are spatial integrals only of their respective densities. We can formalize what we mean by a spatial integral by thinking of space at a fixed time as a hypersurface in spacetime, just as we did when considering the general relativistic particle Hamiltonian.

A hypersurface $\Sigma \in \mathbb{T}$ is a submanifold of spacetime defined by all the points $X \in \mathbb{T}$ which satisfy some constraint equation $\zeta(X) = 0$ where ζ is some smooth real valued function of the coordinates. If we are interested in a hypersurface at fixed time t as measured by some observer, then in that coordinate system the function ζ would simply be $\zeta = x^0 - t$. Because $\zeta(X) = 0$ provides a single constraint on the coordinates x^μ , it takes 1 fewer coordinate to parameterize points in Σ than it does a general point in $\mathbb{T}$. In 4-dimensional spacetime then, 3 coordinates are required for Σ . Let y^a be coordinates for Σ . Then, if X is a point in Σ , we can write $x^\mu(y)$ to mean the spacetime coordinates given by the 3-coordinates y^a . A general coordinate displacement dy^a produces corresponding coordinate displacements dx^μ which then must produce a generic displacement vector dX tangent to the hypersurface Σ :

$$dx^\mu(y) = \frac{\partial x^\mu}{\partial y^a} dy^a \implies dX = dx^\mu \vec{e}_\mu = \left(\frac{\partial x^\mu}{\partial y^a} \vec{e}_\mu \right) dy^a. \quad (7.4.25)$$

So, we can define coordinate basis vectors $\vec{e}_a^{(\Sigma)}$ tangent to Σ by:

$$\vec{e}_a^{(\Sigma)} = \frac{\partial x^\mu}{\partial y^a} \vec{e}_\mu \quad (7.4.26)$$

as then every displacement vector tangent to Σ can be written as a linear combination of these vectors.

There is a natural way to construct the normal vector of the hypersurface as well. All coordinate displacements dx^μ which remain on the surface $\zeta(X) = 0$ must automatically have $d\zeta = 0$ and thus:

$$d\zeta = \frac{\partial \zeta}{\partial x^\mu} dx^\mu = 0. \quad (7.4.27)$$

Because dx^μ are the coefficients of arbitrary legal displacements on Σ , we see that the vector k with lowered components:

$$k_\mu = -\frac{\partial \zeta}{\partial x^\mu} \quad (7.4.28)$$

is automatically orthogonal to all such displacements:

$$k \cdot dX = g_{\mu\nu} k^\mu dx^\nu = k_\mu dx^\mu = -\frac{\partial \zeta}{\partial x^\mu} dx^\mu = 0. \quad (7.4.29)$$

Thus, k is a normal vector to the Σ .

We can find a more refined notion of a normal vector if we know a little bit about Σ . The hypersurface Σ is said to be locally spacelike at X if k at X is timelike (it is said to be locally lightlike if k is lightlike and it is said to be locally timelike if k is spacelike). This naming is due to the fact that because there is only ever one negative entry in the diagonal of the metric, if k is timelike then all tangential directions to Σ must be spacelike, if k is lightlike then some tangential directions to Σ must be lightlike, and if k is spacelike then some tangential directions to Σ must be timelike. We will often but not always work with hypersurfaces that have the same causal character (spacelike, timelike, lightlike) everywhere on the surface.

For now, suppose Σ is locally spacelike or timelike and let ε equal the sign of $k \cdot k$ (so -1 if Σ is spacelike

and 1 if Σ is timelike). Then, we can define the unit normal vector $\vec{n}$ as having lowered components n_μ :

$$n_\mu = -\frac{\varepsilon k_\mu}{\sqrt{|k \cdot k|}} \implies n \cdot n = \varepsilon. \quad (7.4.30)$$

The direction pointing normally to Σ in which ζ is increasing is called the outward normal direction to Σ . The outward normal (as familiar from standard vector calculus) appears directly in Stokes' theorem. Note that n_μ as defined here is not only a unit normal but is in fact the outward unit normal vector because for displacements in the $\vec{n}$ direction, ζ is increasing:

$$dX = A\vec{n}, \quad A > 0 \implies d\zeta = \frac{\partial \zeta}{\partial x^\mu} dx^\mu = -k^\mu \frac{-A\varepsilon k_\mu}{\sqrt{|k \cdot k|}} = A\sqrt{|k \cdot k|} > 0. \quad (7.4.31)$$

You should note that for the function $\zeta = x^0$, the given definition of $\vec{n}$ coincides with the definition used when defining the lapse function and shift-vector for the Hamiltonian formalism.

Thinking of Σ as a manifold, using the pseudo-inner product inherited from $\mathbb{T}$, there is a natural induced metric tensor γ_{ab} on Σ :

$$\gamma_{ab} = \vec{e}_a^{(\Sigma)} \cdot \vec{e}_b^{(\Sigma)} = g_{\mu\nu} \frac{\partial x^\mu}{\partial y^a} \frac{\partial x^\nu}{\partial y^b} \implies d\tau^2 = -\gamma_{ab} dy^a dy^b \quad (7.4.32)$$

for all displacements on Σ .

With this thinking of Σ as a manifold, if Σ is timelike or spacelike there is automatically a natural invariant volume element $d\Sigma$ on Σ given by:

$$d\Sigma = \sqrt{|\det \gamma|} d^3y \quad (7.4.33)$$

by copying the argument used to derive the volume element $d\mathbb{T}$ for spacetime. The surface element that appears in Stokes' theorem points normally to the surface with this magnitude, and so it is useful to define the directed surface element $d\Sigma_\mu$:

$$d\Sigma_\mu = \varepsilon n_\mu d\Sigma. \quad (7.4.34)$$

With γ_{ab} acting as the metric tensor on Σ , we can define the inverse metric γ^{ab} by the 3x3 inverse matrix of γ_{ab} :

$$\gamma^{ac} \gamma_{cb} = \delta_b^a. \quad (7.4.35)$$

It is possible to define $\gamma^{\mu\nu}$ as a tensor on spacetime from the inverse metric γ^{ab} by:

$$\gamma^{\mu\nu} = \gamma^{ab} \frac{\partial x^\mu}{\partial y^a} \frac{\partial x^\nu}{\partial y^b}. \quad (7.4.36)$$

This procedure of turning a tensor on Σ into a tensor on $\mathbb{T}$ is called lifting. This lifted tensor has several interesting and useful properties. Using that $\vec{n}$ is orthogonal to each of the $\vec{e}_a^{(\Sigma)}$:

$$\vec{n} \cdot \vec{e}_a^{(\Sigma)} = n_\mu \frac{\partial x^\mu}{\partial y^a} = 0. \quad (7.4.37)$$

Therefore:

$$\gamma^{\mu\nu} n_\nu = \gamma^{ab} \frac{\partial x^\mu}{\partial y^a} \frac{\partial x^\nu}{\partial y^b} n_\nu = 0. \quad (7.4.38)$$

Consider a generic vector $\vec{v}$ at X on spacetime. Then, it can be resolved into a part parallel to Σ and a part orthogonal to it:

$$\vec{v} = v_n \vec{n} + v^a \vec{e}_a^{(\Sigma)} = v^\mu \vec{e}_\mu. \quad (7.4.39)$$

Taking the inner product of both sides with $\vec{n}$ gives:

$$v_n = \varepsilon v^\mu n_\mu \quad (7.4.40)$$

while taking the inner product of both sides with $\vec{e}_a^{(\Sigma)}$ gives:

$$v_a = v_\mu \frac{\partial x^\mu}{\partial y^a}. \quad (7.4.41)$$

Returning these to the expression for $\vec{v}$ gives:

$$v^\mu \vec{e}_\mu = \varepsilon v^\nu n_\nu n^\mu \vec{e}_\mu + \gamma^{ab} v_\nu \frac{\partial x^\nu}{\partial y^b} \frac{\partial x^\mu}{\partial y^a} \vec{e}_\mu. \quad (7.4.42)$$

Because this holds for all coefficients v^μ , we have:

$$\delta_\nu^\mu = \varepsilon n^\mu n_\nu + \gamma^{ab} \frac{\partial x^\mu}{\partial y^a} \frac{\partial x^\rho}{\partial y^b} g_{\rho\nu}. \quad (7.4.43)$$

Using the definition of $\gamma^{\mu\nu}$:

$$g^{\mu\nu} = \gamma^{\mu\nu} + \varepsilon n^\mu n^\nu. \quad (7.4.44)$$

Automatically, it follows that $\gamma^\mu{}_\nu$ eliminates any component of a vector which is orthogonal to Σ but preserves all components tangent to Σ :

$$\gamma^\mu{}_\nu v^\nu = v^\mu - v_n n^\mu \quad (7.4.45)$$

and that $\gamma^\mu{}_\nu$ squares to itself as a matrix:

$$\gamma^\mu{}_\rho \gamma^\rho{}_\nu = (\delta_\rho^\mu - \varepsilon n^\mu n_\rho)(\delta_\nu^\rho - \varepsilon n^\rho n_\nu) = \delta_\nu^\mu - \varepsilon n^\mu n_\nu - \varepsilon n^\mu n_\nu + \varepsilon n^\mu n_\nu = \gamma^\mu{}_\nu. \quad (7.4.46)$$

Therefore, $\gamma^\mu{}_\nu$ is a projection matrix that projects vectors onto spacetime onto vectors on Σ .

There is another useful form for the surface element. To find it, consider the vector F with lower components F_μ defined by:

$$F_\mu = \epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3}. \quad (7.4.47)$$

This vector is automatically orthogonal to each $\vec{e}_a^{(\Sigma)}$ due to the antisymmetry of the Levi-Civita pseudotensor:

$$F \cdot \vec{e}_a^{(\Sigma)} = F_\mu \frac{\partial x^\mu}{\partial y^a} = \epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\mu}{\partial y^a} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = 0 \quad (7.4.48)$$

(because a must take the value 1, 2, or 3, which already occurs in the product). Because F is orthogonal to Σ , it must be parallel to the normal vector k , for some coefficient:

$$\epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = C n_\mu. \quad (7.4.49)$$

The coefficient is thus determined by:

$$C = \varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} \quad (7.4.50)$$

and so automatically is invariant with respect to orientation preserving coordinate transformations of the spacetime coordinates x^μ . However, it is not a scalar with respect to changes of the coordinates y^a on Σ . In particular, consider a transformation $y'^a(y)$:

$$C' = \varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y'^1} \frac{\partial x^\rho}{\partial y'^2} \frac{\partial x^\sigma}{\partial y'^3} = \varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^a} \frac{\partial x^\rho}{\partial y^b} \frac{\partial x^\sigma}{\partial y^c} \frac{\partial y^a}{\partial y'^1} \frac{\partial y^b}{\partial y'^2} \frac{\partial y^c}{\partial y'^3}. \quad (7.4.51)$$

For some coefficient D :

$$\varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^a} \frac{\partial x^\rho}{\partial y^b} \frac{\partial x^\sigma}{\partial y^c} = D[abc] \quad (7.4.52)$$

where $[abc]$ is the fully antisymmetric numerical Levi-Civita symbol for only three indices. This form is necessary because the left hand side is fully antisymmetric under interchanging a , b , and c . Thus:

$$\varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^a} \frac{\partial x^\rho}{\partial y^b} \frac{\partial x^\sigma}{\partial y^c} [abc] = D[abc][abc] \quad (7.4.53)$$

$$\implies 6\varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = 6D \quad (7.4.54)$$

$$\implies D = \varepsilon \epsilon_{\mu\nu\rho\sigma} n^\mu \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = C. \quad (7.4.55)$$

Thus:

$$C' = C[abc] \frac{\partial y^a}{\partial y'^1} \frac{\partial y^b}{\partial y'^2} \frac{\partial y^c}{\partial y'^3} = C \det \frac{\partial y}{\partial y'}. \quad (7.4.56)$$

As well, under this transformation:

$$\gamma'_{ab} = g_{\mu\nu} \frac{\partial x^\mu}{\partial y'^a} \frac{\partial x^\nu}{\partial y'^b} = g_{\mu\nu} \frac{\partial x^\mu}{\partial y^c} \frac{\partial x^\nu}{\partial y^d} \frac{\partial y^c}{\partial y'^a} \frac{\partial y^d}{\partial y'^b} = \gamma_{cd} \frac{\partial y^c}{\partial y'^a} \frac{\partial y^d}{\partial y'^b} \quad (7.4.57)$$

$$\implies \det \gamma' = \det \gamma \left(\det \frac{\partial y}{\partial y'} \right)^2. \quad (7.4.58)$$

So, under orientation preserving coordinate transformations on Σ :

$$\frac{C'}{\sqrt{|\det \gamma'|}} = \frac{C}{\sqrt{|\det \gamma|}}. \quad (7.4.59)$$

Thus, for some coefficient κ which is invariant under all transformations of coordinates on spacetime or Σ :

$$\epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = \kappa n_\mu \sqrt{|\det \gamma|}. \quad (7.4.60)$$

Because of its invariance, κ can be computed in a convenient coordinate system and then its value will be preserved. Contracting both sides with n^μ :

$$\kappa = \epsilon \frac{\sqrt{-\det g}}{\sqrt{|\det \gamma|}} [\mu\nu\rho\sigma] n^\mu \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3}. \quad (7.4.61)$$

Now let us specialize our coordinates. For the moment, don't assume that x^0 is the timelike coordinate. Instead, define coordinates so that locally $x^0 = \zeta(X)$ and the coordinates $x^a = y^a$ coincide with those on Σ . In such coordinates, automatically:

$$k_\mu = -\frac{\partial \zeta}{\partial x^\mu} = -\delta_\mu^0 \implies k \cdot k = g^{00} \implies n^\mu = \epsilon \frac{g^{0\mu}}{\sqrt{|g^{00}|}}. \quad (7.4.62)$$

As well, in these coordinates:

$$\frac{\partial x^\mu}{\partial y^a} = \delta_a^\mu \implies \gamma^{00} = \gamma^{0a} = 0, \quad \gamma^{ab} \text{ unambiguous.} \quad (7.4.63)$$

So, the full metric determinant satisfies:

$$\frac{1}{\det g} = \det(g^{-1}) = [\mu\nu\rho\sigma] g^{\mu 0} g^{\nu 1} g^{\rho 2} g^{\sigma 3} \quad (7.4.64)$$

$$= [\mu\nu\rho\sigma] (\gamma^{\mu 0} + \epsilon n^\mu n^0) g^{\nu 1} g^{\rho 2} g^{\sigma 3} = \epsilon n^0 [\mu\nu\rho\sigma] n^\mu g^{\nu 1} g^{\rho 2} g^{\sigma 3} \quad (7.4.65)$$

$$= \epsilon n^0 [\mu\nu\rho\sigma] n^\mu \gamma^{\nu 1} \gamma^{\rho 1} \gamma^{\sigma 3} = \epsilon n^0 [\mu abc] n^\mu \gamma^{a 1} \gamma^{b 1} \gamma^{c 1} \quad (7.4.66)$$

$$= \epsilon (n^0)^2 [0 abc] \gamma^{1a} \gamma^{2b} \gamma^{3c} = \epsilon |g^{00}| \det(\gamma^{-1}) = \frac{g^{00}}{\det \gamma} \quad (7.4.67)$$

$$\implies \det g = \frac{\det \gamma}{g^{00}}. \quad (7.4.68)$$

Then, we find:

$$\kappa = \epsilon \frac{\sqrt{|\det \gamma|}}{n^0 \sqrt{|\det \gamma|}} [\mu 123] n^\mu = \epsilon. \quad (7.4.69)$$

With this we have that in all coordinates:

$$\epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} = \epsilon n_\mu \sqrt{|\det \gamma|}. \quad (7.4.70)$$

Consequently, the directed surface element can be written:

$$d\Sigma_\mu = \epsilon_{\mu\nu\rho\sigma} \frac{\partial x^\nu}{\partial y^1} \frac{\partial x^\rho}{\partial y^2} \frac{\partial x^\sigma}{\partial y^3} dy^1 dy^2 dy^3. \quad (7.4.71)$$

We can now consider the notion of a lightlike surface. On a lightlike surface, there is no way to define a unit normal vector, because the norm of k is 0. The sign we chose for k was picked so that for a lightlike surface, the vector k is future oriented whenever ζ increases toward the future. If Σ is lightlike, then $\det \gamma = 0$ automatically, and so the surface element $d\Sigma$ becomes useless. However, the directed surface element as expressed in (7.4.71) remains well-defined for a lightlike surface and so remains the appropriate integration measure.

Thus, altogether, for a vector field with components f^μ , we can define its integral over a hypersurface Σ (whether that surface is spacelike, timelike, or lightlike) by:

$$I = \int_\Sigma f^\mu d\Sigma_\mu \quad (7.4.72)$$

where the directed integration measure $d\Sigma_\mu$ is defined by (7.4.71).

7.4.3 Stokes' Theorem

We now have the ingredients necessary to derive the appropriate form of Stokes' theorem on our manifold. Suppose we have some vector field with components f^μ whose divergence $\nabla_\mu f^\mu$ we integrate over a compact simply-connected region $\mathbb{M}$ of spacetime:

$$I = \int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T}. \quad (7.4.73)$$

In the case of Minkowski space, we know that this integral can be turned into a surface integral of f^μ over the boundary $\partial\mathbb{M}$ of the region $\mathbb{M}$. We will now see that this result can be generalized to a generic spacetime.

In order to simplify this integral, there is a useful identity relating the derivatives of the metric determinant and the divergence of a generic vector field. Using (5.2.30):

$$\partial_\mu \det g = g^{\alpha\beta} \partial_\mu g_{\alpha\beta} \det g \quad (7.4.74)$$

$$\implies \partial_\mu \sqrt{-\det g} = \frac{1}{2} g^{\rho\sigma} \partial_\mu g_{\rho\sigma} \sqrt{-\det g}. \quad (7.4.75)$$

Thus:

$$\nabla_\mu f^\mu = \partial_\mu f^\mu + \Gamma_{\nu\mu}^\mu f^\nu = \partial_\mu f^\mu + \frac{1}{2} g^{\mu\rho} (\partial_\nu g_{\rho\mu} + \partial_\mu g_{\rho\nu} - \partial_\rho g_{\mu\nu}) f^\nu \quad (7.4.76)$$

$$= \partial_\mu f^\mu + \frac{1}{2} g^{\rho\sigma} \partial_\mu g_{\rho\sigma} f^\mu = \partial_\mu f^\mu + \frac{\partial_\mu \sqrt{-\det g}}{\sqrt{-\det g}} f^\mu \quad (7.4.77)$$

$$= \frac{\partial_\mu (f^\mu \sqrt{-\det g})}{\sqrt{-\det g}}. \quad (7.4.78)$$

Therefore, our integral may be rewritten as:

$$\int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T} = \int_{\mathbb{M}} \partial_\mu (f^\mu \sqrt{-\det g}) d^4x. \quad (7.4.79)$$

Let us choose coordinates so that $\mathbb{M}$ can be decomposed into a 1-parameter family of closed hypersurfaces $\Sigma(\lambda)$ where $x^0 = \lambda$ on each hypersurface and the coordinates $x^a = y^a$ can be used as coordinates on the hypersurface. We choose this division so that each hypersurface $\Sigma(\lambda')$ encloses all of the other hypersurfaces $\Sigma(\lambda)$ for $\lambda < \lambda'$, meaning these surfaces form layers around some point which eventually reaches $\partial\mathbb{M}$. Choose the parameter λ so that $\Sigma(0)$ corresponds simply to the single point $\mathbb{M}$ gets shrunk down to by this procedure and $\Sigma(1) = \partial\mathbb{M}$. With this coordinate system, the integration of an arbitrary integrand becomes:

$$\int_{\mathbb{M}} F d\mathbb{T} = \int_0^1 \int_{\Sigma(\lambda)} F \sqrt{-\det g} d^3y d\lambda. \quad (7.4.80)$$

Thus, our integral can be written:

$$\int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T} = \int_0^1 \int_{\Sigma(\lambda)} \partial_0 (f^0 \sqrt{-\det g}) d^3y d\lambda + \int_0^1 \int_{\Sigma(\lambda)} \partial_a (f^a \sqrt{-\det g}) d^3y d\lambda. \quad (7.4.81)$$

The y integration in the second term can be rewritten in some way as a surface integral over the boundary of $\Sigma(\lambda)$, however, $\Sigma(\lambda)$ by being a closed hypersurface in our layering scheme has vanishing boundary automatically. Thus, this second term vanishes. Similarly, because the boundary of $\Sigma(\lambda)$ vanishes, the $\partial_0 = \frac{\partial}{\partial\lambda}$ derivative can be moved past the Σ integral in the first term, as the cost of commuting the two for a generic region is an additional term given by integrating over the boundary of $\Sigma(\lambda)$. Thus:

$$\int_{\Sigma(\lambda)} \partial_a (f^a \sqrt{-\det g}) d^3y = 0, \quad \int_{\Sigma(\lambda)} \partial_0 (f^0 \sqrt{-\det g}) d^3y = \frac{\partial}{\partial\lambda} \int_{\Sigma(\lambda)} f^0 \sqrt{-\det g} d^3y. \quad (7.4.82)$$

Then, our integral becomes, using the fundamental theorem of calculus:

$$\int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T} = \int_0^1 \frac{\partial}{\partial\lambda} \int_{\Sigma(\lambda)} f^0 \sqrt{-\det g} d^3y d\lambda = \int_{\Sigma(1)} f^0 \sqrt{-\det g} d^3y - \int_{\Sigma(0)} f^0 \sqrt{-\det g} d^3y. \quad (7.4.83)$$

By definition $\Sigma(1) = \partial\mathbb{M}$ and $\Sigma(0)$ is a single point (and so this second term vanishes):

$$\int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T} = \int_{\partial\mathbb{M}} f^0 \sqrt{-\det g} d^3y \quad (7.4.84)$$

In our coordinates, the hypersurface $\partial\mathbb{M}$ is defined by the constraint $\zeta(X) = x^0 - 1 \stackrel{!}{=} 0$. Therefore, using (7.4.71):

$$d\Sigma_\mu = \sqrt{-\det g} [\mu\nu\rho\sigma] \delta_1^\nu \delta_2^\sigma \delta_3^\sigma d^3y = \delta_\mu^0 \sqrt{-\det g} d^3y \quad (7.4.85)$$

$$\implies f^\mu d\Sigma_\mu = f^0 \sqrt{-\det g} d^3y. \quad (7.4.86)$$

With this result, we have:

$$\boxed{\int_{\mathbb{M}} \nabla_\mu f^\mu d\mathbb{T} = \int_{\partial\mathbb{M}} f^\mu d\Sigma_\mu} \quad (7.4.87)$$

which although we derived this in a particular coordinate system, because it is manifestly coordinate invariant, it is valid in all coordinate systems. This is the generalization of Stokes' theorem to manifolds.

Using the product rule for the covariant derivative and the generalized Stokes' theorem, we can now formulate the manifold generalization of integration by parts. Consider two tensors A and B where the rank of A is one more than the rank of B . Then:

$$\begin{aligned} \nabla_\mu (A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n} B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m}) \\ = \nabla_\mu (A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n}) B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m} \\ + A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n} \nabla_\mu (B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m}). \end{aligned} \quad (7.4.88)$$

Integrating both sides over some region $\mathbb{M}$ and using Stokes' theorem:

$$\boxed{\begin{aligned} \int_{\mathbb{M}} \nabla_\mu (A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n}) B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m} d\mathbb{T} \\ = - \int_{\mathbb{M}} A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n} \nabla_\mu (B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m}) d\mathbb{T} \\ + \int_{\partial\mathbb{M}} A^{\rho_1 \dots \rho_{k-1} \mu \rho_{k+1} \dots \rho_m}{}_{\sigma_1 \dots \sigma_n} B^{\sigma_1 \dots \sigma_n}{}_{\rho_1 \dots \rho_{k-1} \rho_{k+1} \dots \rho_m} d\Sigma_\mu. \end{aligned}} \quad (7.4.89)$$

Exercises

Problem 7.5: Convenient coordinates on a lightlike surface. Consider a lightlike hypersurface Σ defined by a constraint $\zeta(X) = 0$ and with normal vector k with components $k_\mu = -\nabla_\mu \zeta$.

- Show that k is both normal to Σ and tangent to Σ (a very peculiar feature of lightlike surfaces).
- Show that for some scalar field $\kappa(X)$:

$$k^\nu \nabla_\nu k^\mu = 2\kappa k^\mu.$$

- Let $x^\mu(\lambda)$ be a path along Σ satisfying $\frac{dx^\mu}{d\lambda} = k^\mu$. Show that $x^\mu(\lambda)$ is a lightlike geodesic (but λ is not an affine parameter).
- The parameter λ is a useful coordinate on Σ . Let our coordinates on Σ , $y = (\lambda, \theta)$ where λ is a coordinate satisfying $\frac{\partial x^\mu}{\partial \lambda} = k^\mu$ and θ^i (with i taking values 1 or 2) are remaining coordinates on Σ . Show that the proper time element on Σ is:

$$d\tau^2 = \sigma_{ij} d\theta^i d\theta^j$$

where σ_{ij} , the induced metric on Σ , is:

$$\sigma_{AB} = g_{\mu\nu} \frac{\partial x^\mu}{\partial \theta^i} \frac{\partial x^\nu}{\partial \theta^j}.$$

- Show that there exists a lightlike vector field ℓ with components ℓ^μ satisfying $\ell_\mu k^\mu = -1$ and $\ell_\mu \frac{\partial x^\mu}{\partial \theta^i} = 0$. Show that the inverse metric can be expressed as:

$$g^{\mu\nu} = -\ell^\mu k^\nu - k^\mu \ell^\nu + \sigma^{ij} \frac{\partial x^\mu}{\partial \theta^i} \frac{\partial x^\nu}{\partial \theta^j}$$

where σ^{ij} is the matrix inverse of σ_{ij} .

7.5 Spacetime Curvature

7.5.1 Riemann Curvature Tensor

Partial derivatives commute. Covariant derivatives do not. There is a natural geometric reason why. A covariant derivative differs from a partial derivative only by the additional act of parallel transporting the appropriate quantity to the correct base point so that one never subtracts tensors in different tangent spaces. But, parallel transports in different directions do not commute. To understand this, let us think about parallel transport geometrically.

Imagine you have a sheet of paper on which you have drawn a vector. Imagine now the act of taking that vector and translating its location around on the page while keeping its angle above horizontal fixed. No matter what path on the page you translate the vector through, if you return it back to where you started the vector will be pointing exactly the way it originally pointed. This is because a piece of paper is flat. Even if you curve a piece of paper in your hands this remains true because the paper is flat in an intrinsic sense. The curvature you get from bending the paper is only extrinsic. (A manifold is said to be extrinsically curved if it is not simply Euclidean when viewed from outside in a larger space. Something is called intrinsically curved if within that manifold itself it does not behave as simply Euclidean space.) The fact that the vector always returns to how it originally pointed when going around a closed loop shows that parallel transport on a flat space is trivial. Now imagine you are looking at a globe and facing it so that the equator going west to east runs from left to right and the prime meridian going south to north runs from bottom to top. Imagine you have drawn a tangent vector at the north pole which from your perspective is pointing directly to the right (east). Now imagine pulling that vector down from the north pole toward you on the sphere along the prime meridian until it reaches the intersection of the equator and prime meridian while always making sure not to twist the vector at all. When it gets to the equator, the vector is still pointing to the right. Now imagine pushing the vector along the equator until it reaches the 90° W meridian, again without twisting. When it gets there, the vector is now pointing directly from the globe to you. Finally, now imagine pushing the vector up the 90° W meridian from the equator back to the north pole without twisting. Now you have parallel transported this vector in a closed loop around the globe and it went from pointing directly to the right to now pointing directly at you. Therefore, a sphere is intrinsically curved. These parallel transports formed a closed loop but were not trivial.

By the preceding argument, the behavior of parallel transporting a vector around a closed loop tells us about the curvature of a space. By considering parallel transport around a small loop we can learn about the curvature in a small neighborhood of the space and thus develop a notion of a local curvature. Suppose we consider a small rectangle formed by transporting in one direction, then a second, backward back along the first, and then backward back along the second. We could then compute our final vector back at its original location with the initial vector, and compare the difference. To make this explicit, define the transformation $T(\alpha)$ that parallel transports quantities along a vector field $\xi^\mu(x)$ by an amount α . By this, we mean that $T(\alpha)$ acts on position as:

$$T(\alpha)x^\mu = x^\mu + \alpha\xi^\mu(x) + \mathcal{O}(\alpha^2) \quad (7.5.1)$$

and that if ϕ^μ is a vector at X then $T(\alpha)\phi^\mu$ produces a vector at $T(\alpha)X$ by parallel transport:

$$T(\alpha)\phi^\mu = \Upsilon^\mu(\phi, x, T(\alpha)x). \quad (7.5.2)$$

Explicitly using the parallel transport equation (7.2.16) and (7.2.100):

$$\frac{\partial}{\partial \alpha}(T(\alpha)\phi^\rho) + \Gamma^\rho_{\mu\sigma}(T(\alpha)x)\xi^\sigma(T(\alpha)x)T(\alpha)\phi^\mu = 0 \quad (7.5.3)$$

Thus, we can capture the full action of our parallel transport along ξ^μ by the transformation:

$$T(\alpha) \begin{pmatrix} x^\mu \\ \phi^\rho \end{pmatrix} = \begin{pmatrix} x^\mu + \alpha\xi^\mu(x) + \mathcal{O}(\alpha^2) \\ \phi^\rho - \alpha\Gamma^\rho_{\mu\sigma}(x)\xi^\sigma(x)\phi^\mu + \mathcal{O}(\alpha^2) \end{pmatrix}. \quad (7.5.4)$$

Now suppose we have a second such transformation $S(\beta)$ which parallel transports along $\psi^\mu(x)$:

$$S(\beta) \begin{pmatrix} x^\mu \\ \phi^\rho \end{pmatrix} = \begin{pmatrix} x^\mu + \beta\psi^\mu(x) + \mathcal{O}(\beta^2) \\ \phi^\rho - \beta\Gamma^\rho_{\mu\sigma}(x)\psi^\sigma(x)\phi^\mu + \mathcal{O}(\beta^2) \end{pmatrix}. \quad (7.5.5)$$

To see how ϕ^μ changes under parallel transport around a small closed loop, we first transport along ξ^μ , then

ψ^μ , then backward along ξ^μ , and finally backward along ψ^μ . Thus, we consider:

$$S(-\beta)T(-\alpha)S(\beta)T(\alpha) \begin{pmatrix} x^\mu \\ \phi^\rho \end{pmatrix} = S(-\beta)T(-\alpha)S(\beta) \begin{pmatrix} x^\mu + \alpha\xi^\mu + \mathcal{O}(\alpha^2) \\ \phi^\rho - \alpha\Gamma^\rho_{\mu\sigma}\xi^\sigma\phi^\mu + \mathcal{O}(\alpha^2) \end{pmatrix} \quad (7.5.6)$$

$$= S(-\beta)T(-\alpha) \begin{pmatrix} x^\mu + \alpha\xi^\mu + \beta\psi^\mu(x + \alpha\xi) + \mathcal{O}(\alpha^2, \beta^2) \\ \phi^\rho - \alpha\Gamma^\rho_{\mu\sigma}\xi^\sigma\phi^\mu - \beta\Gamma^\rho_{\lambda\nu}(x + \alpha\xi)\psi^\nu(x + \alpha\xi)(\phi^\lambda - \alpha\Gamma^\lambda_{\mu\sigma}\xi^\sigma\phi^\mu) + \mathcal{O}(\alpha^2, \beta^2) \end{pmatrix} \quad (7.5.7)$$

$$= S(-\beta) \begin{pmatrix} x^\mu + \beta\psi^\mu + \alpha\beta(\xi^\nu\partial_\nu\psi^\mu - \psi^\nu\partial_\nu\psi^\mu) + \mathcal{O}(\alpha^2, \beta^2) \\ \phi^\rho - \beta\Gamma^\rho_{\lambda\sigma}\psi^\sigma\phi^\lambda - \alpha\beta\xi^\nu\partial_\nu(\Gamma^\rho_{\lambda\sigma}\psi^\sigma)\phi^\lambda + \alpha\beta\Gamma^\rho_{\lambda\sigma}\Gamma^\lambda_{\mu\nu}\psi^\sigma\xi^\nu\phi^\mu \\ + \alpha\beta\psi^\nu\partial_\nu(\Gamma^\rho_{\mu\sigma}\xi^\sigma)\phi^\mu - \alpha\beta\Gamma^\rho_{\mu\sigma}\Gamma^\lambda_{\lambda\nu}\xi^\sigma\psi^\nu\phi^\lambda + \mathcal{O}(\alpha^2, \beta^2) \end{pmatrix} \quad (7.5.8)$$

$$= \begin{pmatrix} x^\mu + \alpha\beta(\xi^\nu\partial_\nu\psi^\mu - \psi^\nu\partial_\nu\xi^\mu) + \mathcal{O}(\alpha^2, \beta^2) \\ \phi^\rho - \alpha\beta(\partial_\sigma\Gamma^\rho_{\mu\nu} - \partial_\nu\Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\lambda\sigma}\Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\lambda\nu}\Gamma^\lambda_{\mu\sigma})\xi^\sigma\psi^\nu\phi^\mu \\ - \alpha\beta\Gamma^\rho_{\mu\sigma}(\xi^\nu\partial_\nu\psi^\sigma - \psi^\nu\partial_\nu\xi^\sigma)\phi^\mu + \mathcal{O}(\alpha^2, \beta^2) \end{pmatrix} \quad (7.5.9)$$

(in the last two equations, the third line is to be understood as overflow from the previous line, not an additional matrix element). Notice that these four transformations do not in general take us around in a complete loop! The final position x'^μ in fact differs from the initial position to lowest order precisely by the Lie bracket of the vector fields used:

$$x'^\mu - x^\mu = \alpha\beta[\hat{\xi}, \hat{\psi}]^\mu + \mathcal{O}(\alpha^2, \beta^2). \quad (7.5.10)$$

This makes perfect sense, because a translation by a vector field at one point and the inverse translation by that same vector field at a different point will generally not be inverses. They will only be inverses if the translation connecting those points preserved the vector field, hence is a symmetry of that vector field, hence has vanishing Lie bracket with that vector field. In order to close our loop in general then, we need to perform one final translation back to where we started, accounting for this discrepancy. So, define the vector field:

$$\zeta^\mu = \xi^\nu\partial_\nu\psi^\mu - \psi^\nu\partial_\nu\xi^\mu \quad (7.5.11)$$

and the transformation:

$$U(\varepsilon) \begin{pmatrix} x^\mu \\ \phi^\rho \end{pmatrix} = \begin{pmatrix} x^\mu + \varepsilon\zeta^\mu + \mathcal{O}(\varepsilon^2) \\ \phi^\rho - \varepsilon\Gamma^\rho_{\mu\sigma}\zeta^\sigma\phi^\mu + \mathcal{O}(\varepsilon^2) \end{pmatrix} \quad (7.5.12)$$

Then, after the transformation $U(-\alpha\beta)S(-\beta)T(-\alpha)S(\beta)T(\alpha)$ we will have gone in a small closed loop. Altogether then:

$$U(-\alpha\beta)S(-\beta)T(-\alpha)S(\beta)T(\alpha) \begin{pmatrix} x^\mu \\ \phi^\rho \end{pmatrix} = \begin{pmatrix} x^\mu + \mathcal{O}(\alpha^2, \beta^2) \\ \phi^\rho - \alpha\beta R^\rho_{\mu\sigma\nu}\xi^\sigma\psi^\nu\phi^\mu + \mathcal{O}(\alpha^2, \beta^2) \end{pmatrix} \quad (7.5.13)$$

where here we defined the **Riemann curvature tensor** (also just called the Riemann tensor) $R^\rho_{\mu\sigma\nu}$:

$$\boxed{R^\rho_{\mu\sigma\nu} = \partial_\sigma\Gamma^\rho_{\mu\nu} - \partial_\nu\Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\lambda\sigma}\Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\lambda\nu}\Gamma^\lambda_{\mu\sigma}.} \quad (7.5.14)$$

The vector ϕ^ρ has not perfectly returned to itself when transported around a closed loop. Thus, the Riemann curvature tensor measures the local extent to which parallel transports in different directions fail to commute. Equivalently, it measures the local intrinsic curvature of the manifold.

Let us now see how the Riemann tensor relates precisely to the non-commutation of covariant derivatives. First notice that for scalar fields, covariant derivatives do commute:

$$[\nabla_\mu, \nabla_\nu]\phi = \nabla_\mu\nabla_\nu\phi - \nabla_\nu\nabla_\mu\phi \quad (7.5.15)$$

$$= \partial_\mu(\nabla_\nu\phi) - \Gamma^\rho_{\nu\mu}\nabla_\rho\phi - \partial_\nu(\nabla_\mu\phi) + \Gamma^\rho_{\mu\nu}\nabla_\rho\phi \quad (7.5.16)$$

$$= \partial_\mu\partial_\nu\phi - \partial_\nu\partial_\mu\phi = 0. \quad (7.5.17)$$

However, for vector fields we find something more interesting:

$$[\nabla_\sigma, \nabla_\nu]\phi^\rho = \nabla_\sigma\nabla_\nu\phi^\rho - \nabla_\nu\nabla_\sigma\phi^\rho \quad (7.5.18)$$

$$= \partial_\sigma(\nabla_\nu\phi^\rho) + \Gamma^\rho_{\lambda\sigma}\nabla_\nu\phi^\lambda - \Gamma^\lambda_{\nu\sigma}\nabla_\lambda\phi^\rho - \partial_\nu(\nabla_\sigma\phi^\rho) - \Gamma^\rho_{\lambda\nu}\nabla_\sigma\phi^\lambda + \Gamma^\lambda_{\sigma\nu}\nabla_\lambda\phi^\rho \quad (7.5.19)$$

$$= \partial_\sigma(\partial_\nu\phi^\rho + \Gamma^\rho_{\mu\nu}\phi^\mu) + \Gamma^\rho_{\lambda\sigma}(\partial_\nu\phi^\lambda + \Gamma^\lambda_{\mu\nu}\phi^\mu) - \partial_\nu(\partial_\sigma\phi^\rho + \Gamma^\rho_{\mu\sigma}\phi^\mu) - \Gamma^\rho_{\lambda\nu}(\partial_\sigma\phi^\lambda + \Gamma^\lambda_{\mu\sigma}\phi^\mu) \quad (7.5.20)$$

$$= \partial^2_{\sigma\nu}\phi^\rho + \partial_\sigma\Gamma^\rho_{\mu\nu}\phi^\mu + \Gamma^\rho_{\mu\nu}\partial_\sigma\phi^\mu + \Gamma^\rho_{\mu\sigma}\partial_\nu\phi^\mu + \Gamma^\rho_{\lambda\sigma}\Gamma^\lambda_{\mu\nu}\phi^\mu \\ - \partial^2_{\sigma\nu}\phi^\rho - \partial_\nu\Gamma^\rho_{\mu\sigma}\phi^\mu - \Gamma^\rho_{\mu\sigma}\partial_\nu\phi^\mu - \Gamma^\rho_{\mu\nu}\partial_\sigma\phi^\mu - \Gamma^\rho_{\lambda\nu}\Gamma^\lambda_{\mu\sigma}\phi^\mu \quad (7.5.21)$$

$$= (\partial_\sigma \Gamma^\rho_{\mu\nu} - \partial_\nu \Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\lambda\sigma} \Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\lambda\nu} \Gamma^\lambda_{\mu\sigma}) \phi^\mu. \quad (7.5.22)$$

So:

$$[\nabla_\sigma, \nabla_\nu] \phi^\rho = R^\rho_{\mu\sigma\nu} \phi^\mu. \quad (7.5.23)$$

Because both $\nabla_\sigma \nabla_\nu \phi^\rho$ and $\nabla_\nu \nabla_\sigma \phi^\rho$ are the components of proper tensors, their difference $R^\rho_{\mu\sigma\nu} \phi^\mu$ also forms the components of a tensor and so because ϕ^μ is an arbitrary vector field, $R^\rho_{\mu\sigma\nu}$ in fact is a proper tensor. This can also be verified in a more painful way by using the transformation property of the connection coefficients in (7.2.23). Thus:

$$R'^\rho_{\mu\sigma\nu}(x') = \frac{\partial x'^\rho}{\partial x^\delta} \frac{\partial x}{\partial x'^\alpha} \frac{\partial x}{\partial x'^\gamma} \frac{\partial x^\beta}{\partial x'^\nu} R^\delta_{\alpha\gamma\beta}(x). \quad (7.5.24)$$

One may worry that for higher rank tensors, even more structures may appear from the non-commutation of covariant derivatives. Let us now show that this is not the case. Let ϕ^a be the components of an arbitrary tensor field, where a is a compound index serving as a shorthand for whatever list of tensor indices that tensor would have. In order to continue, we need two helpful properties of the index shuffler. Explicitly writing tensor indices:

$$\begin{aligned} \hat{G}^\alpha_{\beta} \nabla_\mu \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n} &= -\delta^\alpha_\mu \nabla_\beta \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n} + \delta^\rho_1_\beta \nabla_\mu \phi^{\alpha \rho_2 \dots \rho_m}_{\sigma_1 \dots \sigma_n} + \dots + \delta^{\rho_m}_\beta \nabla_\mu \phi^{\rho_1 \dots \rho_{m-1} \alpha}_{\sigma_1 \dots \sigma_n} \\ &\quad - \delta^\alpha_{\sigma_1} \nabla_\mu \phi^{\rho_1 \dots \rho_m}_{\beta \sigma_2 \dots \sigma_n} - \dots - \delta^\alpha_{\sigma_n} \nabla_\mu \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_{n-1} \beta} \end{aligned} \quad (7.5.25)$$

$$= -\delta^\alpha_\mu \nabla_\beta \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n} + \nabla_\mu \hat{G}^\alpha_{\beta} \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n}. \quad (7.5.26)$$

Thus, we have:

$$\boxed{\hat{G}^\alpha_{\beta} \nabla_\mu \phi^a = -\delta^\alpha_\mu \nabla_\beta \phi^a + \nabla_\mu \hat{G}^\alpha_{\beta} \phi^a.} \quad (7.5.27)$$

As well, expand the covariant derivatives appearing on both sides and use the product rule property of the index shuffler:

$$\hat{G}^\alpha_{\beta} (\partial_\mu \phi^a + \Gamma^\lambda_{\gamma\mu} \hat{G}^\gamma_{\lambda} \phi^a) = -\delta^\alpha_\mu (\partial_\beta \phi^a + \Gamma^\lambda_{\gamma\beta} \hat{G}^\gamma_{\lambda} \phi^a) + \partial_\mu (\hat{G}^\alpha_{\beta} \phi^a) + \Gamma^\lambda_{\gamma\mu} \hat{G}^\gamma_{\lambda} \hat{G}^\alpha_{\beta} \phi^a \quad (7.5.28)$$

$$\begin{aligned} \implies & -\delta^\alpha_\mu \partial_\beta \phi^a + \partial_\mu (\hat{G}^\alpha_{\beta} \phi^a) + \hat{G}^\alpha_{\beta} (\Gamma^\lambda_{\gamma\mu} \hat{G}^\gamma_{\lambda} \phi^a) + \Gamma^\lambda_{\gamma\mu} \hat{G}^\alpha_{\beta} \hat{G}^\gamma_{\lambda} \phi^a \\ & = -\delta^\alpha_\mu \partial_\beta \phi^a - \delta^\alpha_\mu \Gamma^\lambda_{\gamma\beta} \hat{G}^\gamma_{\lambda} \phi^a + \partial_\mu (\hat{G}^\alpha_{\beta} \phi^a) + \Gamma^\lambda_{\gamma\mu} \hat{G}^\alpha_{\beta} \hat{G}^\gamma_{\lambda} \phi^a \end{aligned} \quad (7.5.29)$$

$$\implies \Gamma^\lambda_{\gamma\mu} (\hat{G}^\alpha_{\beta} \hat{G}^\gamma_{\lambda} - \hat{G}^\gamma_{\lambda} \hat{G}^\alpha_{\beta}) \phi^a + \Gamma^\alpha_{\gamma\mu} \hat{G}^\gamma_{\beta} \phi^a - \Gamma^\lambda_{\beta\mu} \hat{G}^\alpha_{\lambda} \phi^a - \delta^\alpha_\mu \Gamma^\lambda_{\gamma\beta} \hat{G}^\gamma_{\lambda} \phi^a + \delta^\alpha_\mu \Gamma^\lambda_{\gamma\beta} \hat{G}^\gamma_{\lambda} \phi^a = 0 \quad (7.5.30)$$

$$\implies \Gamma^\lambda_{\gamma\mu} ([\hat{G}^\alpha_{\beta}, \hat{G}^\gamma_{\lambda}] \phi^a - \delta^\gamma_\beta \hat{G}^\alpha_{\lambda} \phi^a + \delta^\alpha_\lambda \hat{G}^\gamma_{\beta} \phi^a) = 0. \quad (7.5.31)$$

Because this equation is true in all coordinate systems and the connection coefficients can be set to an arbitrary value by appropriate choice of coordinate system, their coefficient must vanish and so:

$$\boxed{[\hat{G}^\alpha_{\beta}, \hat{G}^\gamma_{\lambda}] \phi^a = \delta^\gamma_\beta \hat{G}^\alpha_{\lambda} \phi^a - \delta^\alpha_\lambda \hat{G}^\gamma_{\beta} \phi^a.} \quad (7.5.32)$$

Then, using (7.5.27) and (7.5.32):

$$[\nabla_\sigma, \nabla_\nu] \phi^a = \nabla_\sigma \nabla_\nu \phi^a - \nabla_\nu \nabla_\sigma \phi^a \quad (7.5.33)$$

$$= \partial_\sigma (\nabla_\nu \phi^a) + \Gamma^\beta_{\alpha\sigma} \hat{G}^\alpha_{\beta} \nabla_\nu \phi^a - \partial_\nu (\nabla_\sigma \phi^a) - \Gamma^\beta_{\alpha\nu} \hat{G}^\alpha_{\beta} \nabla_\sigma \phi^a \quad (7.5.34)$$

$$\begin{aligned} &= \partial_\sigma (\partial_\nu \phi^a + \Gamma^\beta_{\alpha\nu} \hat{G}^\alpha_{\beta} \phi^a) + \Gamma^\beta_{\alpha\sigma} (-\delta^\alpha_\nu \nabla_\beta \phi^a + \nabla_\nu \hat{G}^\alpha_{\beta} \phi^a) \\ &\quad - \partial_\nu (\partial_\sigma \phi^a + \Gamma^\beta_{\alpha\sigma} \hat{G}^\alpha_{\beta} \phi^a) - \Gamma^\beta_{\alpha\nu} (-\delta^\alpha_\sigma \nabla_\beta \phi^a + \nabla_\sigma \hat{G}^\alpha_{\beta} \phi^a) \end{aligned} \quad (7.5.35)$$

$$\begin{aligned} &= \partial_\sigma^2 \phi^a + \partial_\sigma \Gamma^\beta_{\alpha\nu} \hat{G}^\alpha_{\beta} \phi^a + \Gamma^\beta_{\alpha\nu} \partial_\sigma \hat{G}^\alpha_{\beta} \phi^a - \Gamma^\beta_{\sigma\nu} \nabla_\beta \phi^a + \Gamma^\beta_{\alpha\sigma} (\partial_\nu \hat{G}^\alpha_{\beta} \phi^a + \Gamma^\lambda_{\gamma\nu} \hat{G}^\gamma_{\lambda} \phi^a) \\ &\quad - \partial_\nu^2 \phi^a - \partial_\nu \Gamma^\beta_{\alpha\sigma} \hat{G}^\alpha_{\beta} \phi^a - \Gamma^\beta_{\alpha\sigma} \partial_\nu \hat{G}^\alpha_{\beta} \phi^a + \Gamma^\beta_{\sigma\nu} \nabla_\beta \phi^a - \Gamma^\beta_{\alpha\nu} (\partial_\sigma \hat{G}^\alpha_{\beta} \phi^a + \Gamma^\lambda_{\gamma\sigma} \hat{G}^\gamma_{\lambda} \phi^a) \end{aligned} \quad (7.5.36)$$

$$= (\partial_\sigma \Gamma^\beta_{\alpha\nu} - \partial_\nu \Gamma^\beta_{\alpha\sigma}) \hat{G}^\alpha_{\beta} \phi^a + \Gamma^\beta_{\alpha\sigma} \Gamma^\lambda_{\gamma\nu} [\hat{G}^\alpha_{\beta}, \hat{G}^\gamma_{\lambda}] \phi^a \quad (7.5.37)$$

$$= (\partial_\sigma \Gamma^\beta_{\alpha\nu} - \partial_\nu \Gamma^\beta_{\alpha\sigma} + \Gamma^\beta_{\lambda\sigma} \Gamma^\lambda_{\alpha\nu} - \Gamma^\beta_{\lambda\nu} \Gamma^\lambda_{\alpha\sigma}) \hat{G}^\alpha_{\beta} \phi^a. \quad (7.5.38)$$

Therefore, for an arbitrary tensor field:

$$\boxed{[\nabla_\sigma, \nabla_\nu] \phi^a = R^\rho_{\mu\sigma\nu} \hat{G}^\mu_{\rho} \phi^a.} \quad (7.5.39)$$

The Riemann tensor has many index interchange symmetries. Most of them are easiest to see when

in a LIRF. Suppose we are in a coordinate system which is a LIRF at the point X_0 . Then, at that point $g_{\mu\nu}(x_0) = \eta_{\mu\nu}$ and $\Gamma^\rho_{\mu\nu}(x_0) = 0$ (equivalently $\partial_\rho g_{\mu\nu}(x_0) = 0$). Automatically:

$$\partial_\sigma \Gamma^\rho_{\mu\nu}(x_0) = \partial_\sigma \left(\frac{1}{2} g^{\rho\lambda} (\partial_\mu g_{\lambda\nu} + \partial_\nu g_{\lambda\mu} - \partial_\lambda g_{\mu\nu}) \right) \Big|_{x=x_0} \quad (7.5.40)$$

$$= \frac{1}{2} \eta^{\rho\lambda} (\partial_{\mu\sigma}^2 g_{\lambda\nu}(x_0) + \partial_{\nu\sigma}^2 g_{\lambda\mu}(x_0) - \partial_{\lambda\sigma}^2 g_{\mu\nu}(x_0)). \quad (7.5.41)$$

Thus, in a LIRF:

$$R_{\rho\mu\sigma\nu}(x_0) = \frac{1}{2} (\partial_{\mu\sigma}^2 g_{\rho\nu}(x_0) + \partial_{\nu\sigma}^2 g_{\rho\mu}(x_0) - \partial_{\rho\sigma}^2 g_{\mu\nu}(x_0) - \partial_{\mu\nu}^2 g_{\rho\sigma}(x_0) - \partial_{\nu\rho}^2 g_{\sigma\mu}(x_0) + \partial_{\rho\nu}^2 g_{\sigma\mu}(x_0)) \quad (7.5.42)$$

$$\implies R_{\rho\sigma\mu\nu}(x_0) = \frac{1}{2} (\partial_{\sigma\mu}^2 g_{\rho\nu}(x_0) + \partial_{\rho\nu}^2 g_{\sigma\mu}(x_0) - \partial_{\rho\mu}^2 g_{\sigma\nu}(x_0) - \partial_{\sigma\nu}^2 g_{\rho\mu}(x_0)). \quad (7.5.43)$$

From this last expression we can see directly:

$$\boxed{R_{\rho\sigma\mu\nu} = -R_{\rho\sigma\nu\mu} = -R_{\sigma\rho\mu\nu} = R_{\mu\nu\rho\sigma}.} \quad (7.5.44)$$

While these symmetries were derived in a LIRF, because all of the quantities in this equation transform correctly as tensor components, this equation remains true in all coordinate systems. There is one other so-called “algebraic” identity (meaning not involving derivatives) satisfied by the Riemann tensor. A brief calculation from (7.5.43) gives:

$$\boxed{R_{\rho\sigma\mu\nu} + R_{\rho\mu\nu\sigma} + R_{\rho\nu\sigma\mu} = 0.} \quad (7.5.45)$$

This is known as the algebraic Bianchi identity.

There is one other nontrivial identity satisfied by the Riemann tensor but it is a differential identity (meaning it relates the derivatives of the Riemann tensor). Consider a tensor field ϕ^a and recall that the commutator of linear operators automatically satisfies the Jacobi identity (1.3.27):

$$[\nabla_\lambda, [\nabla_\sigma, \nabla_\nu]]\phi^a + [\nabla_\sigma, [\nabla_\nu, \nabla_\lambda]]\phi^a + [\nabla_\nu, [\nabla_\lambda, \nabla_\sigma]]\phi^a = 0. \quad (7.5.46)$$

Let us simplify one of these three terms (using (7.5.27) and (7.5.39)):

$$[\nabla_\lambda, [\nabla_\sigma, \nabla_\nu]]\phi^a = \nabla_\lambda[\nabla_\sigma, \nabla_\nu]\phi^a - [\nabla_\sigma, \nabla_\nu]\nabla_\lambda\phi^a \quad (7.5.47)$$

$$= \nabla_\lambda(R^\rho_{\mu\sigma\nu}\hat{G}^\mu_{\rho}\phi^a) - R^\rho_{\mu\sigma\nu}\hat{G}^\mu_{\rho}(\nabla_\lambda\phi^a) \quad (7.5.48)$$

$$= \nabla_\lambda R^\rho_{\mu\sigma\nu}\hat{G}^\mu_{\rho}\phi^a + R^\rho_{\mu\sigma\nu}\nabla_\lambda\hat{G}^\mu_{\rho}\phi^a - R^\rho_{\mu\sigma\nu}(-\delta^\mu_\lambda\nabla_\rho\phi^a + \nabla_\lambda\hat{G}^\mu_{\rho}\phi^a) \quad (7.5.49)$$

$$= \nabla_\lambda R^\rho_{\mu\sigma\nu}\hat{G}^\mu_{\rho}\phi^a + R^\rho_{\lambda\sigma\nu}\nabla_\rho\phi^a. \quad (7.5.50)$$

Returning this to the full Jacobi identity and using (7.5.45):

$$(\nabla_\lambda R^\rho_{\mu\sigma\nu} + \nabla_\sigma R^\rho_{\mu\nu\lambda} + \nabla_\nu R^\rho_{\mu\lambda\sigma})\hat{G}^\mu_{\rho}\phi^a = 0. \quad (7.5.51)$$

This holds for all tensor fields, and so the coefficient must vanish:

$$\boxed{\nabla_\lambda R^\rho_{\mu\sigma\nu} + \nabla_\sigma R^\rho_{\mu\nu\lambda} + \nabla_\nu R^\rho_{\mu\lambda\sigma} = 0.} \quad (7.5.52)$$

This is known as the differential Bianchi identity.

In (7.2.113) we found that the antisymmetric partial derivatives of the connection coefficients cannot be altered by further coordinate transformations once one has gone to a LIRF. That combination we now see is precisely the Riemann curvature! This really starts to make the Riemann tensor look like something directly observable, because one cannot get rid of it by going to the right coordinates. We found that a free particle experiencing a background gravitational field follows geodesics of spacetime. In a LIRF at that particle’s position, the particle’s acceleration is always 0, and so there is no experience of motion. However, we will now see that the displacement between nearby particles evolves in a way that cannot be transformed away, and that it does so in a way dependent upon the Riemann tensor. Let $x^\mu(\lambda, s)$ be a smooth 1-parameter family of geodesics. By this I mean that for each fixed s , $x^\mu(\lambda, s)$ is a geodesic viewed as a function of λ (which we take to be an affine parameter by definition). Changing s changes which geodesic we are talking about. We could imagine such a function $x^\mu(\lambda, s)$ by considering a fluid of free particles each following geodesics and s labeling which fluid element is being tracked. Then, define:

$$u^\mu(\lambda, s) = \frac{\partial x^\mu}{\partial \lambda}, \quad \xi^\mu(\lambda, s) = \frac{\partial x^\mu}{\partial s}. \quad (7.5.53)$$

The vector u^μ gives the four-velocity of particle s at parameter λ (viewing λ as the time). The vector ξ^μ gives

the displacement per unit s between nearby fluid elements. ξ^μ is called the geodesic deviation. Recalling the covariant parameter derivative and using the equality of mixed partials:

$$\frac{D\xi^\mu}{D\lambda} = \frac{\partial\xi^\mu}{\partial\lambda} + \Gamma^\mu_{\rho\sigma}\xi^\rho \frac{\partial x^\sigma}{\partial\lambda} = \frac{\partial u^\mu}{\partial s} + \Gamma^\mu_{\rho\sigma}u^\rho \xi^\sigma = \frac{Du^\mu}{Ds}. \quad (7.5.54)$$

Now taking the covariant λ derivative of ξ^μ (and recalling that these are geodesics and so $\frac{Du^\mu}{D\lambda} = 0$):

$$\frac{D^2\xi^\mu}{D\lambda^2} = \frac{D}{D\lambda} \frac{Du^\mu}{Ds} = \frac{D}{D\lambda} \frac{D}{Ds} u^\mu - \frac{D}{Ds} \frac{D}{D\lambda} u^\mu \quad (7.5.55)$$

$$= \frac{\partial}{\partial\lambda} \frac{Du^\mu}{Ds} + \Gamma^\mu_{\rho\sigma}u^\rho \frac{Du^\sigma}{Ds} - \frac{\partial}{\partial s} \frac{Du^\mu}{D\lambda} - \Gamma^\mu_{\rho\sigma}\xi^\rho \frac{Du^\sigma}{D\lambda} \quad (7.5.56)$$

$$= \frac{\partial}{\partial\lambda} \left(\frac{\partial u^\mu}{\partial s} + \Gamma^\mu_{\rho\sigma}u^\rho \xi^\sigma \right) + \Gamma^\mu_{\rho\sigma}u^\rho \left(\frac{\partial u^\sigma}{\partial s} + \Gamma^\sigma_{\alpha\beta}u^\alpha \xi^\beta \right) - \frac{\partial}{\partial s} \left(\frac{\partial u^\mu}{\partial\lambda} + \Gamma^\mu_{\rho\sigma}u^\rho u^\sigma \right) - \Gamma^\mu_{\rho\sigma}\xi^\rho \left(\frac{\partial u^\sigma}{\partial\lambda} + \Gamma^\sigma_{\alpha\beta}u^\alpha u^\beta \right) \quad (7.5.57)$$

$$= \frac{\partial^2 u^\mu}{\partial\lambda\partial s} + u^\nu \partial_\nu \Gamma^\mu_{\rho\sigma} u^\rho \xi^\sigma + \Gamma^\mu_{\rho\sigma}\xi^\rho \frac{\partial u^\sigma}{\partial\lambda} + \Gamma^\mu_{\rho\sigma}u^\sigma \frac{\partial u^\sigma}{\partial s} + \Gamma^\mu_{\rho\sigma}u^\rho \frac{\partial u^\sigma}{\partial s} + \Gamma^\mu_{\rho\sigma}\Gamma^\sigma_{\alpha\beta}u^\rho u^\alpha \xi^\beta \quad (7.5.58)$$

$$- \frac{\partial^2 u^\mu}{\partial\lambda\partial s} - \xi^\nu \partial_\nu \Gamma^\mu_{\rho\sigma} u^\rho u^\sigma - 2\Gamma^\mu_{\rho\sigma}u^\rho \frac{\partial u^\sigma}{\partial s} - \Gamma^\mu_{\rho\sigma}\xi^\rho \frac{\partial u^\sigma}{\partial\lambda} - \Gamma^\mu_{\rho\sigma}\Gamma^\sigma_{\alpha\beta}\xi^\rho u^\alpha u^\beta \quad (7.5.59)$$

$$= (\partial_\rho \Gamma^\mu_{\nu\sigma} - \partial_\sigma \Gamma^\mu_{\nu\rho} + \Gamma^\mu_{\rho\lambda}\Gamma^\lambda_{\nu\sigma} - \Gamma^\mu_{\sigma\lambda}\Gamma^\lambda_{\nu\rho}) u^\rho u^\nu \xi^\sigma. \quad (7.5.60)$$

Thus, the geodesic deviation satisfies:

$$\boxed{\frac{D^2\xi^\mu}{D\lambda^2} + R^\mu_{\rho\nu\sigma}u^\rho \xi^\nu u^\sigma = 0} \quad (7.5.61)$$

which is a second order differential equation for ξ^μ known as the geodesic deviation equation. So, one physical consequence of the Riemann tensor is that it captures the rate at which nearby particles accelerate away from each other.

The Riemann tensor is a rank-4 tensor. We will repeatedly find that the rank-2 tensor known as the **Ricci tensor** $R_{\mu\nu}$ defined by:

$$\boxed{R_{\mu\nu} = R^\rho_{\mu\rho\nu}} \quad (7.5.62)$$

appears in important equations, and so is worth introducing the above shorthand. Due to the index interchange properties of the Riemann tensor, the Ricci tensor is symmetric:

$$R_{\nu\mu} = R^\rho_{\nu\rho\mu} = R_{\rho\mu}{}^\rho{}_\nu = R_{\mu\nu}. \quad (7.5.63)$$

It will also be a convenient shorthand to define the **Ricci scalar** R by:

$$\boxed{R = R^\mu{}_\mu}. \quad (7.5.64)$$

It may seem dangerous to use the symbol R for so many different meanings, but when indices are written one can always uniquely identify whether the Riemann tensor, Ricci tensor, or Ricci scalar is intended by whether the object has 4, 2, or 0 indices.

7.5.2 Wilson Loops

The Riemann tensor captures the local curvature of the manifold through the change in tensor fields when transported around a small closed loop. It is a nontrivial question whether there is more information to be found in the transport around large loops. Essentially, the question is whether all curvature information can be extracted from local curvature information.

It turns out it cannot. Suppose we have some path $x^\mu(\lambda)$ in spacetime along which we parallel transport some vector $\phi^\mu(\lambda)$. That is, we define $\phi^\mu(\lambda)$ according to:

$$\frac{D\phi^\mu}{D\lambda} = 0 \implies \frac{\partial\phi^\mu}{\partial\lambda} = -\Gamma^\mu_{\nu\rho}(x(\lambda)) \frac{dx^\rho}{d\lambda} \phi^\nu(\lambda) \quad (7.5.65)$$

with some initial condition $\phi^\mu(0)$ at the start of the path. This is a linear differential equation and so at least formally can be solved. Define the list of matrices $\hat{\Gamma}_\mu(x)$ to have components given by the connection

coefficients:

$$(\hat{\Gamma}_\mu(x))^\rho{}_\sigma = \Gamma^\rho{}_{\sigma\mu}(x). \quad (7.5.66)$$

Then, let $\hat{U}(\lambda)$ be the matrix with components $U^\mu{}_\nu(\lambda)$ satisfying:

$$U^\mu{}_\nu(0) = \delta^\mu_\nu, \quad \frac{\partial U^\mu{}_\nu}{\partial \lambda} = -\Gamma^\mu{}_{\rho\sigma}(x(\lambda)) \frac{dx^\sigma}{d\lambda} U^\rho{}_\nu(\lambda). \quad (7.5.67)$$

Then, at $\lambda = 0$:

$$\phi^\mu(0) - U^\mu{}_\nu(0)\phi^\nu(0) = 0 \quad (7.5.68)$$

and for all λ :

$$\frac{\partial}{\partial \lambda}(\phi^\mu(\lambda) - U^\mu{}_\nu(\lambda)\phi^\nu(0)) = -\Gamma^\mu{}_{\nu\sigma} \frac{dx^\sigma}{d\lambda}(\phi^\nu(\lambda) - U^\nu{}_\rho(\lambda)\phi^\rho(0)). \quad (7.5.69)$$

Thus, $\phi^\mu(\lambda) - U^\mu{}_\nu(\lambda)\phi^\nu(0)$ is initially zero and it satisfies a homogeneous linear differential equation. So, it remains 0 for all λ and we have:

$$\phi^\mu(\lambda) = U^\mu{}_\nu(\lambda)\phi^\nu(0). \quad (7.5.70)$$

Parallel transport along this path is therefore determined fully by the matrix $\hat{U}(\lambda)$.

Rewritten in terms of matrices rather than components, $\hat{U}$ satisfies:

$$\hat{U}(0) = \mathbb{1}, \quad \frac{\partial \hat{U}(\lambda)}{\partial \lambda} = -\hat{\Gamma}_\mu(x(\lambda)) \frac{dx^\mu}{d\lambda} \hat{U}(\lambda). \quad (7.5.71)$$

Evaluating both sides at λ' and integrating from 0 to λ :

$$\hat{U}(\lambda) - \mathbb{1} = - \int_0^\lambda \hat{\Gamma}_\mu(x(\lambda')) \frac{dx^\mu(\lambda')}{d\lambda'} \hat{U}(\lambda') d\lambda'. \quad (7.5.72)$$

This equation is inconvenient because $\hat{U}$ appears on both sides of the equation. Notice what happens when we insert this equation into itself on the right hand side under the integral:

$$\hat{U}(\lambda) = \mathbb{1} - \int_0^\lambda \hat{\Gamma}_\mu(x(\lambda')) \frac{dx^\mu(\lambda')}{d\lambda'} d\lambda' + \int_0^\lambda \int_0^{\lambda'} \hat{\Gamma}_\mu(x(\lambda')) \frac{dx^\mu(\lambda')}{d\lambda'} \hat{\Gamma}_\nu(x(\lambda'')) \frac{dx^\nu(\lambda'')}{d\lambda''} \hat{U}(\lambda'') d\lambda'' d\lambda'. \quad (7.5.73)$$

We can continue to do so iteratively. Doing so finitely many times gives:

$$\begin{aligned} \hat{U}(\lambda) = & \mathbb{1} - \int_0^\lambda \hat{\Gamma}_\mu(x(\lambda')) \frac{dx^\mu(\lambda')}{d\lambda'} d\lambda' + \dots \\ & + (-1)^n \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_n)) \frac{dx^{\mu_n}}{d\lambda_n} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_1)) \frac{dx^{\mu_1}}{d\lambda_1} \hat{U}(\lambda_1) d\lambda_1 \dots d\lambda_n. \end{aligned} \quad (7.5.74)$$

Under very mild hypothesis on the smoothness of the connection coefficients, it is guaranteed that these iterated terms get smaller quite quickly for large n . Intuitively, $\hat{U}(\lambda_1)$ is always evaluated at the least value among $\lambda_1, \dots, \lambda_n$ and as the number n becomes large, then in the integration region λ_1 is almost always very small and thus $\hat{U}(\lambda_1)$ is almost always very close to $\mathbb{1}$. With these assumptions, we can apply this iteratively process infinitely to arrive at:

$$\hat{U}(\lambda) = \sum_{n=0}^{\infty} (-1)^n \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_n)) \frac{dx^{\mu_n}}{d\lambda_n} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_1)) \frac{dx^{\mu_1}}{d\lambda_1} d\lambda_1 \dots d\lambda_n. \quad (7.5.75)$$

This equation is the most useful form for perturbatively computing the operator $\hat{U}$. However, it can be simplified in terms of notation (though made less useful for calculation), by introducing the path ordering transformation $\mathcal{P}$: which is a transformation that acts on a product of operators which are functions of λ and is defined by reordering all of the operators into order from last to first in terms of when they occur on the path $x^\mu(\lambda)$. That is, for 2 operators $\hat{A}(\lambda_1)$ and $\hat{B}(\lambda_2)$:

$$\mathcal{P} : \hat{A}(\lambda_1) \hat{B}(\lambda_2) = \begin{cases} \hat{A}(\lambda_1) \hat{B}(\lambda_2), & \lambda_1 > \lambda_2 \\ \frac{\hat{A}(\lambda_1) \hat{B}(\lambda_2) + \hat{B}(\lambda_2) \hat{A}(\lambda_1)}{2}, & \lambda_1 = \lambda_2 \\ \hat{B}(\lambda_2) \hat{A}(\lambda_1), & \lambda_1 < \lambda_2 \end{cases} \quad (7.5.76)$$

and similarly so for products of 3 or more operators. Then, because $\lambda_1 < \dots < \lambda_n < \lambda$ in our integration, it is

already path ordered and so we can trivially apply the path ordering transformation to it:

$$\hat{U}(\lambda) = \sum_{n=0}^{\infty} (-1)^n \mathcal{P} : \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_n)) \frac{dx^{\mu_n}}{d\lambda_n} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_1)) \frac{dx^{\mu_1}}{d\lambda_1} d\lambda_1 \dots d\lambda_n. \quad (7.5.77)$$

Because of the path ordering, we can reorder the factors of $\hat{\Gamma}$ arbitrarily as the path ordering will just return them back to their original order anyway. There are $n!$ ways to order n factors and so we can sum over all $n!$ orderings and divide by $n!$ because under the path ordering all of the terms in such a sum are equal. Let σ be a list containing each of the numbers 1 to n once each in some order (this is called a permutation of n). Then, let σ_k be the k^{th} entry in that list. Then:

$$\hat{U}(\lambda) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \mathcal{P} : \int_0^\lambda \dots \int_0^{\lambda_2} \sum_{\text{All } \sigma} \hat{\Gamma}_{\mu_n}(x(\lambda_{\sigma_n})) \frac{dx^{\mu_n}}{d\lambda_{\sigma_n}} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_{\sigma_1})) \frac{dx^{\mu_1}}{d\lambda_{\sigma_1}} d\lambda_1 \dots d\lambda_n. \quad (7.5.78)$$

In each term of the sum over all σ , rename λ_{σ_k} to λ_k . Then, the resulting integration region will be the set of all values of $\lambda_1, \dots, \lambda_n$ from 0 to λ with the λ_k ordered so that the k^{th} highest element is λ_{σ_k} . The region of values of $\lambda_1, \dots, \lambda_n$ each from 0 to λ can be divided into $n!$ regions in which the λ_k take a particular ordering on each region. Then, the sum over all such orderings of these integrals is equivalent to simply integrating each λ_k from 0 to λ without having to sum over orderings:

$$\begin{aligned} \sum_{\text{All } \sigma} \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_{\sigma_n})) \frac{dx^{\mu_n}}{d\lambda_{\sigma_n}} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_{\sigma_1})) \frac{dx^{\mu_1}}{d\lambda_{\sigma_1}} d\lambda_1 \dots d\lambda_n \\ = \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_n)) \frac{dx^{\mu_n}}{d\lambda_n} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_1)) \frac{dx^{\mu_1}}{d\lambda_1} d\lambda_1 \dots d\lambda_n. \end{aligned} \quad (7.5.79)$$

Then, $\hat{U}(\lambda)$ becomes:

$$\hat{U}(\lambda) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \mathcal{P} : \int_0^\lambda \dots \int_0^{\lambda_2} \hat{\Gamma}_{\mu_n}(x(\lambda_n)) \frac{dx^{\mu_n}}{d\lambda_n} \dots \hat{\Gamma}_{\mu_1}(x(\lambda_1)) \frac{dx^{\mu_1}}{d\lambda_1} d\lambda_1 \dots d\lambda_n \quad (7.5.80)$$

$$= \mathcal{P} : \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\int_0^\lambda \hat{\Gamma}_{\mu}(x(\lambda')) \frac{dx^{\mu}}{d\lambda'} d\lambda' \right)^n \quad (7.5.81)$$

$$= \mathcal{P} : e^{-\int_0^\lambda \hat{\Gamma}_{\mu}(x(\lambda')) \frac{dx^{\mu}}{d\lambda'} d\lambda'}. \quad (7.5.82)$$

This final expression, called a path ordered exponential, is not very helpful for calculations and effectively just acts as a shorthand for (7.5.75).

We can construct $\hat{U}$ along a generic smooth curve on our manifold. If X_0 and $X_f = X$ are the initial and final points along such a curve γ (with $\lambda = 0$ at X_0 and $\lambda = 1$ at X_f by convention), then parallel transporting a vector ϕ^μ from X_0 to X_f along this curve is given by:

$$\Upsilon^\mu(\phi)[\gamma] = U^\mu{}_\nu(1)\phi^\nu \quad (7.5.83)$$

where we have written the usual parallel transport map as a functional of the path rather than solely as a function of the end points because it is only a simple function of the endpoints for very short paths (when one considers nearby points and follows the geodesic between them). So, define the **parallel transport propagator** or **gravitational Wilson line** $\Upsilon^\mu{}_\nu[\gamma]$ by:

$$\Upsilon^\mu{}_\nu[\gamma] = \left(\mathcal{P} : e^{-\int_\gamma \hat{\Gamma}_\rho(x) dx^\rho} \right)^\mu{}_\nu. \quad (7.5.84)$$

Then, the parallel transport map is fully given by:

$$\Upsilon^\mu(\phi)[\gamma] = \Upsilon^\mu{}_\nu[\gamma]\phi^\nu. \quad (7.5.85)$$

The object $\Upsilon^\mu{}_\nu[\gamma]$ is called a **bitensor** because it is a tensor with respect to two different tangent spaces. This is because ϕ^μ is a vector at the initial point X_0 whereas $\Upsilon^\mu(\phi)[\gamma]$ is a vector at the final point X_f . Therefore, the μ index on $\Upsilon^\mu{}_\nu[\gamma]$ is an index on the tangent space at X_f whereas the ν index is on the tangent space at X_0 . Consequently, under a change of coordinates:

$$\Upsilon'^\mu{}_\nu[\gamma] = \frac{\partial x'^\mu}{\partial x^\rho}(X_f) \frac{\partial x^\sigma}{\partial x'^\nu}(X_0) \Upsilon^\rho{}_\sigma[\gamma]. \quad (7.5.86)$$

Now let us consider a closed loop γ . Then, $\Upsilon^\mu{}_\nu[\gamma]$ becomes purely a tensor at the initial point of the loop and is known as the **holonomy** of the loop. The trace $\Upsilon^\mu{}_\mu[\gamma]$ would then be a scalar functional of

the closed loop and completely coordinate invariant. That quantity is known as the **Wilson loop** $W[\gamma]$ (confusingly, the standard naming is that the loop γ itself is not the Wilson loop; the Wilson loop is the trace of the parallel transport propagator when going around γ):

$$W[\gamma] = \text{Tr } \mathcal{P} : e^{-\oint_{\gamma} \hat{\Gamma}_{\rho}(x) dx^{\rho}}. \quad (7.5.87)$$

The Wilson loops provide an answer to an important geometric question. Suppose I have a set of points X and two different coordinate atlases so that we have coordinates $x^{\mu}(X)$ from the first atlas and $x'^{\mu}(X)$ from the second atlas. Suppose further that associated to each of these coordinate systems we have a metric tensor $g_{\mu\nu}(x)$ (for the first) and $g'_{\mu\nu}(x')$ for the second. These two metrics are physically equivalent and said to be **isometric** to each other if the coordinate transformation $x'^{\mu} = x'^{\mu}(x) = x'^{\mu}(X(x))$ (where we invert $x^{\mu}(X)$) turns the metric $g_{\mu\nu}(x)$ into the metric $g'_{\mu\nu}(x')$. Simply given two metrics without the accompanying coordinate transformation, you may naturally ask how you can tell if the two metrics are isometric to each other. If the Riemann tensor tensors of the two metrics agree everywhere, it turns out that is **NOT** enough information to conclude that the metrics are physically equivalent. Local curvature does not capture everything about the geometry of the manifold. However, if the Wilson loops for two metrics $g_{\mu\nu}$ and $g'_{\mu\nu}$ agree for every loop on a manifold and the metrics have the same signature, then it is always possible to find a coordinate transformation $x'^{\mu}(x)$ so that $g_{\mu\nu}(x)$ is turned into $g'_{\mu\nu}(x')$ under that coordinate transformation. Therefore, **Wilson loops capture all of the gauge invariant information of the metric.**

Exercises

Problem 7.6: Number of independent components of the Riemann Tensor. For the purpose of this question, suppose we are working in a spacetime of d dimensions.

- Consider $R_{\mu\nu\rho\sigma}$ as a generic rank-4 tensor without using any index symmetries for the moment. Explain why a generic rank-4 tensor has d^4 independent components.
- Now consider the index symmetry $R_{\mu\nu\rho\sigma} = -R_{\nu\mu\rho\sigma} = -R_{\mu\nu\sigma\rho}$. Show that a generic rank-2 antisymmetric tensor has $\frac{d(d-1)}{2}$ independent components. Then show that using these index symmetries only such a rank-4 tensor would have $\frac{d^2(d-1)^2}{4}$ independent components.
- Now consider the above index symmetries and additionally $R_{\mu\nu\rho\sigma} = R_{\rho\sigma\mu\nu}$. Show that a generic rank-2 symmetric tensor has $\frac{d(d+1)}{2}$ independent components. Then show that using these index symmetries only such a rank-4 tensor would have $\frac{d(d-1)}{4} \left(\frac{d(d-1)}{2} + 1 \right)$ independent components.
- Finally consider all of the index symmetries of the Riemann tensor (the previous set plus the algebraic Bianchi identity). Show that the algebraic Bianchi identity provides $\binom{d}{4}$ linearly independent constraints on the Riemann tensor. Thus, conclude:

$$\# \text{ of algebraically independent components of the Riemann tensor} = \frac{d^2(d^2 - 1)}{12}.$$

Show that in 1, 2, 3, and 4 spacetime dimensions the Riemann tensor has 0, 1, 6, and 20 independent components respectively.

Problem 7.7: Riemann tensor in 2 dimensional spacetime. Consider a two dimensional spacetime.

- Show that the Riemann tensor is fully determined by the value of the Ricci scalar R .
- Show that for some scalar function K :

$$R_{\rho\mu\sigma\nu} = K(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho}).$$

Do this by showing that the tensor on the right hand side has the correct index symmetry properties and using that in two dimensions the Riemann tensor has only one independent component. Show that $K = \frac{R}{2}$.

Problem 7.8: Contracted Bianchi identities.

- Show by contracting a pair of indices in the differential Bianchi identity that:

$$\nabla^{\rho} R_{\rho\sigma\mu\nu} = \nabla_{\mu} R_{\sigma\nu} - \nabla_{\nu} R_{\sigma\mu}.$$

This is known as the contracted Riemann identity.

- (b) Show by contracting a second pair of indices in the differential Bianchi identity that:

$$\nabla^\rho R_{\rho\sigma} = \frac{1}{2} \nabla_\sigma R.$$

This is known as the contracted Ricci identity.

Problem 7.9: Flatness and the Riemann tensor.

- (a) Show (very easy) that if there exists coordinates so that the metric becomes the Minkowski metric everywhere then the Riemann tensor of the manifold vanishes everywhere.
- (b) Suppose that the Riemann tensor of spacetime vanishes everywhere. Show that it is possible to construct coordinates so that the metric becomes the Minkowski metric everywhere. Thus conclude a spacetime is flat if and only if its Riemann tensor vanishes everywhere.

Problem 7.10: Normal Coordinates. Consider a point X_0 in spacetime. We wish to define a coordinate system which is as nice as possible in the neighborhood of X_0 .

- (a) Suppose we already have some coordinate system x^μ . Let V be a vector in $T_{X_0}(\mathbb{T})$ with components v^μ . Let $\zeta^\mu(\lambda)$ be the geodesic beginning at X_0 at $\lambda = 0$ with affine parameter λ and initial tangent V . That is:

$$\zeta^\mu(0) = x_0^\mu, \quad \frac{d\zeta^\mu}{d\lambda}(0) = v^\mu, \quad \frac{d^2\zeta^\mu}{d\lambda^2}(\lambda) + \Gamma^\mu_{\rho\sigma}(\zeta(\lambda)) \frac{d\zeta^\rho}{d\lambda} \frac{d\zeta^\sigma}{d\lambda} = 0.$$

The **exponential map** at X_0 of V , written $\exp_{X_0}(V)$ is defined to be the point X given by $\zeta^\mu(1)$. That is:

$$\exp_{x_0}^\mu(v) = \zeta^\mu(1).$$

Explain that for X in a finite size neighborhood around X_0 , each X is smoothly and invertibly related to a choice of V , thus one may define the map $x^\mu(v)$ which gives a coordinate system in this neighborhood with the components of V acting as our new coordinates. Such a coordinate system is called a **normal coordinate system** around X_0 .

- (b) Let $x^\mu(v)$ be the coordinate transformation defined in the previous part. Show that:

$$x^\mu = x_0^\mu + v^\mu - \frac{1}{2} \Gamma^\mu_{\rho\sigma}(x_0) v^\rho v^\sigma - \frac{1}{6} (\partial_\nu \Gamma^\mu_{\rho\sigma}(x_0) - 2\Gamma^\mu_{\lambda\nu}(x_0) \Gamma^\lambda_{\rho\sigma}(x_0)) v^\nu v^\rho v^\sigma + \mathcal{O}(v^4).$$

- (c) For convenience, suppose we have chosen our original coordinates x^μ to be coordinates of a LIRF at X_0 . Show by Taylor expanding $g_{\mu\nu}(x)$ near x_0 and simplifying $x^\mu(v)$ that:

$$x^\mu = x_0^\mu + v^\mu - \frac{1}{6} \partial_\nu \Gamma^\mu_{\rho\sigma}(x_0) v^\nu v^\rho v^\sigma + \mathcal{O}(v^4)$$

$$g_{\mu\nu}(x) = \eta_{\mu\nu} + \frac{1}{2} (\eta_{\nu\lambda} \partial_\sigma \Gamma^\lambda_{\mu\rho}(x_0) + \eta_{\mu\lambda} \partial_\sigma \Gamma^\lambda_{\nu\rho}(x_0)) v^\rho v^\sigma + \mathcal{O}(v^3).$$

Let $g'_{\mu\nu}(x')$ be the transformed metric in the transformed coordinates $x'^\mu = v^\mu$. Show that:

$$g'_{\mu\nu}(x') = \eta_{\mu\nu} - \frac{1}{3} R'^{\mu\rho\nu\sigma}(0) x'^\rho x'^\sigma + \mathcal{O}(x'^3).$$

A coordinate system which is both normal and a LIRF at the same point (such as these x'^μ coordinates) is called a **Fermi normal coordinate system**.

- (d) Let x^μ be Fermi normal coordinates at X_0 . Show that the volume element $d\mathbb{T}(x)$ nearby X_0 is given by:

$$d\mathbb{T}(x) = \left(1 - \frac{1}{6} R_{\mu\nu} x^\mu x^\nu + \mathcal{O}(x^3) \right) d\mathbb{T}(0)$$

thus conclude that the Ricci tensor $R_{\mu\nu}$ captures the rate of expansion of a small initial volume in spacetime as one flows along a geodesic in a particular initial direction. Show similarly that the Ricci scalar R characterizes the directional average of that rate of expansion.

Problem 7.11: The Weyl tensor. Based on the previous problem, the Ricci tensor characterizes volume changing curvature. The rest of the Riemann tensor thus must contain information about curvature due to changes in direction, rather than changes in scale.

- (a) Attempt to find a tensor $W_{\mu\nu\rho\sigma}$ which depends linearly on the Riemann tensor $R_{\mu\nu\rho\sigma}$, which has the same index symmetries, and which satisfies $W^\rho_{\mu\rho\nu} = 0$. Show that in d spacetime dimensions the

unique such tensor (up to a single overall numerical multiple) is:

$$W_{\mu\nu\rho\sigma} = R_{\mu\nu\rho\sigma} - \frac{1}{d-2}(R_{\mu\rho}g_{\nu\sigma} - R_{\nu\rho}g_{\mu\sigma} - R_{\mu\sigma}g_{\nu\rho} + R_{\nu\sigma}g_{\mu\rho}) + \frac{1}{(d-1)(d-2)}R(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho}).$$

This tensor is known as the **Weyl tensor**. Show that it has all of the index interchange symmetries as the Riemann tensor and that it satisfies the algebraic Bianchi identity. Explain why we would expect the Weyl tensor to tell us about directional curvature but nothing about volume changing curvature.

- (b) Consider a transformation of our manifold in which volumes are locally rescaled but the angles between all tangent vectors are preserved (this is a transformation from one metric to a new metric, not a coordinate transformation). Show that for some scalar function $\phi(x)$ the transformed metric is given by:

$$g'_{\mu\nu}(x) = e^{2\phi(x)}g_{\mu\nu}(x).$$

Such a transformation is called a **conformal transformation**. $\phi(x)$ is called the conformal factor. Show that the Christoffel symbol transforms as (where we only raise or lower indices using the untransformed metric):

$$\Gamma'^{\rho}{}_{\mu\nu} = \Gamma^{\rho}{}_{\mu\nu} + \delta_{\mu}^{\rho}\nabla_{\nu}\phi + \delta_{\nu}^{\rho}\nabla_{\mu}\phi - g_{\mu\nu}\nabla^{\rho}\phi.$$

Show further that the Riemann tensor transforms as:

$$\begin{aligned} R'^{\rho}{}_{\mu\sigma\nu} = & R^{\rho}{}_{\mu\sigma\nu} + \delta_{\nu}^{\rho}\nabla_{\sigma}\nabla_{\mu}\phi - \delta_{\sigma}^{\rho}\nabla_{\nu}\nabla_{\mu}\phi - g_{\mu\nu}\nabla^{\rho}\nabla_{\sigma}\phi + g_{\mu\sigma}\nabla^{\rho}\nabla_{\nu}\phi + \delta_{\sigma}^{\rho}\nabla_{\mu}\phi\nabla_{\nu}\phi - \delta_{\nu}^{\rho}\nabla_{\mu}\phi\nabla_{\sigma}\phi \\ & - \delta_{\sigma}^{\rho}g_{\mu\nu}\nabla^{\lambda}\phi\nabla_{\lambda}\phi + \delta_{\nu}^{\rho}g_{\mu\sigma}\nabla^{\lambda}\phi\nabla_{\lambda}\phi - g_{\sigma\mu}\nabla^{\rho}\phi\nabla_{\nu}\phi + g_{\mu\nu}\nabla^{\rho}\phi\nabla_{\sigma}\phi. \end{aligned}$$

Finally, show that the Weyl tensor is conformally invariant:

$$W'^{\rho}{}_{\mu\sigma\nu} = W^{\rho}{}_{\mu\sigma\nu}.$$

- (c) Suppose a Lorentzian manifold is conformally flat, meaning it is possible to choose coordinates so that for some scalar field $\phi(x)$: $g_{\mu\nu} = e^{2\phi}\eta_{\mu\nu}$. Show that the Weyl tensor of this manifold vanishes everywhere. The converse is also true in spacetime dimension 4 or greater (if a manifold's Weyl tensor vanishes everywhere then it is conformally flat).

7.6 Classical Field Theory in Curved Spacetime

7.6.1 Covariant Equations of Motion

Before we begin trying to find the theory of how the metric should evolve, let us first understand how we can formulate our existing fields as interacting with the metric. We want to know how to pose classical field theories on our spacetime manifold. Suppose that our fields $\phi^a(X)$ are some list of tensor fields (of potentially various ranks) and we want to find the Lagrangian density for those fields given a metric (we are looking for the action 1|2 with system 1 being the ϕ^a fields and 2 being the metric). The partial derivatives $\partial_\mu \phi^a$ which would normally appear in the Lagrangian density are pretty inconvenient, because the partial derivative of a tensor is not a tensor. However, we can rewrite the Lagrangian density in terms of the actual tensors $\nabla_\mu \phi^a$ with the only cost being the introduction of terms proportional to ϕ^a (and depending on the connection coefficients). All of the first derivatives of the metric can be rewritten in terms of the connection coefficients. Therefore, instead of a consider a Lagrangian density for the theory which depends on our fields $\phi^a, g_{\mu\nu}$ up through their first derivatives as $\phi^a, \partial_\mu \phi^a, g_{\mu\nu}, \partial_\rho g_{\mu\nu}$ we repackage this dependence as $\mathfrak{L}(x, g, \Gamma, \phi, \nabla \phi)$.

The only pieces in $\mathfrak{L}$ as described which are not true tensors are its explicit x^μ dependence and its explicit connection coefficient dependence. Consider some particular coordinate system with coordinates x_0^μ and Lagrangian density as described. In this particular coordinate system, we introduce a set of “background fields” $B_a(x)$ which include among them each of the coordinates x^μ and all of the connection coefficients as well as the vector fields with components $\delta_0^\mu, \delta_1^\mu, \delta_2^\mu, \delta_3^\mu$. We define these background fields specifically in this base coordinate system but define them to transform differently than the quantities they are related to in this base coordinate system. We define the background fields associated to the coordinates to transform as scalars, the background fields associated to the connection coefficients to transform like a genuine tensor with the same index placements, and the background fields associated to the mentioned vector fields to transform like genuine vector fields. Therefore, outside of this base coordinate system the background fields will not be same as the transformed versions of the various quantities mentioned. However, we now can write the Lagrangian density as $\mathfrak{L}(B, g, \phi, \nabla \phi)$ because we have simply repackaged the dependence. We have by construction introduced enough background fields that we can now write the function $\mathfrak{L}(B, g, \phi, \nabla \phi)$ in a way which is manifestly coordinate invariant.

For example, if we were in 2 spacetime dimensions (1 space and 1 time) with a single scalar field ϕ and had the Lagrangian density:

$$\mathfrak{L} = (\partial_t \phi)^2 + tx \partial_t \phi \partial_x \phi \quad (7.6.1)$$

then we could rewrite this in a coordinate invariant way by introducing, in an arbitrary coordinate system of our choice, the fields:

$$u = t, \quad v = x, \quad \mathfrak{U}^\mu = (1, 0)^\mu, \quad \mathfrak{V}^\mu = (0, 1)^\mu \quad (7.6.2)$$

which are then all required to transform correctly like tensors with their respective index placement when taken to another coordinate system. With these:

$$\mathfrak{L} = (\mathfrak{U}^\mu \nabla_\mu \phi)^2 + uv \mathfrak{U}^\mu \mathfrak{V}^\nu \nabla_\mu \phi \nabla_\nu \phi \quad (7.6.3)$$

which is now plainly coordinate invariant but depends on the unvaried background fields $u, v, \mathfrak{U}^\mu, \mathfrak{V}^\mu$.

We proved in section 7.1 that there are no nontrivial background tensors consistent with diff symmetry. Therefore, the only way for the Lagrangian density $\mathfrak{L}(B, g, \phi, \nabla \phi)$ to have diff symmetry (which it must as these are the gauge symmetries of general relativity) while also being coordinate invariant (which it is by construction) is for it to actually have no dependence on the background fields. That is, starting from a Lagrangian density which has explicit x and Γ dependence and introducing background fields as described will produce a new function and any pieces of that function which depend on the introduced background fields are guaranteed to violate diff symmetry. Consequently, when looking for a diff symmetric action for our fields on some region $\mathbb{M}$ of spacetime, we actually only have to consider:

$$S = \int_{\mathbb{M}} \mathfrak{L}(g, \phi, \nabla \phi) d\mathbb{T} \quad (7.6.4)$$

where the Lagrangian density is a coordinate scalar. Then, under variations of our fields which vanish on $\partial \mathbb{M}$ (using Stokes’ theorem and that we are not varying the metric so by formula for the covariant derivative of a

tensor field $\delta\nabla_\mu\phi^a = \nabla_\mu\delta\phi^a$):

$$\delta S = \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} \delta\phi^a + \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\mu \delta\phi^a \right) d\mathbb{T} \quad (7.6.5)$$

$$= \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} \delta\phi^a + \nabla_\mu \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \delta\phi^a \right) - \delta\phi^a \nabla_\mu \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \right) \right) d\mathbb{T} \quad (7.6.6)$$

$$= \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} - \nabla_\mu \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \right) \delta\phi^a d\mathbb{T} + \int_{\partial\mathbb{M}} \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \delta\phi^a d\Sigma_\mu \quad (7.6.7)$$

$$= \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial \phi^a} - \nabla_\mu \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \right) \delta\phi^a d\mathbb{T}. \quad (7.6.8)$$

Be careful with this next step! The measure $d\mathbb{T} = \sqrt{-\det g} d^4x$ contains a factor of the metric and so the functional derivative of the action (which plucks off the full integrand under variation) is:

$$\frac{1}{\sqrt{-\det g}} \frac{\delta S}{\delta \phi^a} = \frac{\partial \mathfrak{L}}{\partial \phi^a} - \nabla_\mu \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \stackrel{!}{=} 0. \quad (7.6.9)$$

This is the covariant form of the Euler-Lagrange equations for classical field theory. It might seem like a clever idea to define the functional derivative to absorb this factor of the metric, but doing so makes calculations using the Poisson bracket in the Hamiltonian formalism uglier. It is fully possible in our analysis to include higher derivatives of the fields and of the metric (which can then be rewritten in terms of the Riemann tensor). The result is unsurprising; you will find that the Lagrangian density in order to have diff invariance can necessarily be expressed in terms of our fields and their covariant derivatives, the metric, and the Riemann tensor and its covariant derivatives. This is proven in detail in section 2 of [51].

Using minimal replacement, we can lift any field theory on Minkowski space to a field theory on curved spacetime. In particular, suppose we have written our Lagrangian density $\mathfrak{L}_0(\eta, \phi, \partial\phi)$ for a special relativistic field theory so that the Lagrangian density is invariant under connected Poincare transformations. Because the Lagrangian density $\mathfrak{L}(g, \phi, \nabla\phi)$ for the general relativistic theory is coordinate invariant, at any given point X_0 we can go to a LIRF and in that frame $g_{\mu\nu}(X_0) = \eta_{\mu\nu}$ and $\Gamma^\rho_{\mu\nu}(X_0) = 0$ and so $\nabla_\mu\phi^a(X_0) = \partial_\mu\phi^a(X_0)$. Thus, in that frame:

$$\mathfrak{L}(g, \phi, \nabla\phi)|_{\text{LIRF}} = \mathfrak{L}_0(\eta, \phi, \partial\phi). \quad (7.6.10)$$

When transformed away from that frame, $\eta_{\mu\nu}$ will get replaced by $g_{\mu\nu}$ and $\partial_\mu\phi^a$ will get replaced by $\nabla_\mu\phi^a$ when transformed properly as tensors. Therefore, all we end up having to do is take the special relativistic theory Lagrangian density and replace each copy of the Minkowski metric $\eta_{\mu\nu}$ with the spacetime metric $g_{\mu\nu}$ and replace each partial derivative ∂_μ with the covariant derivative ∇_μ to arrive at the appropriate general relativistic Lagrangian density.

For an example, let us use minimal replacement to lift electromagnetism to general relativity:

$$\eta_{\mu\nu} \rightarrow g_{\mu\nu}, \quad \mathcal{F}_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \rightarrow \mathcal{F}_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu. \quad (7.6.11)$$

Because the torsion of our connection is 0, the second of these replacements actually doesn't change the definition of $\mathcal{F}_{\mu\nu}$ at all. Then, the Lagrangian density of electromagnetism becomes:

$$\mathfrak{L} = -\frac{1}{4} \mathcal{F}^{\mu\nu} \mathcal{F}_{\mu\nu} + J^\mu A_\mu \quad (7.6.12)$$

where we have raised the indices on the field strength using the metric $g_{\mu\nu}$, not the Minkowski metric. Viewed as a Lagrangian density for A_μ only, J^μ is a background field. The resulting equations of motion (Maxwell's equations in curved spacetime) are given by:

$$\frac{\partial \mathfrak{L}}{\partial A_\mu} = J^\mu, \quad \frac{\partial \mathfrak{L}}{\partial \nabla_\nu A_\mu} = \mathcal{F}^{\mu\nu} \quad (7.6.13)$$

$$\nabla_\nu \frac{\partial \mathfrak{L}}{\partial \nabla_\nu A_\mu} = \frac{\partial \mathfrak{L}}{\partial A_\mu} \implies \boxed{\nabla_\nu \mathcal{F}^{\mu\nu} = J^\mu}. \quad (7.6.14)$$

You should suspect that the covariant divergence of both sides should give 0, so that the current density is covariantly conserved. Let us verify this by explicit calculation, using the index antisymmetry of the $\mathcal{F}^{\mu\nu}$, the index symmetry of the Ricci tensor $R_{\mu\nu}$, and that the commutator of covariant derivatives gives the Riemann tensor:

$$\nabla_\mu \nabla_\nu \mathcal{F}^{\mu\nu} = \frac{1}{2} \nabla_\mu \nabla_\nu \mathcal{F}^{\mu\nu} - \frac{1}{2} \nabla_\nu \nabla_\mu \mathcal{F}^{\mu\nu} = \frac{1}{2} [\nabla_\mu, \nabla_\nu] \mathcal{F}^{\mu\nu} \quad (7.6.15)$$

$$= \frac{1}{2} R^\mu{}_{\rho\mu\nu} \mathcal{F}^{\rho\nu} + \frac{1}{2} R^\nu{}_{\rho\mu\nu} \mathcal{F}^{\mu\rho} = \frac{1}{2} R_{\mu\nu} \mathcal{F}^{\mu\nu} - \frac{1}{2} R_{\mu\nu} \mathcal{F}^{\nu\mu} \quad (7.6.16)$$

$$= \frac{1}{2} (R_{\mu\nu} - R_{\nu\mu}) \mathcal{F}^{\mu\nu} = 0. \quad (7.6.17)$$

Therefore, Maxwell's equations automatically imply the covariant conservation of the current density:

$$\nabla_\mu J^\mu = 0 \quad (7.6.18)$$

exactly as you should have expected. You may have dared to assert $\nabla_\mu \nabla_\nu \mathcal{F}^{\mu\nu} = 0$ based on the antisymmetry of $\mathcal{F}^{\mu\nu}$ but remember that for curved spacetimes, covariant derivatives do **NOT** commute.

7.6.2 Field Canonical Transformations

Let us now study the transformation properties of classical fields. Suppose we have a local classical field theory with fields $\phi^a(x)$ which has Lagrangian density $\mathcal{L}(B, g, \phi, \nabla\phi)$. Here we have only included terms in the Lagrangian density containing 1 or fewer derivatives on the fields which as always can be generalized straightforwardly if you need higher derivative dependence in your theory. We also include the possibility of background fields $B_a(x)$ (like how the current density is a background field to electromagnetism) and we will treat the metric as a background field in this and the next subsection. We will be agnostic as to whether this Lagrangian density is written in terms of only the canonical coordinate fields (meaning $\phi(x) = Q(x)$) of theory or is written in terms of both the canonical coordinate fields and their conjugate momenta fields (meaning $\phi(x) = (Q(x), P(x))$). Let $\mathbb{M}$ be the region of spacetime on which we are presently formulating our theory:

$$S_{\mathbb{M}}[\phi] = \int_{\mathbb{M}} \mathcal{L}(B, g, \phi, \nabla\phi) \sqrt{-\det g} d^4x. \quad (7.6.19)$$

If the integrand is written in terms of canonical coordinate fields only then this action is in the Lagrangian action form, as described in section 1.7, whereas if it is in terms of canonical coordinate and conjugate momenta fields then it is in the Hamiltonian action form. Much like in the arguments of section 1.8, which is used will not matter here.

Suppose we have a local canonical transformation from our fields $\phi^a(x)$ into new fields $\phi'^a(x')$, generically transforming the coordinates as well. That is, we have some functions $x'(x, \phi)$ and $\phi'(x, \phi)$ so that:

$$x'^\mu = x'^\mu(x, \phi), \quad \phi'^a(x') = \phi'^a(x, \phi). \quad (7.6.20)$$

It is perfectly legal to include derivatives of ϕ in the functions defining x' and ϕ' , though doing so will generally add higher derivatives to the Lagrangian density under the transformation.

Under this canonical transformation, $\phi'^a(x')$ will now be a field theory on a new region $\mathbb{M}'$ with some new action $S'_{\mathbb{M}'}[\phi']$. That action will be the integral of some new Lagrangian density $\mathcal{L}'(x', \phi', \nabla\phi')$:

$$S'_{\mathbb{M}'}[\phi'] = \int_{\mathbb{M}'} \mathcal{L}'(B(x'), g(x'), \phi', \nabla\phi') \sqrt{-\det g(x')} d^4x' \quad (7.6.21)$$

The background quantities $B^a(x)$ and $g_{\mu\nu}(x)$ are not transformed because they are not dynamically independent variables in our theory at the moment. Requiring that this is a canonical transformation, as explained in section 1.9, means that if $S'_{\mathbb{M}'}[\phi']$ were to be reexpressed as a functional of ϕ , then it would produce the same equations of motion as $S_{\mathbb{M}}[\phi]$. In order for it to do so, the two can only differ by a functional of the boundary conditions of ϕ , so that their functional derivatives on the interior of $\mathbb{M}$ agree. Thus, there must exist a functional $F_{\partial\mathbb{M}}[\phi]$ depending on ϕ only through its values on the boundary $\partial\mathbb{M}$ of the region $\mathbb{M}$ so that:

$$S'_{\mathbb{M}'}[\phi'] = S_{\mathbb{M}}[\phi] + F_{\partial\mathbb{M}}[\phi]. \quad (7.6.22)$$

A generic local functional $F_{\partial\mathbb{M}}[\phi]$ as described can be written as an integral over $\partial\mathbb{M}$ of some integrand vector field $f^\mu(x, \phi)$:

$$F_{\partial\mathbb{M}}[\phi] = \int_{\partial\mathbb{M}} f^\mu(x, \phi(x)) d\Sigma_\mu. \quad (7.6.23)$$

This just states that $F_{\partial\mathbb{M}}$ depends in some generic way on the boundary data. Importantly, the vector field $f^\mu(x, \phi)$ is not unique, even for a given $F_{\partial\mathbb{M}}$. Consider two vector fields f'^μ and f^μ which differ by a divergence free vector field J^μ (meaning $f'^\mu = f^\mu + J^\mu$ and $\nabla_\mu J^\mu = 0$). Then, using Stokes' theorem:

$$\int_{\partial\mathbb{M}} f'^\mu d\Sigma_\mu = \int_{\partial\mathbb{M}} f^\mu d\Sigma_\mu + \int_{\partial\mathbb{M}} J^\mu d\Sigma_\mu = \int_{\partial\mathbb{M}} f^\mu d\Sigma_\mu + \int_{\mathbb{M}} \nabla_\mu J^\mu d\mathbb{T} = \int_{\partial\mathbb{M}} f^\mu d\Sigma_\mu. \quad (7.6.24)$$

Therefore, f^μ and f'^μ produce the same functional $F_{\partial\mathbb{M}}$. This argument also shows that if f'^μ and f^μ produce the same $F_{\partial\mathbb{M}}$ then their difference must be divergence free.

Every divergence free vector field J^μ (meaning $\nabla_\mu J^\mu = 0$) can be expressed in the form:

$$J^\mu = \nabla_\nu \chi^{\mu\nu} \quad (7.6.25)$$

for an antisymmetric tensor $\chi^{\mu\nu}$. One way to see this is that we can treat a divergence free vector field as a source in Maxwell's equations and existence theorems of solutions to Maxwell's equations guarantee a corresponding field strength exists, with the field strength then being $\chi^{\mu\nu}$. Conversely, the vector field $\nabla_\nu \chi^{\mu\nu}$ is automatically divergence free as we showed from Maxwell's equations. Therefore, for two vector fields f'^μ and f^μ which produce the same $F_{\partial\mathbb{M}}$, there must exist a tensor field $\chi^{\mu\nu}$ so that:

$$f'^\mu = f^\mu + \nabla_\nu \chi^{\mu\nu}, \quad \chi^{\mu\nu} = -\chi^{\nu\mu}. \quad (7.6.26)$$

When the transformed action is reexpressed in terms of ϕ , it becomes:

$$S'_{\mathbb{M}'}[\phi'] = \int_{\mathbb{M}} \mathcal{L}'(B(x'), g(x'), \phi', \nabla\phi') \sqrt{-\det g(x')} \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| d^4x \quad (7.6.27)$$

by using the Jacobian transformation property of the integration measure d^4x . Returning this to (7.6.22) and using Stokes theorem gives:

$$\begin{aligned} \int_{\mathbb{M}} \mathcal{L}'(B(x'), g(x'), \phi', \nabla\phi') \sqrt{-\det g(x')} \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| \\ = \int_{\mathbb{M}} (\mathcal{L}(B(x), g(x), \phi, \nabla\phi) + \nabla_\mu f^\mu(x, \phi)) \sqrt{-\det g} d^4x. \end{aligned} \quad (7.6.28)$$

Because the field theory is local, this construction can be made for arbitrary region $\mathbb{M}$ and so we may equate the integrands themselves:

$$\mathcal{L}'(B(x'), g(x'), \phi', \nabla\phi') \sqrt{-\det g(x')} \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| = (\mathcal{L}(B(x), g(x), \phi, \nabla\phi) + \nabla_\mu f^\mu(x, \phi)) \sqrt{-\det g}. \quad (7.6.29)$$

This is true whether the transformation of interest is to be a symmetry of our system or not. By the same argument given immediately before theorem 1.8, a transformation is a symmetry if and only if the transformed and untransformed fields have the Hamiltonian functions. If the Hamiltonian function is unchanged, the resulting Lagrangian and Lagrangian density are also unchanged through the Legendre transformation. Therefore, we have:

Theorem 7.2: Field Canonical Transformations

In a local classical field theory, the transformation:

$$x'^\mu = x'^\mu(x, \phi(x)), \quad \phi'^a(x') = \phi'^a(x, \phi(x)) \quad (7.6.30)$$

is canonical if and only if there exists a vector field $f^\mu(x, \phi)$ so that:

$$\mathcal{L}'(B(x'), g(x'), \phi', \nabla\phi') \frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \left| \det \left(\frac{\partial x'(x, \phi(x))}{\partial x} \right) \right| = \mathcal{L}(B(x), g(x), \phi, \nabla\phi) + \nabla_\mu f^\mu(x, \phi). \quad (7.6.31)$$

If such a vector field exists, it is not unique. Any two such vector fields f'^μ and f^μ must be related by:

$$f'^\mu = f^\mu + \nabla_\nu \chi^{\mu\nu} \quad (7.6.32)$$

for some antisymmetric tensor field $\chi^{\mu\nu}$.

The transformation is a symmetry if and only if the transformed ($\mathcal{L}'$) and untransformed ($\mathcal{L}$) Lagrangian densities are the same function.

7.6.3 Noether's Theorem (Version 3)

Suppose now that we have a continuous 1-parameter family of local canonical transformations depending on the parameter ε so that $\varepsilon = 0$ corresponds to the identity transformation. That is, we have some functions

$x'(\varepsilon, x, \phi)$ and $\phi'(\varepsilon, x, \phi)$ so that:

$$x'^\mu = x'^\mu(\varepsilon, x, \phi), \quad \phi'^a(x') = \phi'^a(\varepsilon, x, \phi). \quad (7.6.33)$$

We define the functions $\mathcal{D}x^\mu$ and $\mathcal{D}\phi^a$ by the ε derivative of this quantities at the identity:

$$\mathcal{D}x^\mu(x, \phi) \stackrel{\text{def}}{=} \left. \frac{\partial x'^\mu(\varepsilon, x, \phi)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \mathcal{D}\phi^a(x, \phi) \stackrel{\text{def}}{=} \left. \frac{\partial \Upsilon(\phi'^a(\varepsilon, x, \phi), x', x)}{\partial \varepsilon} \right|_{\varepsilon=0}. \quad (7.6.34)$$

For a generic quantity which depends on x' and $\phi'(x')$ we define $\mathcal{D}$ as its total ε derivative parallel transported back to x , evaluated at $\varepsilon = 0$.

The transformed Lagrangian density $\mathcal{L}'$ depends on ε in a nontrivial way in general. So, we write $\mathcal{L}'(\varepsilon, B(x'), g(x'), \phi', \nabla\phi')$ to explicitly indicate that $\mathcal{L}'$ changes directly with ε (as its functional form changes) and indirectly with ε (through the ε dependence of $x', \phi', \nabla\phi'$). We will use the notation $\delta\mathcal{L}$ to indicate the change in the form of $\mathcal{L}'$ as a function as ε is changed near the identity. That is, we define:

$$\delta\mathcal{L} \stackrel{\text{def}}{=} \left. \frac{\partial}{\partial \varepsilon} \mathcal{L}'(\varepsilon, B(x'), g(x'), \phi', \nabla\phi') \right|_{\varepsilon=0} \quad (7.6.35)$$

where the partial derivative is taken at fixed $x', \phi', \nabla\phi'$.

The total covariant derivative of the Lagrangian density is:

$$\nabla_\mu \mathcal{L} = \frac{\partial \mathcal{L}}{\partial B^a} \nabla_\mu B^a + \frac{\partial \mathcal{L}}{\partial \phi^a} \nabla_\mu \phi^a + \frac{\partial \mathcal{L}}{\partial \nabla_\nu \phi^a} \nabla_\mu \nabla_\nu \phi^a. \quad (7.6.36)$$

We consider our fields ϕ^a as the components of some geometric object Φ (so that ϕ^a is a list of tensors). It is useful to define the ε derivative at fixed x for the fields by parallel transporting back from x' to x :

$$\mathcal{D}\Phi|_x \stackrel{\text{def}}{=} \left. \frac{\partial}{\partial \varepsilon} \Upsilon(\Phi(x'), x', x) \right|_{\varepsilon=0}. \quad (7.6.37)$$

Using the chain rule:

$$\mathcal{D}\phi^a = \mathcal{D}\phi^a|_x + \nabla_\mu \phi^a \mathcal{D}x^\mu. \quad (7.6.38)$$

The ε derivative at fixed x automatically commutes with x^μ derivatives because it doesn't change x . So:

$$\nabla_\mu \mathcal{D}\phi^a|_x = \mathcal{D} \nabla_\mu \phi^a|_x. \quad (7.6.39)$$

With these pieces together, the the total ε derivative of $\mathcal{L}'$ evaluated at $\varepsilon = 0$ gives:

$$\mathcal{D}\mathcal{L} = \delta\mathcal{L} + \frac{\partial \mathcal{L}}{\partial B^a} \nabla_\mu B^a \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a + \frac{\partial \mathcal{L}}{\partial \nabla_\mu \phi^a} \mathcal{D}\nabla_\mu \phi^a \quad (7.6.40)$$

$$= \delta\mathcal{L} + \left(\nabla_\mu \mathcal{L} - \frac{\partial \mathcal{L}}{\partial \phi^a} \nabla_\mu \phi^a - \frac{\partial \mathcal{L}}{\partial \nabla_\nu \phi^a} \nabla_\mu \nabla_\nu \phi^a \right) \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a + \frac{\partial \mathcal{L}}{\partial \nabla_\mu \phi^a} \mathcal{D}\nabla_\mu \phi^a \quad (7.6.41)$$

$$= \delta\mathcal{L} + \nabla_\mu \mathcal{L} \mathcal{D}x^\mu + \frac{\partial \mathcal{L}}{\partial \phi^a} \mathcal{D}\phi^a|_x + \frac{\partial \mathcal{L}}{\partial \nabla_\mu \phi^a} \mathcal{D}\nabla_\mu \phi^a|_x \quad (7.6.42)$$

$$= \delta\mathcal{L} + \left(\frac{\partial \mathcal{L}}{\partial \phi^a} - \nabla_\mu \frac{\partial \mathcal{L}}{\partial \nabla_\mu \phi^a} \right) \mathcal{D}\phi^a|_x + \nabla_\mu \left(\frac{\partial \mathcal{L}}{\partial \nabla_\mu \phi^a} \mathcal{D}\phi^a|_x + \mathcal{L} \mathcal{D}x^\mu \right) - \mathcal{L} \nabla_\mu \mathcal{D}x^\mu. \quad (7.6.43)$$

Because the transformation is canonical for each ε , by theorem 7.2 there will exist a vector field $f^\mu(\varepsilon, x, \phi(x))$ so that:

$$\mathcal{L}'(\varepsilon, B(x'), g(x'), \phi', \nabla\phi') \frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) = \mathcal{L}(x, \phi, \nabla\phi) + \partial_\mu f^\mu(\varepsilon, x, \phi). \quad (7.6.44)$$

The Jacobian determinant will necessarily be positive in the neighborhood of $\varepsilon = 0$ because at $\varepsilon = 0$ it is equal to 1, therefore we can drop the absolute value around it. Now we would like to take the derivative of this expression at $\varepsilon = 0$. Using (4.11.32):

$$\left. \frac{\partial}{\partial \varepsilon} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right|_{\varepsilon=0} = \partial_\mu \mathcal{D}x^\mu. \quad (7.6.45)$$

As well, using (5.2.30) for how to differentiate the determinant:

$$\left. \frac{\partial}{\partial \varepsilon} \sqrt{-\det g(x'(\varepsilon, x, \phi))} \right|_{\varepsilon=0} = \frac{1}{2} g^{\alpha\beta} \partial_\mu g_{\alpha\beta} \mathcal{D}x^\mu \sqrt{-\det g} = \Gamma^\rho_{\mu\rho} \mathcal{D}x^\mu \sqrt{-\det g}. \quad (7.6.46)$$

Now taking the ε derivative of (7.6.44) at fixed $x, \phi(x)$:

$$\mathcal{D}\mathcal{L} + \Gamma^\rho_{\mu\rho} \mathcal{D}x^\rho \mathcal{L} + \partial_\mu \mathcal{D}x^\mu \mathcal{L} = \nabla_\mu \mathcal{D}f^\mu \quad (7.6.47)$$

$$\implies \mathcal{D}\mathfrak{L} + \mathfrak{L}\nabla_\mu \mathcal{D}x^\mu = \nabla_\mu \mathcal{D}f^\mu. \quad (7.6.48)$$

Then, combining this with (7.6.43):

$$\delta\mathfrak{L} + \left(\frac{\partial\mathfrak{L}}{\partial\phi^a} - \nabla_\mu \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \right) \mathcal{D}\phi^a|_x + \nabla_\mu \left(\frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \mathcal{D}\phi^a|_x + \mathfrak{L}\mathcal{D}x^\mu - \mathcal{D}f^\mu \right) = 0. \quad (7.6.49)$$

This is true for all field configurations (we have not assumed that the equations of motion are satisfied) and is true whether the transformation of interest is a symmetry or not. Under the actual dynamics of the system (meaning applying the equations of motion), if the transformation is a symmetry (and thus $\delta\mathfrak{L} = 0$) we have:

$$\nabla_\mu \left(\frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \mathcal{D}\phi^a|_x + \mathfrak{L}\mathcal{D}x^\mu - \mathcal{D}f^\mu \right) = 0. \quad (7.6.50)$$

Therefore, the current density J^μ , called the Noether current for this transformation, defined by:

$$J^\mu = \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \mathcal{D}\phi^a|_x + \mathfrak{L}\mathcal{D}x^\mu - \mathcal{D}f^\mu \quad (7.6.51)$$

is divergence free under the equations of motion if and only if the transformation is a symmetry of the action. Generally $\mathcal{D}\phi^a$ is simpler than the fixed x variation, and so it is useful to express the Noether current in terms of it rather than $\mathcal{D}\phi^a|_x$. Doing so:

$$J^\mu = \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \mathcal{D}\phi^a + \left(\mathfrak{L}\delta_\nu^\mu - \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \nabla_\nu\phi^a \right) \mathcal{D}x^\nu - \mathcal{D}f^\mu \quad (7.6.52)$$

The usual generator G in the sense of the global version of Noether's theorem can be recovered by integrating J^μ over a time slice $\Sigma(t)$ of all points in spacetime at $x^0 = t$. Then:

$$G(t) = \int_{\Sigma(t)} J^\mu d\Sigma_\mu \quad (7.6.53)$$

is the natural covariant lifting of the special relativistic formula.

If the transformation is a symmetry of the action then we can replace the function $\mathfrak{L}'$ with the function $\mathfrak{L}$ in equation (7.6.44). Then, the ε derivative near the identity of that equation becomes:

$$\frac{\partial}{\partial\varepsilon} \left(\mathfrak{L}(B(x'), g(x'), \phi', \nabla\phi') \frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right) \Big|_{\varepsilon=0} = \nabla_\mu \mathcal{D}f^\mu(x, \phi). \quad (7.6.54)$$

Conversely, if a $\mathcal{D}f^\mu(x, \phi)$ can be identified so that this is true, then the transformation is a symmetry of the action. Altogether we have:

Theorem 7.3: Noether's Theorem – Local Conservation

For a continuous transformation $x' = x'(\varepsilon, x, \phi)$, $\phi'(x') = \phi'(\varepsilon, x, \phi)$ (with parameter ε so that $\varepsilon = 0$ corresponds to the identity transformation) so that:

$$S'_{\mathbb{M}'}[\phi'] - S_{\mathbb{M}}[\phi] = \int_{\partial\mathbb{M}} f^\mu(\varepsilon, x, \phi(x)) d\Sigma_\mu \quad (7.6.55)$$

over any region of spacetime $\mathbb{M}$, the Noether current of that transformation is given by:

$$J^\mu = \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \mathcal{D}\phi^a + \left(\mathfrak{L}\delta_\nu^\mu - \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a} \nabla_\nu\phi^a \right) \mathcal{D}x^\nu - \mathcal{D}f^\mu \quad (7.6.56)$$

where:

$$\mathcal{D}x^\mu(x, \phi) = \frac{\partial x'^\mu(\varepsilon, x, \phi)}{\partial\varepsilon} \Big|_{\varepsilon=0}, \quad \mathcal{D}\phi^a(x, \phi) = \frac{\partial \phi'^a(\varepsilon, x, \phi)}{\partial\varepsilon} \Big|_{\varepsilon=0}, \quad \mathcal{D}f^\mu = \frac{\partial f^\mu(\varepsilon, x, \phi)}{\partial\varepsilon} \Big|_{\varepsilon=0}. \quad (7.6.57)$$

The definition of $\mathcal{D}f^\mu$ is not unique and may be modified by:

$$\mathcal{D}f'^\mu = \mathcal{D}f^\mu + \nabla_\nu \chi^{\mu\nu} \quad (7.6.58)$$

for any antisymmetric tensor field $\chi^{\mu\nu}$. The phase space generator of the transformation is given by:

$$G = \int_{\mathbb{S}} J^\mu d\Sigma_\mu. \quad (7.6.59)$$

The on-shell divergence of the Noether current is given by:

$$\nabla_\mu J^\mu = -\delta\mathfrak{L} \quad (7.6.60)$$

where $\delta\mathfrak{L}$ is the rate of change of the functional form of the Lagrangian density under the transformation. Hence, the Noether current is locally conserved if and only if the transformation is a symmetry of the action.

The symmetry condition is equivalent to requiring the existence of a vector field $\mathcal{D}f^\mu(x, \phi)$ so that:

$$\left. \frac{\partial}{\partial \varepsilon} \left(\mathfrak{L}(B(x'), g(x'), \phi', \nabla \phi') \frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right) \right|_{\varepsilon=0} = \nabla_\mu \mathcal{D}f^\mu(x, \phi). \quad (7.6.61)$$

Equivalently, a continuous transformation is a symmetry if and only if when the untransformed action is evaluated at the transformed fields the result differs from the untransformed action evaluated at the untransformed fields only by a functional of the boundary conditions.

7.6.4 Spacetime Symmetries

Sometimes, our metric and background fields will have a symmetry under some diffeomorphism generated by a vector field $\xi^\mu(X)$. That is, by the definition of the Lie derivative:

$$\xi^\mu \text{ generates a symmetry} \implies L_\xi B^a = 0, \quad L_\xi g_{\mu\nu} = 0. \quad (7.6.62)$$

For now hold off on assuming any particular symmetry. Under a generic diffeomorphism a generic tensor field satisfies:

$$B'^a(x') = B^a(x) + \varepsilon \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta B^a + \mathcal{O}(\varepsilon^2) \quad (7.6.63)$$

$$= B^a(x' - \varepsilon \xi) + \varepsilon \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta B^a + \mathcal{O}(\varepsilon^2) \quad (7.6.64)$$

$$= B^a(x') + \varepsilon \xi^\mu \partial_\mu B^a + \varepsilon \partial_\alpha \xi^\beta \hat{G}^\alpha_\beta B^a + \mathcal{O}(\varepsilon^2) \quad (7.6.65)$$

$$= B^a(x') - \varepsilon L_\xi B^a + \mathcal{O}(\varepsilon^2). \quad (7.6.66)$$

In particular for the metric tensor:

$$g'_{\mu\nu}(x') = g_{\mu\nu}(x') - \varepsilon L_\xi g_{\mu\nu} + \mathcal{O}(\varepsilon^2). \quad (7.6.67)$$

Because we have written our Lagrangian density in a coordinate invariant way by definition, under a coordinate transformation:

$$\mathfrak{L}(B'(x'), g'(x'), \phi'(x'), \nabla \phi'(x')) = \mathfrak{L}(B(x), g(x), \phi(x), \nabla \phi(x)) \quad (7.6.68)$$

$$\implies \mathfrak{L}(B(x') - \varepsilon L_\xi B, g(x') - \varepsilon L_\xi g, \phi', \nabla \phi') = \mathfrak{L}(B, g, \phi, \nabla \phi) + \mathcal{O}(\varepsilon^2) \quad (7.6.69)$$

$$\implies \mathfrak{L}(B(x'), g(x'), \phi', \nabla \phi') - \varepsilon \frac{\partial \mathfrak{L}}{\partial B^a} L_\xi B^a - \varepsilon \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} L_\xi g_{\mu\nu} = \mathfrak{L}(B, g, \phi, \nabla \phi) + \mathcal{O}(\varepsilon^2) \quad (7.6.70)$$

$$\implies \left. \frac{\partial}{\partial \varepsilon} \mathfrak{L}(B(x'), g(x'), \phi', \nabla \phi') \right|_{\varepsilon=0} = \frac{\partial \mathfrak{L}}{\partial B^a} L_\xi B^a + \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} L_\xi g_{\mu\nu}. \quad (7.6.71)$$

Therefore, if our background quantities have symmetry under a particular diffeomorphism, then the Lagrangian density satisfies:

$$\left. \frac{\partial}{\partial \varepsilon} \mathfrak{L}(B(x'), g(x'), \phi', \nabla \phi') \right|_{\varepsilon=0} = 0. \quad (7.6.72)$$

As well, because the determinant of a product is the product of determinants, the transformation property of the metric under orientation preserving coordinate transformation determines:

$$\sqrt{-\det g(x')} \det \left(\frac{\partial x'}{\partial x} \right) = \sqrt{-\det g(x)} \quad (7.6.73)$$

and so for a metric symmetric under ξ^μ :

$$\frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \det \left(\frac{\partial x'}{\partial x} \right) = \frac{\sqrt{-\det g'(x')}}{\sqrt{-\det g}} \det \left(\frac{\partial x'}{\partial x} \right) + \mathcal{O}(\varepsilon^2) = 1 + \mathcal{O}(\varepsilon^2). \quad (7.6.74)$$

Thus, under a diffeomorphism which is a symmetry of our background quantities:

$$\frac{\partial}{\partial \varepsilon} \left(\mathfrak{L}(B(x'), g(x'), \phi', \nabla \phi') \frac{\sqrt{-\det g(x')}}{\sqrt{-\det g(x)}} \det \left(\frac{\partial x'(\varepsilon, x, \phi(x))}{\partial x} \right) \right) \Big|_{\varepsilon=0} = 0 \quad (7.6.75)$$

which by Noether's theorem means that diffeomorphism is a symmetry of our theory, with $\mathcal{D}f^\mu = \nabla_\nu \chi^{\mu\nu}$ for some antisymmetric tensor field $\chi^{\mu\nu}$. The covariant changes in coordinates and tensor fields under a diffeomorphism are given by:

$$\mathcal{D}x^\mu = \xi^\mu, \quad \mathcal{D}\phi^a = \nabla_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^a. \quad (7.6.76)$$

Thus, by Noether's theorem, the conserved current associated to symmetry is:

$$J^\mu = \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\alpha \xi^\beta \hat{G}^\alpha_\beta \phi^a + \left(\mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\nu \phi^a \right) \xi^\nu - \nabla_\nu \chi^{\mu\nu}. \quad (7.6.77)$$

One may wonder if there is a natural choice of $\chi^{\mu\nu}$. Certainly the choice may depend on ξ^ρ , and because J^μ is linear in ξ^ρ and its first derivative apart from the $\chi^{\mu\nu}$ term, if that choice is to preserve this linearity, then $\chi^{\mu\nu}$ must be linear in ξ^ρ . If J_1^μ and J_2^μ are the conserved currents corresponding to diffeomorphisms ξ_1^μ and ξ_2^μ , then automatically $\xi_1^\mu + \xi_2^\mu$ also produces a diffeomorphism which is a symmetry and has generator given by the sum of the generators of its constituents. As we would like J^μ to integrate to that generator, it is natural to choose $\chi^{\mu\nu}$ to preserve that linearity so that J^μ corresponding to $\xi_1^\mu + \xi_2^\mu$ is simply $J_1^\mu + J_2^\mu$. Then, for some tensor $\Theta^{\mu\nu\rho}$ which is antisymmetric in its first two indices:

$$\chi^{\mu\nu} = \Theta^{\mu\nu\rho} \xi_\rho. \quad (7.6.78)$$

With this form, the current becomes:

$$J^\mu = \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}^{\alpha\beta} \phi^a - \Theta^{\mu\alpha\beta} \right) \nabla_\alpha \xi_\beta + \left(\mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\nu \phi^a + \nabla_\rho \Theta^{\rho\mu}_\nu \right) \xi^\nu. \quad (7.6.79)$$

We can give a nice interpretation to this quantity. Let X_0 be some particular point of interest and let us consider the behavior of the vector field ξ^μ near that point. At that point define:

$$a^\mu = \xi^\mu(x_0). \quad (7.6.80)$$

Recall (7.2.80) that for a symmetry of our metric:

$$L_\xi g_{\mu\nu} = 0 \implies \nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu = 0. \quad (7.6.81)$$

Define then:

$$\theta_{\mu\nu} = \frac{1}{2} \nabla_\mu \xi_\nu(x_0) = -\frac{1}{2} \nabla_\nu \xi_\mu(x_0) \implies \theta_{\mu\nu}(x_0) = -\theta_{\nu\mu}(x_0). \quad (7.6.82)$$

In a LIRF at X_0 , the covariant derivative becomes simply the partial derivative, and so the vector field $\xi^\mu(x)$ in such coordinates nearby X_0 becomes:

$$\xi^\mu(x) = a^\mu - 2\theta^\mu_\nu (x^\nu - x_0^\nu) + \mathcal{O}(x - x_0)^2. \quad (7.6.83)$$

Recall that ξ^μ is precisely the rate of change of spacetime position under our diffeomorphism. Further, notice that a^μ then represents a uniform shift of spacetime position and so correspond to a spacetime translation, while the $\theta^{\mu\nu}$ term is precisely the differential expression of a Lorentz transformation with Lorentz transformation parameters $\theta^{\alpha\beta}$. Thus, any symmetry of a metric, at any particular point of interest, can be understood as a combination of some amount of spacetime translation and some amount of Lorentz transformation about that point of interest. At the point X_0 then, our conserved current becomes:

$$J^\mu = a^\nu \left(\mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\nu \phi^a + \nabla_\rho \Theta^{\rho\mu}_\nu \right) + \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}^{\alpha\beta} \phi^a - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}^{\beta\alpha} \phi^a - \Theta^{\mu\alpha\beta} + \Theta^{\mu\beta\alpha} \right) \theta_{\alpha\beta}. \quad (7.6.84)$$

Thus, we can see that the portion of the conserved quantity originating from spacetime translations at the point X_0 is:

$$T^\mu_\nu = \mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\nu \phi^a + \nabla_\rho \Theta^{\rho\mu}_\nu \quad (7.6.85)$$

whereas the portion of the conserved quantity originating from Lorentz transformations about the point X_0 is:

$$\mathcal{J}^\mu_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}_{\alpha\beta} \phi^a - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}_{\beta\alpha} \phi^a - \Theta^\mu_{\alpha\beta} + \Theta^\mu_{\beta\alpha}. \quad (7.6.86)$$

Because $T^\mu{}_\nu a^\nu$ then corresponds to the current of spacetime translations by an amount a^ν at X_0 , we identify $T^\mu{}_\nu$ as the energy-momentum tensor at X_0 . Similarly, because $\mathcal{T}^\mu{}_{\alpha\beta}\theta^{\alpha\beta}$ corresponds to the current of Lorentz transformations by an amount $\theta^{\alpha\beta}$ at X_0 , we identify $\mathcal{T}^\mu{}_{\alpha\beta}(X)$ as the total angular momentum current tensor about the point X_0 . It is not possible on a general spacetime to define orbital angular momentum in a meaningful way without some additional structure, because one cannot add tensors at different spacetime locations and so we have to live with an angular momentum current tensor that corresponds to a local generator of transformations about each point. So far, we have developed no fundamental criterion for how to choose the (at this point arbitrary) tensor $\Theta^{\rho\mu\nu}$. One might suspect we can perform a similar construction to the Belinfante-Rosenfeld tensor from the special relativistic case. In fact we can, and we can give a physics reason why such a construction exists and is important.

The current J^μ corresponding to ξ^μ is conserved whenever the spacetime and background variables have symmetry under the diffeomorphism generated by ξ^μ . When considering Minkowski space and no background fields, this produces the local conservation laws of energy-momentum and angular momentum. However, a general spacetime manifold has no Killing vectors, and so no corresponding conserved currents J^μ from diffeomorphisms. Does this mean there is no notion of conserved energy in general relativity? **NO!** It should be obvious that the energy or momentum or angular momentum of our fields will not be conserved in a generic spacetime; this is because they will be interacting with the metric which itself will have energy, momentum, angular momentum and so only the combined system will satisfy the conservation law! We will see in the coming sections that unequivocally energy is conserved in the full interacting theory of general relativity.

7.6.5 Energy-Momentum Tensor

There is something initially puzzling about the lack of a conserved Noether current corresponding to energy-momentum in a generic spacetimes. Our reasoning in section 7.1 that derived diffeomorphism symmetry as the appropriate group of symmetries for gravity relied on the local conservation of energy and momentum. Was that thinking wrong? No, it wasn't. We know that in Minkowski spacetime, the energy-momentum tensor of our fields satisfies the conservation law $\partial_\nu T^{\mu\nu} = 0$ due to spacetime translational symmetry. At a point of interest, a generic spacetime can be made to look like Minkowski spacetime (in the sense that $g_{\mu\nu}(X_0) = \eta_{\mu\nu}$ and $\partial_\rho g_{\mu\nu}(X_0) = 0$ in LIRF coordinates). Then, one would expect that because the point-wise effects of gravity can be transformed away, the energy momentum tensor should still satisfy $\partial_\mu T^\mu{}_\nu = 0$ in LIRF coordinates. Transformed to general coordinates this becomes $\nabla_\mu T^\mu{}_\nu = 0$. This is a local conservation law, however it is different from the conservation form gotten by Noether's theorem. Noether's theorem always gives a divergence free *vector* current. Such a conserved vector current only exists in spacetimes which have a Killing vector. A $T^\mu{}_\nu$ satisfying $\nabla_\mu T^\mu{}_\nu = 0$ is a divergence free rank-2 *tensor* current (and explicitly has a different dependence on Christoffel symbols than a vector current conservation law). We will see in this section that this form of the conservation law is valid in a generic spacetime and serves as the general relativistic statement of local energy-momentum conservation.

Based on our thinking in section 7.1, we will eventually have an action S which describes the interactions of our fields ϕ^a with the metric tensor $g_{\mu\nu}$. We can divide that action into the action S_ϕ for the fields given the metric plus the free action for the metric S_g (following the usual decomposition from theorem 2.11):

$$S[\phi, g] = S_\phi[\phi, g] + S_g[g]. \quad (7.6.87)$$

The equations of motion for the metric will be given by:

$$\frac{\delta S}{\delta g_{\mu\nu}} = \frac{\delta S_\phi}{\delta g_{\mu\nu}} + \frac{\delta S_g}{\delta g_{\mu\nu}} \stackrel{!}{=} 0. \quad (7.6.88)$$

Thus, with S_g the free action for the metric, we see that the external force (as defined in (2.7.49)) acting on the metric is given by $\frac{\delta S_\phi}{\delta g_{\mu\nu}}$. As reasoned in section 7.1, this quantity which now acts as the source term in the equations of motion for the metric must be closely related to the energy-momentum tensor of our fields. Let us now compute $\frac{\delta S_\phi}{\delta g_{\mu\nu}}$ to actually see this.

The action for the fields given the metric will be some integral of the field's Lagrangian density $\mathfrak{L}(g, \phi, \nabla\phi)$ over the region of spacetime we are considering:

$$S_\phi = \int_{\mathbb{M}} \mathfrak{L}(g, \phi, \nabla\phi) d\mathbb{T}. \quad (7.6.89)$$

Under a variation of the metric, of course g is varied, but also $\nabla\phi$ is varied because the covariant derivative depends on the connection coefficients, which depend on the metric. As well, the spacetime measure $d\mathbb{T}$ is

varied because it depends on the metric determinant. Thus:

$$\delta S_\phi = \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} \delta g_{\mu\nu} \sqrt{-\det g} + \frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} \delta \nabla_\rho \phi^a \sqrt{-\det g} + \mathfrak{L} \delta \sqrt{-\det g} \right) d^4x. \quad (7.6.90)$$

The variation of the metric determinant can be completed using the now familiar determinant derivative formula:

$$\delta \sqrt{-\det g} = \frac{-\delta \det g}{2\sqrt{-\det g}} = \frac{-g^{\mu\nu} \delta g_{\mu\nu} \det g}{2\sqrt{-\det g}} = \frac{1}{2} g^{\mu\nu} \delta g_{\mu\nu} \sqrt{-\det g}. \quad (7.6.91)$$

The variation of the covariant derivative can be accomplished using the definition of the Levi-Civita connection:

$$\delta \nabla_\mu \phi^a = \delta (\partial_\mu \phi^a + \Gamma^\beta_{\alpha\mu} \hat{G}^\alpha_\beta \phi^a) = \delta \Gamma^\beta_{\alpha\mu} \hat{G}^\alpha_\beta \phi^a \quad (7.6.92)$$

where the last step follows because $\hat{G}^\alpha_\beta \phi^a$ by its definition does not on the metric (only on the fields and combinations of Kronecker deltas). Then:

$$\delta \Gamma^\beta_{\alpha\mu} = \delta \left(\frac{1}{2} g^{\beta\gamma} (\partial_\alpha g_{\gamma\mu} + \partial_\mu g_{\gamma\alpha} - \partial_\gamma g_{\alpha\mu}) \right) \quad (7.6.93)$$

$$= \frac{1}{2} \delta g^{\beta\gamma} (\partial_\alpha g_{\gamma\mu} + \partial_\mu g_{\gamma\alpha} - \partial_\gamma g_{\alpha\mu}) + \frac{1}{2} g^{\beta\gamma} (\partial_\alpha \delta g_{\gamma\mu} + \partial_\mu \delta g_{\gamma\alpha} - \partial_\gamma \delta g_{\alpha\mu}). \quad (7.6.94)$$

In order to vary the metric inverse, simply use the definition of the matrix inverse:

$$g^{\mu\rho} g_{\rho\nu} = \delta^\mu_\nu \implies \delta g^{\mu\rho} g_{\rho\nu} + g^{\mu\rho} \delta g_{\rho\nu} = 0 \implies \delta g^{\mu\nu} = -g^{\mu\alpha} g^{\nu\beta} \delta g_{\alpha\beta}. \quad (7.6.95)$$

Then:

$$\delta \Gamma^\beta_{\alpha\mu} = -g^{\beta\gamma} \delta g_{\gamma\lambda} \Gamma^\lambda_{\alpha\mu} + \frac{1}{2} g^{\beta\gamma} (\partial_\alpha \delta g_{\gamma\mu} + \partial_\mu \delta g_{\gamma\alpha} - \partial_\gamma \delta g_{\alpha\mu}) \quad (7.6.96)$$

$$= \frac{1}{2} g^{\beta\gamma} (\partial_\alpha \delta g_{\gamma\mu} - \Gamma^\lambda_{\gamma\alpha} \delta g_{\lambda\mu} - \Gamma^\lambda_{\mu\alpha} \delta g_{\gamma\lambda} + \partial_\mu \delta g_{\gamma\alpha} - \Gamma^\lambda_{\gamma\mu} \delta g_{\lambda\alpha} - \Gamma^\lambda_{\mu\alpha} \delta g_{\gamma\lambda} - \partial_\gamma \delta g_{\alpha\mu} + \Gamma^\lambda_{\alpha\gamma} \delta g_{\lambda\mu} + \Gamma^\lambda_{\mu\gamma} \delta g_{\alpha\lambda}) \quad (7.6.97)$$

$$= \frac{1}{2} g^{\beta\gamma} (\nabla_\alpha \delta g_{\gamma\mu} + \nabla_\mu \delta g_{\gamma\alpha} - \nabla_\gamma \delta g_{\alpha\mu}). \quad (7.6.98)$$

Note that even though the connection coefficients/Christoffel symbols are not a tensor, the variation $\delta \Gamma^\rho_{\mu\nu}$ is in fact a tensor. This can also be noticed by using the transformation property of the connection coefficients in (7.2.23) from which it is clear that the nontensorial part of the Christoffel symbols cancels out in a difference of two different Christoffel symbols. Returning these to the variation of our action, we have:

$$\delta S_\phi = \int_{\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} \delta g_{\mu\nu} + \frac{1}{2} \frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} (\nabla_\mu \delta g_{\nu\rho} + \nabla_\rho \delta g_{\mu\nu} - \nabla_\nu \delta g_{\mu\rho}) \hat{G}^{\mu\nu} \phi^a + \frac{\mathfrak{L}}{2} g^{\mu\nu} \delta g_{\mu\nu} \right) d\mathbb{T}. \quad (7.6.99)$$

It is useful to keep the variations of our metric generic and to not assume the equations of motion hold for the ϕ^a fields for now. Rearranging our action slightly:

$$\delta S_\phi = \frac{1}{2} \int_{\mathbb{M}} \left(\left(2 \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} + \mathfrak{L} g^{\mu\nu} \right) \delta g_{\mu\nu} + \frac{1}{2} \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} (\hat{G}^{\mu\nu} \phi^a + \hat{G}^{\nu\mu} \phi^a) - S^{\mu\nu\rho} - S^{\nu\mu\rho} \right) \nabla_\rho \delta g_{\mu\nu} \right) d\mathbb{T} \quad (7.6.100)$$

where we have deliberately written the coefficients of $\delta g_{\mu\nu}$ and $\nabla_\rho \delta g_{\mu\nu}$ to be symmetric in exchanging $\mu\nu$, because $\delta g_{\mu\nu}$ is and we have introduced (just as with the special relativistic case) the covariant version of the spin current tensor:

$$S^\mu_{\alpha\beta} = \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} (\hat{G}_{\alpha\beta} \phi^a - \hat{G}_{\beta\alpha} \phi^a). \quad (7.6.101)$$

For calculation purposes it is also useful to define the Noether stress tensor:

$$N^\mu_\nu = \mathfrak{L} \delta^\mu_\nu - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\nu \phi^a. \quad (7.6.102)$$

The form (7.6.100) doesn't look especially insightful, but we have not used that the Lagrangian density is coordinate invariant. Using that fact, under a coordinate transformation $x'^\mu = x^\mu + \varepsilon \xi^\mu(x) + \mathcal{O}(\varepsilon^2)$ for arbitrary vector field $\xi^\mu(x)$:

$$\mathfrak{L}(g'(x'), \phi'(x'), \nabla \phi'(x')) = \mathfrak{L}(g(x), \phi(x), \nabla \phi(x)) \quad (7.6.103)$$

$$\implies \Upsilon(\mathfrak{L}(g'(x'), \phi'(x'), \nabla \phi'(x')), x', x) = \mathfrak{L}(g(x), \phi(x), \nabla \phi(x)) \quad (7.6.104)$$

$$\Rightarrow \left. \frac{\partial}{\partial \varepsilon} \Upsilon(\mathfrak{L}(g'(x'), \phi'(x'), \nabla \phi'(x')), x', x) \right|_{\varepsilon=0} = 0 \quad (7.6.105)$$

$$\Rightarrow \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} \nabla_\alpha \xi^\beta \hat{G}^\alpha{}_\beta g_{\mu\nu} + \frac{\partial \mathfrak{L}}{\partial \phi^a} \nabla_\alpha \xi^\beta \hat{G}^\alpha{}_\beta \phi^a + \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla_\alpha \xi^\beta \hat{G}^\alpha{}_\beta \nabla_\mu \phi^a = 0. \quad (7.6.106)$$

Because this is true for all choices of ξ^α , the coefficient of $\nabla_\alpha \xi^\beta$ must vanish:

$$\boxed{\frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} \hat{G}^\alpha{}_\beta g_{\mu\nu} + \frac{\partial \mathfrak{L}}{\partial \phi^a} \hat{G}^\alpha{}_\beta \phi^a + \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \hat{G}^\alpha{}_\beta \nabla_\mu \phi^a = 0.} \quad (7.6.107)$$

For now hold off from assuming the equations of motion of ϕ^a are satisfied, and let E_a be the equation of motion functions:

$$E_a = \frac{\partial \mathfrak{L}}{\partial \phi^a} - \nabla_\mu \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a}. \quad (7.6.108)$$

Then, using (7.5.27) to simplify (7.6.107), we have that:

$$-2 \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} + E_a \hat{G}^{\mu\nu} \phi^a + \nabla_\rho \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} \right) \hat{G}^{\mu\nu} \phi^a - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla^\nu \phi^a + \frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} \nabla_\rho \hat{G}^{\mu\nu} \phi^a = 0 \quad (7.6.109)$$

$$\Rightarrow 2 \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} + \mathfrak{L} g^{\mu\nu} = E_a \hat{G}^{\mu\nu} \phi^a + N^{\mu\nu} + \nabla_\rho \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} \hat{G}^{\mu\nu} \phi^a \right) \quad (7.6.110)$$

$$\Rightarrow 2 \frac{\partial \mathfrak{L}}{\partial g_{\mu\nu}} + \mathfrak{L} g^{\mu\nu} = E_a \hat{G}^{\mu\nu} \phi^a + N^{\mu\nu} + \frac{1}{2} \nabla_\rho \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} (\hat{G}^{\mu\nu} \phi^a + \hat{G}^{\nu\mu} \phi^a) + S^{\rho\mu\nu} \right). \quad (7.6.111)$$

The right hand side here doesn't look symmetric in $\mu\nu$, but the left hand side is and so the right must be so as well. Equating that right hand side with itself after swapping $\mu\nu$ gives:

$$\nabla_\rho S^{\rho\mu\nu} = N^{\nu\mu} - N^{\mu\nu} + E_a \hat{G}^{\nu\mu} \phi^a - E_a \hat{G}^{\mu\nu} \phi^a. \quad (7.6.112)$$

Now returning (7.6.111) to (7.6.100) and using Stokes' theorem:

$$\begin{aligned} \delta S_\phi = & \frac{1}{2} \int_{\mathbb{M}} \left(E_a \hat{G}^{\mu\nu} \phi^a + N^{\mu\nu} + \frac{1}{2} \nabla_\rho (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \right) \delta g_{\mu\nu} d\mathbb{T} \\ & + \frac{1}{2} \int_{\partial\mathbb{M}} \left(\frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} \hat{G}^{\mu\nu} \phi^a - \frac{1}{2} (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \right) \delta g_{\mu\nu} d\Sigma_\rho \end{aligned} \quad (7.6.113)$$

where we have consistently kept the coefficients of $\delta g_{\mu\nu}$ symmetric in $\mu\nu$ (even though they may not be obviously so, due to (7.6.111)). Equation (7.6.113) is the fully general variation of the field action with respect to the metric, valid off-shell and without any conditions on the metric variations. Now applying the equations of motion $E_a = 0$ (going on-shell for the fields ϕ^a) and considering variations of the metric which vanish on the boundary of our integration region, we have:

$$\boxed{\frac{2}{\sqrt{-\det g}} \frac{\delta S_\phi}{\delta g_{\mu\nu}} = N^{\mu\nu} + \frac{1}{2} \nabla_\rho (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}).} \quad (7.6.114)$$

Therefore, **the action's functional derivative with respect to the metric on-shell is directly proportional to the energy-momentum tensor as constructed by Belinfante-Rosenfeld**. This explains why the Belinfante-Rosenfeld definition of the energy-momentum is the natural one – it is the only one which corresponds to the source of the gravitational interaction/it is the one that appears in the gravitational equations of motion. Identifying:

$$\Theta^{\rho\mu\nu} = \frac{1}{2} (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (7.6.115)$$

which in fact has the correct index symmetry properties, we can see that (7.6.85) becomes:

$$T^{\mu\nu} = \frac{2}{\sqrt{-\det g}} \frac{\delta S_\phi}{\delta g_{\mu\nu}} \quad (7.6.116)$$

and that (7.6.86) becomes:

$$\mathcal{J}^\mu{}_{\alpha\beta} = 0. \quad (7.6.117)$$

Because $g_{\mu\nu}$ is symmetric, $T^{\mu\nu}$ is automatically symmetric due to (7.6.116). Let us now compute the

divergence of the energy-momentum tensor. Using (7.6.112) with (7.6.114):

$$T^{\mu\nu} = \frac{N^{\mu\nu} + N^{\nu\mu}}{2} + \frac{1}{2}\nabla_\rho(S^{\mu\nu\rho} + S^{\nu\mu\rho}). \quad (7.6.118)$$

Then, again using (7.6.112) and the definitions and index symmetry properties of the Riemann and Ricci tensors:

$$\nabla_\mu T^{\mu\nu} = \frac{1}{2}\nabla_\mu N^{\mu\nu} + \frac{1}{2}\nabla_\mu N^{\nu\mu} + \frac{1}{2}\nabla_\mu \nabla_\rho S^{\mu\nu\rho} + \frac{1}{2}\nabla_\mu \nabla_\rho S^{\nu\mu\rho} \quad (7.6.119)$$

$$= \frac{1}{2}\nabla_\mu N^{\mu\nu} + \frac{1}{2}\nabla_\mu N^{\nu\mu} + \frac{1}{2}\nabla_\rho \nabla_\mu S^{\mu\nu\rho} + \frac{1}{2}[\nabla_\mu, \nabla_\rho]S^{\mu\nu\rho} + \frac{1}{4}[\nabla_\mu, \nabla_\rho]S^{\nu\mu\rho} \quad (7.6.120)$$

$$= \frac{1}{2}\nabla_\mu N^{\mu\nu} + \frac{1}{2}\nabla_\mu N^{\nu\mu} + \frac{1}{2}\nabla_\rho N^{\rho\nu} - \frac{1}{2}\nabla_\rho N^{\nu\rho} + \frac{1}{2}R^\beta_{\alpha\mu\rho}\hat{G}^\alpha_{\beta}S^{\mu\nu\rho} + \frac{1}{4}R^\beta_{\alpha\mu\rho}\hat{G}^\alpha_{\beta}S^{\nu\mu\rho} \quad (7.6.121)$$

$$= \nabla_\mu N^{\mu\nu} + \frac{1}{2}R_{\alpha\beta}S^{\alpha\nu\beta} - \frac{1}{2}R^\nu_{\gamma\alpha\beta}S^{\alpha\beta\gamma} - \frac{1}{2}R_{\alpha\beta}S^{\alpha\nu\beta} + \frac{1}{4}R^\nu_{\gamma\alpha\beta}S^{\gamma\alpha\beta} + \frac{1}{4}R_{\alpha\beta}S^{\nu\alpha\beta} + \frac{1}{4}R_{\alpha\beta}S^{\nu\alpha\beta} \quad (7.6.122)$$

$$= \nabla_\mu N^{\mu\nu} - \frac{1}{2}R^\nu_{\gamma\alpha\beta}S^{\alpha\beta\gamma} + \frac{1}{4}R^\nu_{\gamma\alpha\beta}S^{\gamma\alpha\beta}. \quad (7.6.123)$$

Using the algebraic Bianchi identity:

$$(R^\nu_{\gamma\alpha\beta} + R^\nu_{\alpha\beta\gamma} + R^\nu_{\beta\gamma\alpha})S^{\alpha\beta\gamma} = 0 \quad (7.6.124)$$

$$\implies R^\nu_{\gamma\alpha\beta}S^{\alpha\beta\gamma} = -\frac{1}{2}R^\nu_{\gamma\alpha\beta}S^{\gamma\alpha\beta}. \quad (7.6.125)$$

Then, using the definition of $S^\mu_{\alpha\beta}$:

$$\nabla_\mu T^{\mu\nu} = \nabla_\mu N^{\mu\nu} + R^\nu_{\gamma\alpha\beta}\frac{\partial\mathfrak{L}}{\partial\nabla_\gamma\phi^a}\hat{G}^{\alpha\beta}\phi^a. \quad (7.6.126)$$

Now explicitly computing the divergence of $N^{\mu\nu}$ and using the equation of motion for ϕ^a :

$$\nabla_\mu N^{\mu\nu} = \nabla_\mu \left(\mathfrak{L}g^{\mu\nu} - \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a}\nabla^\nu\phi^a \right) = \nabla^\nu\mathfrak{L} - \nabla_\mu\frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a}\nabla^\nu\phi^a - \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a}\nabla_\mu\nabla^\nu\phi^a \quad (7.6.127)$$

$$= \frac{\partial\mathfrak{L}}{\partial\phi^a}\nabla^\nu\phi^a + \frac{\partial\mathfrak{L}}{\partial\nabla^\mu\phi^a}\nabla^\nu\nabla^\mu\phi^a - \frac{\partial\mathfrak{L}}{\partial\phi^a}\nabla^\nu\phi^a - \frac{\partial\mathfrak{L}}{\partial\nabla^\mu\phi^a}\nabla^\mu\nabla^\nu\phi^a \quad (7.6.128)$$

$$= \frac{\partial\mathfrak{L}}{\partial\nabla^\mu\phi^a}R^\beta_{\alpha}{}^{\nu\mu}\hat{G}^\alpha_{\beta}\phi^a = -R^\nu_{\gamma\alpha\beta}\frac{\partial\mathfrak{L}}{\partial\nabla_\gamma\phi^a}\hat{G}^{\alpha\beta}\phi^a. \quad (7.6.129)$$

Thus, diffeomorphism symmetry guarantees that the energy-momentum tensor satisfies:

$$\boxed{\nabla_\mu T^{\mu\nu} = 0.} \quad (7.6.130)$$

This is exactly what we wanted! The energy-momentum tensor satisfies the covariant conservation law (7.6.130) in a generic spacetime.

For a vector field ξ^μ then, current J^μ defined by:

$$J^\mu = T^\mu_{\nu}\xi^\nu \quad (7.6.131)$$

automatically satisfies (by using (7.2.79)):

$$\nabla_\mu J^\mu = \frac{1}{2}T^{\mu\nu}L_\xi g_{\mu\nu}. \quad (7.6.132)$$

If ξ^μ is a symmetry of the metric, this current is conserved. As well, in that case this J^μ corresponds exactly with (7.6.84) using the definition of $\Theta^{\rho\mu\nu}$ determined by Belinfante-Rosenfeld. Altogether we have:

Theorem 7.4: Belinfante-Rosenfeld Theorem – General Relativity

If $S[\phi]$ is the action of a local classical field theory in curved spacetime with Lagrangian density $\mathfrak{L}(g, \phi, \nabla\phi)$ written in a coordinate-invariant way, then the Lagrangian density satisfies:

$$\frac{\partial\mathfrak{L}}{\partial g_{\mu\nu}}\hat{G}^\alpha_{\beta}g_{\mu\nu} + \frac{\partial\mathfrak{L}}{\partial\phi^a}\hat{G}^\alpha_{\beta}\phi^a + \frac{\partial\mathfrak{L}}{\partial\nabla_\mu\phi^a}\hat{G}^\alpha_{\beta}\nabla_\mu\phi^a = 0. \quad (7.6.133)$$

Consequently, the on-shell energy-momentum tensor $T^{\mu\nu}$ of the theory is given by:

$$T^{\mu\nu} = T^{\nu\mu} = \frac{2}{\sqrt{-\det g}} \frac{\delta S}{\delta g_{\mu\nu}} = \mathfrak{L} g^{\mu\nu} - \frac{\partial \mathfrak{L}}{\partial \nabla_\mu \phi^a} \nabla^\nu \phi^a + \frac{1}{2} \nabla_\rho (S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}) \quad (7.6.134)$$

where $S^{\rho\mu\nu}$ is the spin current tensor defined by:

$$S^\rho{}_{\mu\nu} = \frac{\partial \mathfrak{L}}{\partial \nabla_\rho \phi^a} (\hat{G}_{\mu\nu} \phi^a - \hat{G}_{\nu\mu} \phi^a). \quad (7.6.135)$$

The energy-momentum satisfies the covariant conservation law:

$$\nabla_\nu T^{\mu\nu} = 0 \quad (7.6.136)$$

and the spin current tensor satisfies:

$$\nabla_\rho S^\rho{}_{\mu\nu} = \frac{\partial \mathfrak{L}}{\partial \nabla^\mu \phi^a} \nabla_\nu \phi^a - \frac{\partial \mathfrak{L}}{\partial \nabla^\nu \phi^a} \nabla_\mu \phi^a. \quad (7.6.137)$$

If the metric has symmetry under a diffeomorphism $\mathcal{D}x^\mu = \xi^\mu$, then the conserved Noether current for the fields under that transformation is:

$$J^\mu = T^\mu{}_\nu \xi^\nu. \quad (7.6.138)$$

Exercises

Problem 7.12: ★ Familiar energy-momentum tensors in curved spacetime.

- Show by explicit calculation of both expressions for the energy-momentum tensor in the Belinfante-Rosenfeld theorem that the two agree for the Maxwell Lagrangian density $\mathfrak{L} = -\frac{1}{4} \mathcal{F}^{\mu\nu} \mathcal{F}_{\mu\nu}$. Show as well that the resulting energy-momentum tensor is covariantly conserved when Maxwell's equations are applied.
- Show by explicit calculation of both expressions for the energy-momentum tensor in the Belinfante-Rosenfeld theorem that the two agree for the ideal fluid Lagrangian density $\mathfrak{L} = -n\mathcal{U}(n)$. Show as well that the resulting energy-momentum tensor is covariantly conserved when the equations of motion are applied.

7.7 Einstein-Hilbert Action

It is time to find equations of motion for the metric. We would like to write our Lagrangian density as a scalar so that it is coordinate invariant. No nontrivial scalars can be made out of the metric without derivatives because it can pointwise always be transformed into the Minkowski metric. No nontrivial scalars can be made out of the metric's first derivatives because in a LIRF they all vanish. Thus, we must consider a Lagrangian density containing at least second derivatives. All of proper tensors that can be made out of the metric's second derivatives are packaged in the Riemann tensor (which can be seen in Fermi normal coordinates, where the metric's second derivatives are fully determined by the Riemann tensor). Therefore, we seek a Lagrangian density which is a scalar function of the Riemann tensor. We exclude the possibility of derivatives on the Riemann tensor as those would give even higher order derivatives of the metric, and always we consider the lowest order consistent theory first.

The lowest order (meaning involving the fewest powers) scalar that can be made out of the Riemann tensor is the Ricci scalar R , and no other scalars can be formed out of only a single power of $R_{\rho\mu\sigma\nu}$. Therefore, the lowest order Lagrangian density for the metric is simply:

$$\mathcal{L} = a + bR \quad (7.7.1)$$

for constants a and b . It is nicer to give these constants slightly different names. Let $\Omega = \frac{1}{2b}$ and define the **cosmological constant** $\Lambda = -\Omega a$. Then, our Lagrangian density becomes:

$$\mathcal{L} = \frac{R}{2\Omega} - \frac{\Lambda}{\Omega}. \quad (7.7.2)$$

Naively one may believe that Λ has no affect on the equations of motion, but this is incorrect (it is not simply the addition of a constant to the action, because in the integral it gets multiplied by $\sqrt{-\det g}$ and so does add a dynamical term). Because the Ricci scalar depends on the first derivative of the Christoffel symbols and the Christoffel symbols depend on the first derivative of the metric, the Ricci scalar depends on the second derivatives of the metric. Thus, one may believe that using this Lagrangian density will lead to a higher derivative theory. However, the Ricci scalar is only linear in the second derivatives of the metric, and so it is possible to add (non-scalar) terms to the Lagrangian density which do not affect the equations of motion but which make the Lagrangian density only depend on first derivatives of the metric. In particular, define the **Lagrangian coordinate density** $\mathcal{L}$ by:

$$\mathcal{L} = \mathcal{L}\sqrt{-\det g} \quad (7.7.3)$$

so that the action is given by the integral of the Lagrangian coordinate density over the coordinate measure d^4x . The ability to add total covariant divergences $\nabla_\rho f^\rho$ to the Lagrangian density without affecting equations of motion then manifests as the ability to add partial derivative divergences to the Lagrangian coordinate density without affecting the equations of motion due to:

$$\mathcal{L}' = \mathcal{L}'\sqrt{-\det g} = \mathcal{L}\sqrt{-\det g} + \nabla_\rho f^\rho \sqrt{-\det g} = \mathcal{L} + \partial_\rho(f^\rho \sqrt{-\det g}). \quad (7.7.4)$$

Using the definition of the Ricci scalar:

$$\mathcal{L} = \frac{\sqrt{-\det g}}{2\Omega} g^{\mu\nu} (\partial_\rho \Gamma^\rho_{\mu\nu} - \partial_\nu \Gamma^\rho_{\rho\mu} + \Gamma^\rho_{\rho\lambda} \Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\lambda\nu} \Gamma^\lambda_{\rho\mu}) - \frac{\Lambda}{\Omega} \sqrt{-\det g} \quad (7.7.5)$$

$$\begin{aligned} &= -\frac{1}{2\Omega} \Gamma^\rho_{\mu\nu} \partial_\rho (g^{\mu\nu} \sqrt{-\det g}) + \frac{1}{2\Omega} \Gamma^\rho_{\rho\mu} \partial_\nu (g^{\mu\nu} \sqrt{-\det g}) + \frac{\sqrt{-\det g}}{2\Omega} g^{\mu\nu} (\Gamma^\rho_{\rho\lambda} \Gamma^\lambda_{\mu\nu} - \Gamma^\rho_{\lambda\nu} \Gamma^\lambda_{\rho\mu}) \\ &\quad - \frac{\Lambda}{\Omega} \sqrt{-\det g} + \partial_\rho \left(\frac{\sqrt{-\det g}}{2\Omega} g^{\mu\nu} \Gamma^\rho_{\mu\nu} \right) - \partial_\nu \left(\frac{\sqrt{-\det g}}{2\Omega} g^{\mu\nu} \Gamma^\rho_{\rho\mu} \right). \end{aligned} \quad (7.7.6)$$

Then, using the definition of the Christoffel symbols:

$$\partial_\rho (g^{\mu\nu} \sqrt{-\det g}) = \partial_\rho g^{\mu\nu} \sqrt{-\det g} + g^{\mu\nu} \partial_\rho \sqrt{-\det g} \quad (7.7.7)$$

$$= -g^{\mu\alpha} g^{\nu\beta} \partial_\rho g_{\alpha\beta} \sqrt{-\det g} + \frac{1}{2} g^{\mu\nu} g^{\alpha\beta} \partial_\rho g_{\alpha\beta} \sqrt{-\det g} \quad (7.7.8)$$

$$= -\left(g^{\mu\alpha} g^{\nu\beta} - \frac{1}{2} g^{\mu\nu} g^{\alpha\beta} \right) (g_{\alpha\sigma} \Gamma^\sigma_{\beta\rho} + g_{\beta\sigma} \Gamma^\sigma_{\alpha\rho}) \sqrt{-\det g} \quad (7.7.9)$$

$$= (g^{\mu\nu} \Gamma^\sigma_{\sigma\rho} - g^{\mu\sigma} \Gamma^\nu_{\rho\sigma} - g^{\nu\sigma} \Gamma^\mu_{\rho\sigma}) \sqrt{-\det g}. \quad (7.7.10)$$

Now returning this to the Lagrangian coordinate density and simplifying:

$$\mathcal{L} = \frac{\sqrt{-\det g}}{2\Omega} g^{\mu\nu} (\Gamma^\rho_{\sigma\mu} \Gamma^\sigma_{\rho\nu} - \Gamma^\rho_{\rho\sigma} \Gamma^\sigma_{\mu\nu}) - \frac{\Lambda}{\Omega} \sqrt{-\det g} + \partial_\rho \left(\frac{\sqrt{-\det g}}{2\Omega} (g^{\mu\nu} \Gamma^\rho_{\mu\nu} - g^{\mu\rho} \Gamma^\nu_{\mu\nu}) \right). \quad (7.7.11)$$

We see that in fact the Lagrangian coordinate density can be written in terms of pieces only involving first derivatives of the metric (up to terms that don't affect the equations of motion due to being total derivatives). We could in principle remove this total partial derivative terms and use only the remaining Lagrangian coordinate density, which would then give equations of motion in the usual way without higher derivative dependence. However, doing so leaves one with a Lagrangian density which is not coordinate invariant. Our next goal is to show that by the inclusion of the correct boundary term, we have can build a coordinate invariant and first order action.

7.7.1 Gibbons-Hawking-York Boundary Term

Consider our true scalar Lagrangian density (7.7.2). Let S_{EHn} be the action due to the Lagrangian density for the metric only (excluding other fields) on some region $\mathbb{M}$ of spacetime so that:

$$S_{\text{EHn}} = \int_{\mathbb{M}} \left(\frac{R}{2\Omega} - \frac{\Lambda}{\Omega} \right) \sqrt{-\det g} d^4x. \quad (7.7.12)$$

We use the subscript EHn as a shorthand for Einstein-Hilbert (naive). Then, under variations of the metric:

$$\delta S_{\text{EHn}} = \int_{\mathbb{M}} \left(\frac{\delta R}{2\Omega} \sqrt{-\det g} + \frac{R}{2\Omega} \delta \sqrt{-\det g} - \frac{\Lambda}{\Omega} \delta \sqrt{-\det g} \right) d^4x. \quad (7.7.13)$$

Using (7.6.91) and $R = g^{\mu\nu} R_{\mu\nu}$:

$$\delta S_{\text{EHn}} = \int_{\mathbb{M}} \left(\frac{R_{\mu\nu} \delta g^{\mu\nu}}{2\Omega} + \frac{g^{\mu\nu} \delta R_{\mu\nu}}{2\Omega} + \frac{R}{4\Omega} g^{\mu\nu} \delta g_{\mu\nu} - \frac{\Lambda}{2\Omega} g^{\mu\nu} \delta g_{\mu\nu} \right) d\mathbb{T}. \quad (7.7.14)$$

Using the definition of the Riemann tensor:

$$\delta R^\rho_{\mu\sigma\nu} = \partial_\sigma \delta \Gamma^\rho_{\mu\nu} - \partial_\nu \delta \Gamma^\rho_{\mu\sigma} + \delta \Gamma^\rho_{\lambda\sigma} \Gamma^\lambda_{\mu\nu} + \Gamma^\rho_{\lambda\sigma} \delta \Gamma^\lambda_{\mu\nu} - \delta \Gamma^\rho_{\lambda\nu} \Gamma^\lambda_{\mu\sigma} - \Gamma^\rho_{\lambda\nu} \delta \Gamma^\lambda_{\mu\sigma} \quad (7.7.15)$$

$$= \nabla_\sigma \delta \Gamma^\rho_{\mu\nu} - \nabla_\nu \delta \Gamma^\rho_{\mu\sigma} \quad (7.7.16)$$

because the variation of the connection coefficients is a tensor. Now applying (7.6.95) and (7.6.98):

$$g^{\mu\nu} \delta R_{\mu\nu} = \nabla_\rho (g^{\mu\nu} \delta \Gamma^\rho_{\mu\nu} - g^{\mu\rho} \delta \Gamma^\nu_{\mu\nu}) \quad (7.7.17)$$

$$= \nabla_\rho \left(\frac{1}{2} g^{\mu\nu} g^{\rho\sigma} (\nabla_\mu \delta g_{\sigma\nu} + \nabla_\nu \delta g_{\sigma\mu} - \nabla_\sigma \delta g_{\mu\nu}) - \frac{1}{2} g^{\mu\rho} g^{\nu\sigma} (\nabla_\mu \delta g_{\sigma\nu} + \nabla_\nu \delta g_{\sigma\mu} - \nabla_\sigma \delta g_{\mu\nu}) \right) \quad (7.7.18)$$

$$= \nabla_\rho (-\nabla_\sigma \delta g^{\rho\sigma} + g_{\mu\nu} \nabla^\rho \delta g^{\mu\nu}). \quad (7.7.19)$$

Returning this to the action variation and applying Stokes' theorem and (7.6.95) again:

$$\delta S_{\text{EHn}} = \int_{\mathbb{M}} \frac{1}{2\Omega} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right) \delta g^{\mu\nu} d\mathbb{T} - \int_{\partial\mathbb{M}} \frac{1}{2\Omega} (\nabla_\sigma \delta g^{\rho\sigma} - g_{\mu\nu} \nabla^\rho \delta g^{\mu\nu}) d\Sigma_\rho. \quad (7.7.20)$$

When considering variations of our metric which vanish on the boundary of our surface, we have $\delta g^{\mu\nu} = 0$ on $\partial\mathbb{M}$. Automatically then the derivatives of $\delta g^{\mu\nu}$ in the directions tangent to $\mathbb{M}$ will vanish. However, we cannot assume that the derivatives of $\delta g^{\mu\nu}$ in directions normal to $\partial\mathbb{M}$ vanish (that would be a separate and additional boundary condition). We assume our spacetime region is topologically a cylinder, the the sense that we assume $\mathbb{M}$ is a set of equal time time slices of finite spatial extent between some initial and final times. Then, $\partial\mathbb{M}$ is timelike on the initial and final surfaces (the cylindrical end-caps) and spacelike on the spatial boundary (the cylindrical shell). Let n^μ the the usual unit normal vector for a timelike or spacelike surface on $\partial\mathbb{M}$ and let $\gamma^{\mu\nu}$ be the metric on the surface $\partial\mathbb{M}$ lifted to being a tensor on spacetime as done in equation (7.4.36). Let ∇_n be defined by:

$$\nabla_n = n^\mu \nabla_\mu. \quad (7.7.21)$$

Then, the vanishing of $\delta g^{\mu\nu}$ on all of $\partial\mathbb{M}$ gives:

$$\gamma^\sigma_\rho \nabla_\sigma \delta g^{\mu\nu} = 0 \implies \nabla_\rho \delta g^{\mu\nu} = \varepsilon n_\rho \nabla_n \delta g^{\mu\nu} \text{ on } \partial\mathbb{M}. \quad (7.7.22)$$

Using the definition of the surface element, the surface integral becomes:

$$\int_{\partial\mathbb{M}} (\nabla_\sigma \delta g^{\rho\sigma} - g_{\mu\nu} \nabla^\rho \delta g^{\mu\nu}) d\Sigma_\rho = \int_{\partial\mathbb{M}} (n_\rho n_\sigma \nabla_n \delta g^{\rho\sigma} - \varepsilon g_{\mu\nu} \nabla_n \delta g^{\mu\nu}) d\Sigma \quad (7.7.23)$$

$$= \int_{\partial\mathbb{M}} \varepsilon \gamma^{\mu\nu} \nabla_n \delta g_{\mu\nu} d\Sigma. \quad (7.7.24)$$

So, the variation of the naive Einstein-Hilbert action gives:

$$\delta S_{\text{EHn}} = \int_{\mathbb{M}} \frac{1}{2\Omega} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right) \delta g^{\mu\nu} d\mathbb{T} - \int_{\partial\mathbb{M}} \frac{\varepsilon \gamma^{\mu\nu} \nabla_n \delta g_{\mu\nu}}{2\Omega} d\Sigma. \quad (7.7.25)$$

Now we can very clearly see that the naive Einstein-Hilbert action does not give a well-defined variational principle when only the metric is held fixed at the boundary. Let us try to find a boundary term that can be added to the action so that the variational principle on the interior is not affected but which cancels the $\nabla_n \delta g_{\mu\nu}$ term.

If such a term is to exist and maintain the coordinate invariance of the action, then the integrand must be a scalar quantity which can be formed out of quantities only on the boundary of $\partial\mathbb{M}$. The only extra quantity available to us on the boundary which is not available on the interior is the normal vector n_μ . Thinking geometrically for a moment, a surface appears curved from outside if the normal vector to the surface points in different directions in different places on the surface. In other words, a surface appears curved if when we take the normal vector at one point on the surface and parallel transport it to another point, it does not agree with the actual normal vector at that point. Thus, the curvature of a surface as viewed from outside that surface, known as the **extrinsic curvature** is captured by the covariant derivative of the normal vector in the directions tangent to the surface. Based on this, define the extrinsic curvature tensor $K_{\mu\nu}$ by:

$$K_{\mu\nu} = \gamma^\sigma{}_\mu \nabla_\sigma n_\nu = \nabla_\mu n_\nu - \varepsilon n_\mu \nabla_n n_\nu. \quad (7.7.26)$$

We can learn a little bit about the extrinsic curvature by writing it explicitly in terms of the constraint which defines $\partial\mathbb{M}$. Let $\zeta(X)$ be a smooth scalar function which vanishes precisely on $\partial\mathbb{M}$. Then, define the vector k_μ just as when we defined surface integration and define the scalar field M by:

$$k_\mu = -\nabla_\mu \zeta, \quad M = \sqrt{\varepsilon g^{\mu\nu} k_\mu k_\nu} \implies n_\mu = -\frac{\varepsilon k_\mu}{M}. \quad (7.7.27)$$

Because ζ is a scalar function $\nabla_\mu \nabla_\nu \zeta = \nabla_\nu \nabla_\mu \zeta$ and so we write:

$$\nabla_{\mu\nu}^2 \zeta = \nabla_\mu \nabla_\nu \zeta \quad (7.7.28)$$

which is automatically symmetric. Then:

$$\nabla_\mu k_\nu = -\nabla_{\mu\nu}^2 \zeta, \quad \nabla_\mu M = \frac{\varepsilon k^\nu \nabla_\mu k_\nu}{M} = n^\nu \nabla_{\mu\nu}^2 \zeta \quad (7.7.29)$$

$$\implies \nabla_\mu n_\nu = \frac{\varepsilon}{M} \nabla_{\mu\nu}^2 \zeta + \frac{\varepsilon}{M^2} n^\nu \nabla_{\mu\nu}^2 \zeta. \quad (7.7.30)$$

Combining these results in $K_{\mu\nu}$, we find:

$$K_{\mu\nu} = \frac{\varepsilon}{M} (\nabla_{\mu\nu}^2 \zeta - \varepsilon n_\nu n^\rho \nabla_{\mu\rho}^2 \zeta - \varepsilon n_\mu n^\rho \nabla_{\nu\rho}^2 \zeta + n_\mu n_\nu n^\rho n^\sigma \nabla_{\rho\sigma}^2 \zeta). \quad (7.7.31)$$

This expression isn't typically useful for calculations, but it does make it plain to see that the extrinsic curvature is symmetric:

$$K_{\mu\nu} = K_{\nu\mu}. \quad (7.7.32)$$

It follows quickly from the definition of the extrinsic curvature tensor that it contains no components orthogonal to $\partial\mathbb{M}$:

$$K_{\mu\nu} n^\nu = n^\nu \nabla_\mu n_\nu - \varepsilon n_\mu n^\nu \nabla_n n_\nu = \nabla_\mu \left(\frac{1}{2} n^\nu n_\nu \right) - \varepsilon n_\mu \nabla_n \left(\frac{1}{2} n^\nu n_\nu \right) = 0 \quad (7.7.33)$$

because $n^\mu n_\mu = \varepsilon$, which is constant.

The only scalar that can be made out of only a single power of the extrinsic curvature tensor is the extrinsic curvature scalar K defined by:

$$K = g^{\mu\nu} K_{\mu\nu}. \quad (7.7.34)$$

Explicitly in terms of the unit normal:

$$K = \nabla^\mu n_\mu - \varepsilon n^\mu \nabla_n n_\mu = \nabla^\mu n_\mu - \varepsilon \nabla_n \left(\frac{1}{2} n^\mu n_\mu \right) = \nabla^\mu n_\mu. \quad (7.7.35)$$

Now let us study the variations of this scalar due to variations of the metric which vanish on $\partial\mathbb{M}$ and for which $\nabla_n \delta g^{\mu\nu}$ may be nonzero. Under variations of the metric, the function which defines $\partial\mathbb{M}$ is unchanged and so:

$$\delta\zeta = 0 \implies \delta k_\mu = 0 \implies \delta M = \frac{\varepsilon}{2M} \delta g^{\mu\nu} k_\mu k_\nu = \frac{\varepsilon}{2} M \delta g^{\mu\nu} n_\mu n_\nu \quad (7.7.36)$$

$$\implies \delta n_\mu = \frac{\varepsilon k_\mu}{M^2} \delta M = -\frac{\varepsilon}{2} n_\mu n_\rho n_\sigma \delta g^{\rho\sigma} = \frac{\varepsilon}{2} n_\mu n^\rho n^\sigma \delta g_{\rho\sigma}. \quad (7.7.37)$$

Finally then, for our metric variations (using (7.7.22)):

$$\delta K = \delta g^{\mu\nu} \nabla_\mu n_\nu + g^{\mu\nu} (\partial_\mu \delta n_\nu - \Gamma_{\mu\nu}^\rho \delta n_\rho - \delta \Gamma_{\mu\nu}^\rho n_\rho) \quad (7.7.38)$$

$$= 0 + g^{\mu\nu} \nabla_\mu \delta n_\nu - g^{\mu\nu} n_\rho \frac{1}{2} g^{\rho\sigma} (\nabla_\mu \delta g_{\sigma\nu} + \nabla_\nu \delta g_{\sigma\mu} - \nabla_\sigma \delta g_{\mu\nu}) \quad (7.7.39)$$

$$= \nabla^\mu \left(\frac{\varepsilon}{2} n_\mu n^\rho n^\sigma \delta g_{\rho\sigma} \right) - \frac{1}{2} g^{\mu\nu} n^\rho (\varepsilon n_\mu \nabla_n \delta g_{\rho\nu} + \varepsilon n_\nu \nabla_n \delta g_{\rho\mu} - \varepsilon n_\rho \nabla_n \delta g_{\mu\nu}) \quad (7.7.40)$$

$$= \frac{\varepsilon}{2} \nabla^\mu (n_\mu n^\rho n^\sigma) \delta g_{\rho\sigma} + \frac{\varepsilon}{2} n^\rho n^\sigma \nabla_n \delta g_{\rho\sigma} - \frac{\varepsilon}{2} n^\rho n^\sigma \nabla_n \delta g_{\rho\sigma} - \frac{\varepsilon}{2} n^\rho n^\sigma \nabla_n \delta g_{\rho\sigma} + \frac{1}{2} g^{\mu\nu} \nabla_n \delta g_{\mu\nu} \quad (7.7.41)$$

$$= \frac{1}{2} \gamma^{\mu\nu} \nabla_n \delta g_{\mu\nu} \quad (7.7.42)$$

which is precisely of the same form as (7.7.24)! Therefore (because under our variations the measure $d\Sigma$ is not changed since the metric on $\partial\mathbb{M}$ is not changed), we can rewrite (7.7.25) as:

$$\delta \left(S_{\text{EHn}} + \int_{\partial\mathbb{M}} \frac{\varepsilon K}{\Omega} d\Sigma \right) = \int_{\mathbb{M}} \frac{1}{2\Omega} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right) \delta g^{\mu\nu} d\mathbb{T} \quad (7.7.43)$$

which is now a well-defined first-order variational principle!

We could simply add the extrinsic curvature scalar surface integral to the naive Einstein Hilbert action and call it good as it gives a valid coordinate invariant variational principle. However, it is convenient to include another term which will not depend on the actual metric but which does shift the numerical value of the action. Typically, the K boundary term diverges when we consider the action over all of space between two finite times. To see why, let us see what already happens in flat Minkowski spacetime. Consider the region $\mathbb{M}$ to be a finite ball of radius ℓ in space at each time between an initial and final time. That is:

$$\mathbb{M} = \{(t, x, y, z) : t_0 < t < t_f, x^2 + y^2 + z^2 < \ell^2\} \quad (7.7.44)$$

for some constant ℓ . Then, $\partial\mathbb{M}$ is topologically a cylinder. The end-caps are the surfaces $\zeta(X) = t - t_0 \stackrel{!}{=} 0$ and $\zeta(X) = t - t_f \stackrel{!}{=} 0$ which give constant normal vectors and vanishing extrinsic curvature. However, the cylindrical shell is the surface $\zeta(X) = x^2 + y^2 + z^2 - \ell^2 \stackrel{!}{=} 0$ which gives:

$$k_\mu = -\nabla_\mu \zeta = (0, -2x, -2y, -2z)_\mu \implies M = 2\ell \implies n_\mu = \left(0, \frac{x}{\ell}, \frac{y}{\ell}, \frac{z}{\ell}\right)_\mu \quad (7.7.45)$$

$$\implies K = \nabla^\mu n_\mu = \frac{2}{\ell} \quad (7.7.46)$$

$$\implies \int_{\partial\mathbb{M}} \frac{\varepsilon K}{\Omega} d\Sigma = \frac{8\pi\ell}{\Omega} (t_f - t_0). \quad (7.7.47)$$

If a large region of space is considered (and so $\ell \rightarrow \infty$), this integral diverges. It is precisely the spatial boundary behavior that causes the divergence of the K integral. Therefore, if we only include K in our boundary term, the resulting variational principle is reasonable but the value of the action is typically $+\infty$ (this also leads to the value of the Hamiltonian, meaning the energy, being $+\infty$).

The spacetime vacuum⁴ $\mathbb{T}_0$ is defined as the spacetime with the maximally symmetric metric that comes from the complete absence of any external fields (and so with $T_{\mu\nu} = 0$ everywhere at all times). This is exactly

⁴A very confusing point is that vacuum is often used with two different meanings. It is common to use vacuum to mean the state of lowest energy of a system, which typically is also highly symmetric. It is also common to call a solution to equations of motion a vacuum solution if it solves the “source-free” equations. For example, an electromagnetic plane-wave is a “vacuum solution” to Maxwell’s equations (no current) in this second sense but only $A_\mu = 0$ (up to a gauge choice) is the electromagnetic vacuum in the first sense. We will try to consistently use vacuum in the first sense and call the second sense source-free.

like the electromagnetic vacuum $A_\mu = 0$, which comes from the maximally symmetric vector potential in the complete absence of any external current. We will see soon that if $\Lambda = 0$ then $\mathbb{T}_0$ is simply Minkowski space. Maximally symmetric here precisely means the metric which has the highest possible number of symmetries (Killing vectors). In all but one context, we always consider matter and energy to only be in a bounded finite (compact) region of space. Then, far from that source, spacetime will limit to $\mathbb{T}_0$ (as sufficiently far away from the source it cannot have had any effect). If we imagined the surface $\partial\mathbb{M}$ characterized by the constraint $\zeta(X) = 0$ to be hypothetically embedded in $\mathbb{T}_0$ rather than the physical spacetime $\mathbb{T}$, it would have some extrinsic curvature scalar K_0 . This K_0 then only depends on the metric of $\mathbb{T}_0$ and not the actual physical metric, so we can define the **Gibbons-Hawking-York boundary term**:

$$S_{\text{GHY}} = \int_{\partial\mathbb{M}} \frac{\varepsilon(K - K_0)}{\Omega} d\Sigma \quad (7.7.48)$$

and the inclusion of K_0 will not affect our equations of motion at all. However, K_0 has the convenient effect that while the integral of K over $\partial\mathbb{M}$ typically diverges, the integral of $K - K_0$ converges for compact energy-momentum tensors, giving the action and the energy finite reasonable values.

The only context in which $\mathbb{T}_0$ cannot be defined is cosmology. The extremely large scale behavior of the universe is approximately homogeneous and isotropic with energy, momentum, and matter all throughout essentially uniformly in space (once small scale stuff like you and everything you love and another 25 or so orders of magnitude past that are averaged out). Consequently, in cosmological models the universe is not asymptotically a source-free solution because the source term never decays away. The result is that there is no reasonable choice of $\mathbb{T}_0$ and thus no K_0 to be subtracted. This gives a value of $+\infty$ for the action and for the energy, but that should seem obvious. Of course the energy of an infinitely large homogeneous system is infinite!⁵

With all of these pieces, we can finally write the full **Einstein-Hilbert action**:

$$S_{\text{EH}} = \int_{\mathbb{M}} \left(\frac{R}{2\Omega} - \frac{\Lambda}{\Omega} \right) d\mathbb{T} + \int_{\partial\mathbb{M}} \frac{\varepsilon}{\Omega} (K - K_0) d\Sigma \quad (7.7.49)$$

which has metric variation:

$$\frac{1}{\sqrt{-\det g}} \frac{\delta S_{\text{EH}}}{\delta g^{\mu\nu}} = \frac{1}{2\Omega} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right). \quad (7.7.50)$$

Let S be the full action for our theory, which we then write as $S_\phi[\phi, g]$, the action for our non-metric fields for a given metric, plus S_{EH} , the action for our metric when free:

$$S[\phi, g] = S_\phi[\phi, g] + S_{\text{EH}}[g]. \quad (7.7.51)$$

The stationary variation of our action combined with (7.6.134) and (7.7.50) gives:

$$\frac{\delta S}{\delta g^{\mu\nu}} = \frac{\delta S_\phi}{\delta g^{\mu\nu}} + \frac{\delta S_{\text{EH}}}{\delta g^{\mu\nu}} \stackrel{!}{=} 0 \quad (7.7.52)$$

$$\Rightarrow -\frac{1}{2} T_{\mu\nu} + \frac{1}{2\Omega} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right) \stackrel{!}{=} 0 \quad (7.7.53)$$

$$\Rightarrow \boxed{R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} = \Omega T_{\mu\nu}}. \quad (7.7.54)$$

This final equation is known as **Einstein's equation** or (pluralized because it has multiple components) **Einstein's field equations**. These are the equations of motion for gravity, as fundamental to gravity as Maxwell's equations are to electromagnetism. Although Kepler wrote the opening quote to this chapter in 1601, we see how fundamental his insight would be proven to be by Einstein in 1915. Einstein's equations determine the geometry of spacetime (the metric, through the Ricci tensor) from the matter, energy, and momentum present in spacetime (through the energy-momentum tensor). Where there is matter, there is geometry. The constants Ω and Λ remain, at this point in our analysis, undetermined physical constants to be fixed by experiments and the nonrelativistic limit.

We found in the Belinfante-Rosenfeld theorem 7.4 that the energy-momentum tensor is automatically

⁵You will sometimes hear people say cosmology violates energy conservation, which is an unhelpful way to think. General relativity guarantees local covariant conservation of energy-momentum. The issue is that in cosmology the total energy of the system in consideration is by any reasonable definition infinite and there is no natural way to regulate it to a finite value. Everywhere and at all times energy is conserved, its just that the total energy of the model isn't a finite number.

covariant conserved. For consistency of the equations of motion then, we need the left-hand side of Einstein's equations to also be covariantly conserved. Using the contracted Ricci identity:

$$\nabla^\rho R_{\rho\sigma} = \frac{1}{2} \nabla_\sigma R \quad (7.7.55)$$

we automatically have:

$$\nabla^\nu (R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu}) = 0 \quad (7.7.56)$$

and so the covariant conservation of the energy-momentum tensor is in fact consistent with Einstein's equations (just as Maxwell's equations $\nabla_\nu \mathcal{F}^{\mu\nu} = J^\mu$ are automatically consistent with the covariant conservation of charge $\nabla_\mu J^\mu = 0$).

7.7.2 Cosmological Constant

Let us study the spacetime vacuum $\mathbb{T}_0$. Consider the metric in the absence of any external sources. Then, $T_{\mu\nu} = 0$ and we have:

$$R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} = 0. \quad (7.7.57)$$

Then, the trace of this equation gives:

$$R = 4\Lambda \quad (7.7.58)$$

$$\implies R_{\mu\nu} = \Lambda g_{\mu\nu}. \quad (7.7.59)$$

Therefore, for a nonzero cosmological constant Λ , the vacuum spacetime is **NOT** Minkowski space (because Minkowski space has $R_{\mu\nu} = 0$). Due to the experimental success of Minkowski spacetime when gravitational effects are not significant, the cosmological constant must be small enough to have negligible effects on spacetime at the level of such experiments. Let us now understand precisely what the vacuum does look like in the presence of a cosmological constant to see what this requires.

Einstein's equations alone are not enough to fully determine the spacetime, as initial and boundary conditions have to be supplied (just as with any other differential equation) and some coordinate conditions have to be imposed to define a coordinate system (the equivalent of picking a gauge in electromagnetism). By the vacuum spacetime we specifically mean the solution to Einstein's equations in the absence of sources which is maximally symmetric. For example, with $\Lambda = 0$, Minkowski spacetime is one of many spacetimes satisfying $R_{\mu\nu} = 0$, but it is the maximally symmetric one in that Minkowski spacetime is additionally the unique Poincare symmetric such solution. With $\Lambda \neq 0$, we enforce the spacetime be maximally symmetric by requiring that it remains translationally and rotationally symmetric⁶.

Because the vacuum is static, we have a time translationally symmetric metric. This is made precise by the metric having a timelike Killing vector. If we define an arbitrary point X_0 to have $t = 0$ as its time coordinate, we can then define the t direction at X_0 as the direction of that timelike Killing vector. By flowing along that timelike Killing vector, we can form a 1-parameter family of points $X(\lambda)$ where λ is the proper time along such a curve. At each λ , all the directions orthogonal to that Killing vector are the spatial tangent directions, and by flowing along all the geodesics beginning at $X(\lambda)$ with initial tangent vectors orthogonal to the timelike Killing vector we form a surface $\Sigma(\lambda)$ of all points at equal time t to our initial point $X(\lambda)$. For now we leave the precise choice of how t is related to λ unspecified. We define our remaining spatial coordinates so that they are unchanged by moving normally between or equally time slices.

Because $t = x^0$ is one of our coordinates, under translations along our Killing vector $x'^0 = x^0 + \varepsilon$ and $x'^a = x^a$, thus giving $\xi^\mu = \delta_0^\mu$. The Killing equation then requires:

$$\nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu \stackrel{!}{=} 0 \quad (7.7.60)$$

$$\implies \partial_\mu g_{0\nu} + \partial_\nu g_{0\mu} - 2\Gamma^\rho_{\mu\nu} g_{0\rho} = 0 \quad (7.7.61)$$

$$\implies \partial_t g_{\mu\nu} = 0. \quad (7.7.62)$$

Therefore, our metric only depends on x^1, x^2, x^3 . Let $\vec{n}$ be the future oriented normal vector to an equal time

⁶A maximally symmetric spacetime is one with the maximum possible number of Killing vectors. For $\Lambda \neq 0$, there remain Killing vectors that are in a sense like Lorentz boosts, however we will not need them in our calculation of what the vacuum solutions look like.

surface, just as in (7.3.30). Then:

$$n^0 = \sqrt{-g^{00}}, \quad n^a = -\frac{g^{0a}}{\sqrt{-g^{00}}}. \quad (7.7.63)$$

Requiring that our spatial coordinates are unchanged by moving normally between time slices means:

$$dX = A\vec{n} \implies dx^a = 0 \quad (7.7.64)$$

$$\implies dx^a = -A \frac{g^{0a}}{\sqrt{-g^{00}}} = 0 \implies g^{0a} = 0. \quad (7.7.65)$$

Thus, our definition of the time coordinate forces the proper time element to take the form:

$$-d\tau^2 = g_{00}(x^1, x^2, x^3)dt^2 + g_{ab}(x^1, x^2, x^3)dx^a dx^b. \quad (7.7.66)$$

Now let us define our spatial coordinates. Consider a particular equal time slice. On that slice, the line element is purely spatial:

$$ds^2 = g_{ab}(x^1, x^2, x^3)dx^a dx^b \quad (7.7.67)$$

and so at each time, the equal time slice appears as the same fixed spatial manifold. Choose a particular arbitrary point in that space to be the origin (due to translational symmetry, all choices are equally good). The tangent space at the origin is a three dimensional Euclidean vector space, and so any unit direction vector can be specified by standard spherical coordinates θ, φ . We then define the spatial coordinates r, θ, φ of a point on the spatial manifold so that θ, φ are the spherical coordinates of the direction of the initial tangent vector of the geodesic which connects the origin and that point and r is some function of the geodesic distance between the origin and that point. At fixed r then, our space is like a spherical shell of some radius $r(r)$ and so the metric at fixed r becomes:

$$ds^2 = r^2(r)(d\theta^2 + \sin^2 \theta d\varphi^2) \quad (dr = 0) \quad (7.7.68)$$

Alternatively, at fixed θ and φ , the geodesic distance per unit r will be some positive function $\sqrt{S(r)}$ so that:

$$\frac{ds}{dr} = \sqrt{S(r)} \implies ds^2 = S(r)dr^2 \quad (d\theta = d\varphi = 0). \quad (7.7.69)$$

The rotational symmetry of the metric enforces $g_{r\theta} = g_{r\varphi} = 0$, and so the full spatial line element becomes:

$$ds^2 = S(r)dr^2 + r^2(r)(d\theta^2 + \sin^2 \theta d\varphi^2). \quad (7.7.70)$$

So far we have been generic about precisely how the r coordinate is defined. The most convenient choice is simply to take $r = r$, the effective spherical shell radius of the spatial manifold at fixed r . Because the definition of our timelike Killing vector and thus time coordinate is also spherically symmetric, g_{00} cannot depend on the angular variables, and thus for some positive function $T(r)$ the full proper time element becomes:

$$-d\tau^2 = -T(r)dt^2 + S(r)dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2. \quad (7.7.71)$$

In deriving (7.7.71) we used time translational symmetry and rotational symmetry about the origin. We never actually enforced space translational symmetry, and so (7.7.71) is the generic form for the proper time element of a spacetime manifold with time translational symmetry and rotational symmetry in appropriate coordinates. Space translational symmetry will appear in our vacuum solution from the fact that the Ricci scalar R is a uniform constant. It is at this point that any sane person begins using a computer to assist with their algebra. With (7.7.71) as our form of the metric and using ' to indicate r derivatives, the resulting nonzero Christoffel symbols are:

$$\begin{aligned} \Gamma^0_{01} &= \frac{T'}{2T}, & \Gamma^1_{00} &= \frac{T'}{2S}, & \Gamma^1_{11} &= \frac{S'}{2S}, & \Gamma^1_{22} &= -\frac{r}{S}, & \Gamma^1_{33} &= -\frac{r \sin^2 \theta}{S}, \\ \Gamma^2_{12} &= \frac{1}{r}, & \Gamma^2_{33} &= -\sin \theta \cos \theta, & \Gamma^3_{13} &= \frac{1}{r}, & \Gamma^3_{23} &= \frac{\cos \theta}{\sin \theta}. \end{aligned} \quad (7.7.72)$$

The resulting Ricci tensor is purely diagonal, with diagonal entries:

$$R_{00} = \frac{T'}{rS} - \frac{S'T'}{4S^2} - \frac{T'^2}{4ST} + \frac{T''}{2S} \quad (7.7.73)$$

$$R_{11} = \frac{S'}{rS} + \frac{S'T'}{4ST} + \frac{T'^2}{4T^2} - \frac{T''}{2T} \quad (7.7.74)$$

$$R_{22} = 1 - \frac{1}{S} + \frac{rS'}{2S^2} - \frac{rT'}{2ST} \quad (7.7.75)$$

$$R_{33} = R_{22} \sin^2 \theta. \quad (7.7.76)$$

Returning these to (7.7.59) with the form of our metric gives:

$$\frac{T'}{rS} - \frac{S'T'}{4S^2} - \frac{T'^2}{4ST} + \frac{T''}{2S} = -\Lambda T \quad (7.7.77)$$

$$\frac{S'}{rS} + \frac{S'T'}{4ST} + \frac{T'^2}{4T^2} - \frac{T''}{2T} = \Lambda S \quad (7.7.78)$$

$$1 - \frac{1}{S} + \frac{rS'}{2S^2} - \frac{rT'}{2ST} = \Lambda r^2. \quad (7.7.79)$$

Multiplying the first of these by S and the second of these by T and then adding those equations gives:

$$T'S + TS' = 0 \implies \frac{\partial}{\partial r}(TS) = 0 \quad (7.7.80)$$

$$\implies S(r) = \frac{A}{T(r)} \quad (7.7.81)$$

for some constant A . Returning this to (7.7.79) and simplifying gives:

$$1 - \frac{T + rT'}{A} = \Lambda r^2 \quad (7.7.82)$$

$$\implies \frac{\partial}{\partial r}(rT) = A(1 - \Lambda r^2) \quad (7.7.83)$$

$$\implies T = \frac{B}{r} + A - \frac{A\Lambda}{3}r^2 \quad (7.7.84)$$

for some constant B . In order for our time coordinate to be well-defined over the whole time slice, we need T to be a regular function on the slice and so $B = 0$. We can still set the overall scale of our time coordinate. We do so by defining that at the spatial origin $r = 0$, if moving only in the t direction, $dt = d\tau$. Thus, $T(0) = A = 1$. So, our proper time element becomes⁷:

$$-d\tau^2 = -\left(1 - \frac{\Lambda r^2}{3}\right) dt^2 + \frac{dr^2}{1 - \frac{\Lambda r^2}{3}} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2. \quad (7.7.85)$$

When $\Lambda = 0$, this is simply Minkowski space in spherical coordinates. When $\Lambda > 0$, this spacetime is known as de Sitter space. We see that in that case there is a finite r at which g_{11} goes to infinity, and so there is a maximum possible r value (and consequently a maximum spatial geodesic distance). When $\Lambda < 0$, this spacetime is known as anti-de Sitter space. We see in either de Sitter or anti-de Sitter space, for r small compared to $\frac{1}{\sqrt{|\Lambda|}}$, the spacetime is effectively Minkowskian and r is effectively the typical radial spatial coordinate of flat space. Thus, $\frac{1}{\sqrt{|\Lambda|}}$ sets a characteristic length scale on which the Minkowskian approximation of the vacuum becomes inaccurate. For very small values of the cosmological constant, Minkowski space is a good approximation to the gravitational vacuum. We will establish in later sections how Λ is measured; its experimental value is found to be positive, but it is sufficiently small that even on the scale of the entire Milky Way Galaxy it is negligible (the experimental value of Λ has $\frac{1}{\sqrt{\Lambda}} \approx 10^{10}$ lightyears while the size of our galaxy is about 10^5 lightyears). Because Λ is so small, we simply neglect it for all but the most cosmological of purposes.

The cosmological constant can be given another interpretation by moving it to the opposite side of Einstein's equations. In the absence of a cosmological constant, Einstein's equations become:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \Omega T_{\mu\nu}. \quad (7.7.86)$$

Alternatively, in the presence of a cosmological constant, they can be written:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \Omega \left(T_{\mu\nu} - \frac{\Lambda}{\Omega} g_{\mu\nu} \right). \quad (7.7.87)$$

We can interpret this as being of the same form as the no-cosmological-constant equation, if we include the

⁷One may worry that we only solved the metric using two independent combinations of the three conditions we found, but you can check directly that in fact our solution satisfies all of (7.7.77)-(7.7.79).

cosmological constant as part of the energy-momentum tensor:

$$T_{\mu\nu}^{\text{total}} = T_{\mu\nu} + T_{\mu\nu}^{\Lambda}, \quad T_{\mu\nu}^{\Lambda} = -\frac{\Lambda}{\Omega} g_{\mu\nu}. \quad (7.7.88)$$

The thinking behind this is that the term in the action which causes the cosmological constant term in the equations of motion is just a constant in the Lagrangian density, and that constant can be shuffled between the action pieces S_{EH} and S_{ϕ} . If we had included Λ in S_{ϕ} , we would have gotten this $T_{\mu\nu}^{\text{total}}$ as the energy-momentum tensor instead of $T_{\mu\nu}$ as we have been writing so far.

We found when studying relativistic fluid mechanics that the energy-momentum tensor of a relativistic perfect fluid of local average 4-velocity u^{μ} , pressure p , and rest frame energy density ε is simply:

$$T_{\mu\nu} = (\varepsilon + p)u_{\mu}u_{\nu} + pg_{\mu\nu}. \quad (7.7.89)$$

The energy-momentum tensor $T_{\mu\nu}^{\Lambda}$ due to the cosmological constant is precisely of this form but with:

$$\varepsilon = -p = \frac{\Lambda}{\Omega}. \quad (7.7.90)$$

Therefore, the cosmological constant can be thought of as providing spacetime with a completely homogeneous vacuum energy density and an equal in magnitude homogeneous negative pressure. The homogeneous vacuum energy density due to the cosmological constant is called **dark energy**, which is an unnecessarily mysterious sounding but standard name. The negative pressure due to the cosmological constant causes the universe to expand, which we will study later in the homework.

7.7.3 Newtonian Limit

We still need to determine the value of the constant Ω which appears in Einstein's equations precisely as the constant which controls the strength with which energy-momentum influences the gravitational field. Thus, one may reasonably expect that Ω is somehow related to Newton's gravitational constant G , which controls the strength with which mass influences the gravitational field in Newton's theory. This expectation is correct and in this subsection we will find the precise relationship.

Because Newton's gravity is successful on "small" (cosmologically speaking) scales, like for the Earth's orbit around the Sun, the cosmological constant term Λ can be neglected, so that Einstein's equations reduce to:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \Omega T_{\mu\nu}. \quad (7.7.91)$$

Contracting both sides with $g^{\mu\nu}$ gives:

$$-R = \Omega g^{\mu\nu} T_{\mu\nu} \quad (7.7.92)$$

so that Einstein's equations can equivalently be written in so-called "trace-reversed form" as:

$$R_{\mu\nu} = \Omega \left(T_{\mu\nu} - \frac{1}{2} T^{\rho\sigma} g_{\rho\sigma} g_{\mu\nu} \right). \quad (7.7.93)$$

This form is convenient because it decouples the different components of the Ricci tensor from each other.

Several approximations must be made in order to take the Newtonian limit of Einstein's equations. Let us consider the energy-momentum tensor of matter at very low speeds (so that we can take the nonrelativistic limit). For completely noninteracting matter which is all at rest in Minkowski space, the energy density of the matter is simply the mass density ρ , the 4-velocity is simply $u^{\mu} = \delta_0^{\mu}$, and the spatial components of the stress tensor T^{ab} all vanish (T^{ab} must be proportional to the identity due to the rotational symmetry of the physical scenario; that proportionality constant is the pressure which is then 0 due to the assumption of noninteraction). So, in Minkowski space the nonrelativistic approximation of the energy-momentum tensor is:

$$T_{\mu\nu} = \rho u_{\mu} u_{\nu}. \quad (7.7.94)$$

This gives the trace-reversed expression:

$$T_{\mu\nu} - \frac{1}{2} T^{\rho\sigma} g_{\rho\sigma} g_{\mu\nu} = \rho u_{\mu} u_{\nu} + \frac{\rho}{2} g_{\mu\nu}. \quad (7.7.95)$$

In order to achieve the Newtonian limit, we also need spacetime to be nearly flat, as only for weak gravitational fields does the relativistic particle Hamiltonian reduce to the Newtonian particle Hamiltonian in (7.3.44). From (7.3.42) and (7.3.45), the Newtonian scalar potential ϕ appears in the metric through the lapse function L and we found that at lowest order in the nonrelativistic limit only that component of the

metric influences particle motion. Using (7.3.22), the lowest order nonrelativistic approximation of the metric is then:

$$g_{00} = -1 - 2\phi, \quad g_{0a} = 0, \quad g_{ab} = \delta_{ab} + \delta\gamma_{ab}. \quad (7.7.96)$$

Because only ϕ contributes to the particle equation of motion in the Newtonian limit, ϕ is the only piece of the metric we care about in that limit.

Because in the nonrelativistic limit the matter is effectively stationary, the full physical scenario is approximately static and so we approximate ϕ and $\delta\gamma_{ab}$ as time independent: $\phi = \phi(x, y, z)$, $\delta\gamma_{ab} = \delta\gamma_{ab}(x, y, z)$. To lowest order, the resulting Christoffel symbols are:

$$\begin{aligned} \Gamma^0_{00} &= 0, & \Gamma^0_{0a} &= \partial_a \phi, & \Gamma^0_{ab} &= 0 \\ \Gamma^a_{00} &= \delta^{ab} \partial_b \phi, & \Gamma^a_{0b} &= 0, & \Gamma^a_{bc} &= \frac{1}{2} \delta^{ad} (\partial_b \delta\gamma_{dc} + \partial_c \delta\gamma_{db} - \partial_d \delta\gamma_{bc}). \end{aligned} \quad (7.7.97)$$

These give the resulting lowest order Ricci tensor:

$$R_{00} = \partial_x^2 \phi + \partial_y^2 \phi + \partial_z^2 \phi, \quad R_{0a} = 0, \quad R_{ab} = \text{Complicated}. \quad (7.7.98)$$

Conveniently, R_{00} depends only on ϕ . The 00 component of the trace reversed Einstein's equations then becomes at lowest order:

$$R_{00} = \Omega \left(T_{00} - \frac{1}{2} T^{\rho\sigma} g_{\rho\sigma} g_{00} \right) \quad (7.7.99)$$

$$\implies \partial_x^2 \phi + \partial_y^2 \phi + \partial_z^2 \phi = \frac{\Omega}{2} \rho \quad (7.7.100)$$

(where on the right hand side we approximated $g_{\mu\nu} = \eta_{\mu\nu}$ because with both ρ and $\delta g_{\mu\nu}$ first order, $\rho \delta g_{\mu\nu}$ is second order). In order for this to match the equation of motion for Newton's gravitational scalar potential in (3.6.3) we must have:

$$\frac{\Omega}{2} = 4\pi G \implies \boxed{\Omega = 8\pi G}. \quad (7.7.101)$$

The remaining components of Einstein's equations determine the evolution of $\delta\gamma_{ab}$.

With all of this, we can finally state:

Theorem 7.5: Einstein-Hilbert Action

The lowest order diffeomorphism symmetric action for the spacetime metric $g_{\mu\nu}$ interacting with some fields ϕ^a on a region $\mathbb{M}$ of spacetime is:

$$S[g, \phi] = \int_{\mathbb{M}} \left(\frac{R}{16\pi G} - \frac{\Lambda}{8\pi G} \right) d\mathbb{T} + \int_{\partial\mathbb{M}} \frac{\varepsilon(K - K_0)}{8\pi G} d\Sigma + S_\phi[g, \phi] \quad (7.7.102)$$

where R is the Ricci scalar, G is Newton's gravitational constant, Λ is the cosmological constant, K is the extrinsic curvature of the surface $\partial\mathbb{M}$ in spacetime, K_0 is the extrinsic curvature of the surface $\partial\mathbb{M}$ when in vacuum, and S_ϕ is the action of the fields ϕ^a at fixed spacetime metric. The metric variation of this action gives Einstein's field equations:

$$\frac{1}{\sqrt{-\det g}} \frac{\delta S}{\delta g^{\mu\nu}} = \frac{1}{16\pi G} \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} \right) - \frac{1}{2} T_{\mu\nu} \stackrel{!}{=} 0 \quad (7.7.103)$$

$$\implies R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G T_{\mu\nu} \quad (7.7.104)$$

where $T_{\mu\nu}$ is the energy-momentum tensor of the ϕ fields.

7.7.4 Vierbein Description and the Spin Connection

There is another fundamental perspective one can take in understanding general relativity. We will find later in Part II that the perspective of this section brings gravity into extremely close analogy with all of the other fundamental forces in a highly suggestive way. We found in section 7.2 that it is always possible to go to a coordinate system so that at a given point the metric tensor in those coordinates is simply the Minkowski metric. However, even though the metric at that single point is the Minkowski metric, at other points even nearby it is unlikely to still be so. In coordinates so that $g_{\mu\nu} = \eta_{\mu\nu}$ at the point X_0 , the coordinate basis vectors $\vec{e}_\mu$ are automatically Minkowski basis vectors (as that is precisely what is meant by $g_{\mu\nu} = \eta_{\mu\nu}$). When

we have Minkowski basis vectors, we call them $\vec{e}_A$ where capital Latin indices $A, B, C, \dots$ run from 0 to 3 and indicate Lorentz indices (as opposed to Greek letters which indicate coordinate indices and have no allegiance to a particular metric). In generic coordinates, the $\vec{e}_\mu$ will not be a set of $\vec{e}_A$ but instead some linear combination of them (whose coefficients could be determined by explicitly performing the transformation to the Minkowski metric at the point). Thus, at a generic spacetime point in generic coordinates, we may write:

$$\vec{e}_\mu(X) = V^A{}_\mu(X) \vec{e}_A(X) \quad (7.7.105)$$

where $V^A{}_\mu(X)$ are the coefficients of linear combination relating these two bases of the tangent space at X . The coefficients $V^A{}_\mu(X)$ are called the **vierbein** or **tetrad**.

The choice of $\vec{e}_A(X)$ at each X is not unique, because all that we require of them is that they have the Minkowski metric: $\vec{e}_A \cdot \vec{e}_B = \eta_{AB}$. So, at each X it is possible to perform an arbitrary Lorentz transformation on the Minkowski basis:

$$\vec{e}'_A = L_A{}^B \vec{e}_B \quad (7.7.106)$$

to a new Minkowski basis. Automatically, this transforms the vierbein according to:

$$V'^A{}_\mu = L^A{}_B V^B{}_\mu. \quad (7.7.107)$$

This Lorentz transformation can be chosen independently at each point in spacetime. We can think of this geometrically as there being a copy of the Minkowskian tangent space at each point in spacetime and this arbitrary Lorentz transformation simply reorients that tangent space point by point. We call these internal Lorentz transformations or **Lorentz gauge transformations**.

The vectors $\vec{e}_\mu(X)$ of course themselves transform under a change of coordinates, and so $V^A{}_\mu$ does as well. In particular:

$$\vec{e}'_\mu = \frac{\partial x^\nu}{\partial x'^\mu} \vec{e}_\nu \implies V'^A{}_\mu = \frac{\partial x^\nu}{\partial x'^\mu} V^A{}_\nu \quad (7.7.108)$$

giving that $V^A{}_\mu$ transforms like a Lorentz vector with respect to its Lorentz index under internal Lorentz transformations and transforms like a coordinate derivative under coordinate transformations. Thus, both of its indices are properly placed as superscripts/subscripts.

The metric $g_{\mu\nu}$ can be expressed directly in terms of the vierbein by using that $g_{\mu\nu} = \vec{e}_\mu \cdot \vec{e}_\nu$ and $\eta_{AB} = \vec{e}_A \cdot \vec{e}_B$. Automatically then by (7.7.105):

$$\boxed{g_{\mu\nu} = \eta_{AB} V^A{}_\mu V^B{}_\nu.} \quad (7.7.109)$$

We will always choose to orient (in terms of time direction and parity) our choice of Minkowski basis vectors to align everywhere with the orientation of $\vec{e}_\mu$. This way, the Lorentz transformations $L^A{}_B$ we perform are only from the connected Lorentz group. As a consequence, the vierbein as a 4x4 matrix always has positive determinant (because it relates two bases of the same orientation). Thus:

$$\sqrt{-\det g} = \det V \quad (7.7.110)$$

which nicely simplifies the spacetime volume element. Because the metric can be expressed fully in terms of the vierbein, instead of thinking about general relativity as giving us the equations of motion of the metric, we can instead think of it as giving us the equations of motion of the vierbein. Consequently, we can treat the vierbein as the quantity to be varied in the Einstein-Hilbert action. Because $g_{\mu\nu}$ is related holonomically to the vierbein, the variational principle for the metric and vierbein are identical.

The Lorentz index of the vierbein can be lowered using the Minkowski metric and the coordinate index can be raised using the spacetime metric. Doing so, we can immediately identify:

$$V_A{}^\mu V^A{}_\nu = \eta_{AB} g^{\mu\rho} V^B{}_\rho V^A{}_\nu = g^{\mu\rho} g_{\rho\nu} = \delta^\mu_\nu. \quad (7.7.111)$$

Thus $V_A{}^\mu$ is the matrix inverse of $V^A{}_\mu$. Because left and right matrix inverses coincide:

$$V_B{}^\mu V^A{}_\mu = \delta_B^A. \quad (7.7.112)$$

The vierbein can also be used to change the type of an index from Lorentz to coordinate or the other way around. For example, suppose we have a vector field with coordinate components ϕ^μ . Then, we can define the components ϕ^A by simply converting to the Minkowski basis:

$$\phi = \phi^\mu \vec{e}_\mu = \phi^A \vec{e}_A \implies \phi^A = V^A{}_\mu \phi^\mu. \quad (7.7.113)$$

The same transformation can be performed with tensors of arbitrary rank to find that:

$$\phi^{A_1 \dots A_m}{}_{B_1 \dots B_n} = V^{A_1}{}_{\mu_1} \dots V^{A_m}{}_{\mu_m} V_{B_1}{}^{\nu_1} \dots V_{B_n}{}^{\nu_n} \phi^{\mu_1 \dots \mu_m}{}_{\nu_1 \dots \nu_n}. \quad (7.7.114)$$

The connection can also nicely be expressed in terms of the vierbein. Consider the covariant derivative of $\vec{\epsilon}_A(X)$. Because the result is a vector in the tangent space of the spacetime manifold at X , $\nabla_\mu \vec{\epsilon}_A$ must be expressible as a linear combination of the basis vectors $\vec{\epsilon}_B(X)$. Thus, there exist coefficients $\omega^B_{A\mu}$ so that:

$$\nabla_\mu \vec{\epsilon}_A = \omega^B_{A\mu} \vec{\epsilon}_B. \quad (7.7.115)$$

These connection coefficients $\omega^B_{A\mu}$ are called the **spin connection**. Because we know how to transform between the coordinate and Minkowski bases, we can develop a corresponding transformation between the usual connection coefficients $\Gamma^\rho_{\mu\nu}$ and the spin connection. By using (7.7.105) and the product rule (and that the vierbein coefficients in (7.7.105) are acting as scalar coefficients of linear combination):

$$\omega^B_{A\mu} \vec{\epsilon}_B = \nabla_\mu \vec{\epsilon}_A = \nabla_\mu (V_A^\nu \vec{\epsilon}_\nu) = \partial_\mu V_A^\nu \vec{\epsilon}_\nu + V_A^\nu \nabla_\mu \vec{\epsilon}_\nu = \Gamma^\rho_{\nu\mu} V_A^\nu \vec{\epsilon}_\rho + \partial_\mu V_A^\nu \vec{\epsilon}_\nu \quad (7.7.116)$$

$$\implies \omega^B_{A\mu} = \Gamma^\rho_{\nu\mu} V_A^\nu V^B_\rho + \partial_\mu V_A^\nu V^B_\nu \quad (7.7.117)$$

Now using:

$$\partial_\mu V_A^\nu V^B_\nu = \partial_\mu (V_A^\nu V^B_\nu) - V_A^\nu \partial_\mu V^B_\nu = -V_A^\nu \partial_\mu V^B_\nu \quad (7.7.118)$$

we have:

$$\omega^{AB}_\mu = \Gamma^\rho_{\nu\mu} V^A_\rho V^{B\nu} - V^{B\nu} \partial_\mu V^A_\nu. \quad (7.7.119)$$

Now using theorem 7.1, rewriting $g_{\mu\nu}$ in terms of the vierbein, using the product rule and simplifying, we find:

$$\omega^{AB}_\mu = \frac{1}{2} V^{A\nu} (\partial_\mu V^B_\nu - \partial_\nu V^B_\mu) - \frac{1}{2} V^{B\nu} (\partial_\mu V^A_\nu - \partial_\nu V^A_\mu) - \frac{1}{2} V^{A\rho} V^{B\sigma} V_{C\mu} (\partial_\rho V^C_\sigma - \partial_\sigma V^C_\rho). \quad (7.7.120)$$

Automatically we see that the spin connection satisfies:

$$\omega^{BA}_\mu = -\omega^{AB}_\mu. \quad (7.7.121)$$

We could have anticipated this by using the product rule on the covariant derivative:

$$0 = \partial_\mu \eta_{AB} = \partial_\mu (\vec{\epsilon}_A \cdot \vec{\epsilon}_B) = \nabla_\mu \vec{\epsilon}_A \cdot \vec{\epsilon}_B + \vec{\epsilon}_A \cdot \nabla_\mu \vec{\epsilon}_B = \omega_{BA\mu} + \omega_{AB\mu}. \quad (7.7.122)$$

Thus the antisymmetry of the spin connection is ensured by the metricity of the connection.

Now using the spin connection we can develop the vierbein analog of (7.2.55). By definition, for a vector field ϕ :

$$\nabla_\mu \phi = \nabla_\mu \phi^\nu \vec{\epsilon}_\nu = \nabla_\mu \phi^A \vec{\epsilon}_A \implies \nabla_\mu \phi^A = V^A_\nu \nabla_\mu \phi^\nu \quad (7.7.123)$$

$$\implies \nabla_\mu \phi^A = V^A_\nu (\partial_\mu \phi^\nu + \Gamma^\nu_{\rho\mu} \phi^\rho) = \partial_\mu (V^A_\nu \phi^\nu) - \phi^\nu \partial_\mu V^A_\nu + V^A_\nu \Gamma^\nu_{\rho\mu} \phi^\rho \quad (7.7.124)$$

$$\implies \boxed{\nabla_\mu \phi^A = \partial_\mu \phi^A + \omega^A_{B\mu} \phi^B}. \quad (7.7.125)$$

Performing the same calculation for a tensor of generic rank we find:

$$\boxed{\nabla_\mu \phi^{A_1 \dots A_m}_{B_1 \dots B_n} = \partial_\mu \phi^{A_1 \dots A_m}_{B_1 \dots B_n} + \omega^D_{C\mu} \hat{G}^C_D \phi^{A_1 \dots A_m}_{B_1 \dots B_n}} \quad (7.7.126)$$

precisely as you would expect for the connection in analogy with (7.2.55).

There is another consequence of the metricity of the connection, just like the covariant derivative of the metric vanishes $\nabla_\rho g_{\mu\nu} = 0$, so does the covariant derivative of the vierbein (using (7.7.119)):

$$\nabla_\nu V^A_\mu = \partial_\nu V^A_\mu + \omega^A_{B\nu} V^B_\mu - \Gamma^\rho_{\mu\nu} V^A_\rho \quad (7.7.127)$$

$$= \partial_\nu V^A_\mu + (\Gamma^\rho_{\sigma\nu} V^A_\rho V^B_\sigma - V^B_\sigma \partial_\nu V^A_\rho) V^B_\mu - \Gamma^\rho_{\mu\nu} V^A_\rho \quad (7.7.128)$$

$$\implies \boxed{\nabla_\nu V^A_\mu = 0}. \quad (7.7.129)$$

It is also natural to study the curvature implied by the spin connection. The Riemann curvature tensor is given by the commutator of covariant derivatives as in (7.5.39) and takes a nice component form in (7.5.14) in the coordinate basis. However, we can also find a nice expression for it in the Minkowski basis. Consider a vector field ϕ :

$$[\nabla_\mu, \nabla_\nu] \phi = ([\nabla_\mu, \nabla_\nu] \phi^A) \vec{\epsilon}_A = ([\nabla_\mu, \nabla_\nu] \phi^\rho) \vec{\epsilon}_\rho \quad (7.7.130)$$

$$\implies [\nabla_\mu, \nabla_\nu] \phi^A = V^A_\rho [\nabla_\mu, \nabla_\nu] \phi^\rho = V^A_\rho R^\rho_{\sigma\mu\nu} \phi^\sigma = R^A_{B\mu\nu} \phi^B. \quad (7.7.131)$$

Now use (7.7.125):

$$[\nabla_\mu, \nabla_\nu] \phi^A = \nabla_\mu \nabla_\nu \phi^A - \nabla_\nu \nabla_\mu \phi^A \quad (7.7.132)$$

$$= \partial_\mu \nabla_\nu \phi^A + \omega^A_{B\mu} \nabla_\nu \phi^B - \Gamma^\rho_{\nu\mu} \nabla_\rho \phi^A - \partial_\nu \nabla_\mu \phi^A - \omega^A_{B\nu} \nabla_\mu \phi^B + \Gamma^\rho_{\mu\nu} \nabla_\rho \phi^A \quad (7.7.133)$$

$$= \partial_\mu (\partial_\nu \phi^A + \omega^A_{B\nu} \phi^B) + \omega^A_{B\mu} (\partial_\nu \phi^B + \omega^B_{C\nu} \phi^C) - \partial_\nu (\partial_\mu \phi^A + \omega^A_{B\mu} \phi^B) - \omega^A_{B\nu} (\partial_\mu \phi^B + \omega^B_{C\mu} \phi^C) \quad (7.7.134)$$

$$= (\partial_\mu \omega^A_{B\nu} - \partial_\nu \omega^A_{B\mu} + \omega^A_{C\mu} \omega^C_{B\nu} - \omega^A_{C\nu} \omega^C_{B\mu}) \phi^B. \quad (7.7.135)$$

Thus, the Riemann curvature can be written nicely in terms of the spin connection as:

$$R^A_{B\mu\nu} = \partial_\mu \omega^A_{B\nu} - \partial_\nu \omega^A_{B\mu} + \omega^A_{C\mu} \omega^C_{B\nu} - \omega^A_{C\nu} \omega^C_{B\mu}. \quad (7.7.136)$$

Automatically, the Ricci scalar can be written easily as:

$$R = R^{AB}{}_{\mu\nu} V_A{}^\mu V_B{}^\nu. \quad (7.7.137)$$

Using (7.7.120), (7.7.136), and (7.7.137) we can rewrite the Einstein-Hilbert action purely in terms of the vierbein. Thus, we can formulate general relativity purely as a theory in which a copy of Minkowski space is associated to every point in spacetime and the dynamical variable controls how those different copies are glued together by parallel transport (as the spin connection is determined by the vierbein).

There are several other reformulations of classical general relativity which are equivalent under most circumstances but may differ in extreme physical scenarios. At this time none of these nonminimal reformulations have any experimental evidence favoring them over standard general relativity as presented here.

Exercises

Problem 7.13: Gravitational jump conditions. Suppose we have an energy-momentum tensor which contains a surface density. To be precise, suppose there is a hypersurface Σ defined by a constraint $\zeta(X) = 0$. Let the region of spacetime with $\zeta > 0$ be called $\mathbb{T}_+$ and the region with $\zeta < 0$ be called $\mathbb{T}_-$. Assume the hypersurface is either spacelike or timelike and that the constraint function $\zeta(X)$ is normalized so that when leaving Σ normally, $d\zeta$ corresponds to the geodesic distance of the displacement. By a surface density in the energy-momentum tensor, we mean that $T_{\mu\nu}$ in a neighborhood around Σ can be written in the form:

$$T_{\mu\nu} = T_{\mu\nu}^+ \vartheta(\zeta) + T_{\mu\nu}^- \vartheta(-\zeta) + S_{\mu\nu} \delta(\zeta)$$

where $T_{\mu\nu}^+, T_{\mu\nu}^-, S_{\mu\nu}$ are all smooth. In general in this question we use a superscript $+$ for usual quantities on $\mathbb{T}_+$ and $-$ for quantities on $\mathbb{T}_-$. As well, use square brackets around a quantity in indicate the discontinuity in that quantity when approaching Σ from either side normally:

$$[A] = \lim_{\zeta(X) \rightarrow 0^+} A^+(X) - \lim_{\zeta(X) \rightarrow 0^-} A^-(X).$$

- (a) Show that the normalization of $\zeta(X)$ implies that the unit normal vector in the direction of increasing ζ can be written as:

$$n_\mu = \varepsilon \partial_\mu \zeta.$$

- (b) Let $g_{\mu\nu}^+$ and $g_{\mu\nu}^-$ be the metric on each side of our surface and assume we are using coordinates which are defined continuously across the surface. Explain that the metric can be written:

$$g_{\mu\nu} = g_{\mu\nu}^+ \vartheta(\zeta) + g_{\mu\nu}^- \vartheta(-\zeta)$$

and show that the first derivatives of the metric are:

$$\partial_\rho g_{\mu\nu} = \partial_\rho g_{\mu\nu}^+ \vartheta(\zeta) + \partial_\rho g_{\mu\nu}^- \vartheta(-\zeta) + \varepsilon \delta(\zeta) n_\rho [g_{\mu\nu}].$$

- (c) Explain that because the connection on our spacetime must be well-defined, we must have:

$$[g_{\mu\nu}] = 0.$$

Show that this implies the Christoffel symbols take the form:

$$\Gamma^\rho_{\mu\nu} = \Gamma^{+\rho}_{\mu\nu} \vartheta(\zeta) + \Gamma^{-\rho}_{\mu\nu} \vartheta(-\zeta)$$

where $\Gamma^{\pm\rho}_{\mu\nu}$ are the Christoffel symbols of $g_{\mu\nu}^\pm$. Show that the Riemann tensor in a neighborhood of Σ becomes:

$$R^\rho_{\mu\sigma\nu} = R^{+\rho}_{\mu\sigma\nu} \vartheta(\zeta) + R^{-\rho}_{\mu\sigma\nu} \vartheta(-\zeta) + \varepsilon \delta(\zeta) (n_\sigma [\Gamma^\rho_{\mu\nu}] - n_\nu [\Gamma^\rho_{\mu\sigma}])$$

where $R^{\pm\rho}_{\mu\sigma\nu}$ are the Riemann tensors of $g_{\mu\nu}^\pm$.

(d) Show that Einstein's equations become:

$$R_{\mu\nu}^{\pm} - \frac{1}{2}R^{\pm}g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi GT_{\mu\nu}^{\pm}$$

$$Q_{\mu\nu} - \frac{1}{2}Qg_{\mu\nu} = 8\pi G\varepsilon S_{\mu\nu}$$

where $Q_{\mu\nu}$ and Q are defined by:

$$Q_{\mu\nu} = n_{\rho}[\Gamma^{\rho}_{\mu\nu}] - n_{\nu}[\Gamma^{\rho}_{\rho\mu}], \quad Q = g^{\mu\nu}Q_{\mu\nu}.$$

(e) Explain that because $[g_{\mu\nu}] = 0$ on all of Σ , the tangential derivatives of $g_{\mu\nu}^{+}$ and $g_{\mu\nu}^{-}$ agree on Σ . Let $\gamma_{\mu\nu}$ be the induced metric on Σ lifted to a tensor on spacetime, defined as usual by (7.4.44). Show that:

$$\gamma^{\sigma}_{\rho}[\partial_{\sigma}g_{\mu\nu}] = 0 \implies [\partial_{\rho}g_{\mu\nu}] = \varepsilon n_{\rho}[\partial_n g_{\mu\nu}]$$

where $\partial_n = n^{\mu}\partial_{\mu}$. Show further that:

$$[\Gamma^{\rho}_{\mu\nu}] = \frac{\varepsilon}{2}(n_{\mu}g^{\rho\sigma}[\partial_n g_{\sigma\nu}] + n_{\nu}g^{\rho\sigma}[\partial_n g_{\sigma\mu}] - n^{\rho}[\partial_n g_{\mu\nu}])$$

$$Q_{\mu\nu} = -\frac{1}{2}\gamma^{\rho}_{\mu}\gamma^{\sigma}_{\nu}[\partial_n g_{\rho\sigma}] - \frac{\varepsilon}{2}n_{\mu}n_{\nu}\gamma^{\rho\sigma}[\partial_n g_{\rho\sigma}]$$

$$Q_{\mu\nu} - \frac{1}{2}Qg_{\mu\nu} = -\frac{1}{2}\gamma^{\rho}_{\mu}\gamma^{\sigma}_{\nu}[\partial_n g_{\rho\sigma}] + \frac{1}{2}\gamma^{\rho\sigma}[\partial_n g_{\rho\sigma}]\gamma_{\mu\nu}.$$

Show that Einstein's equations require the surface energy-momentum tensor to be tangent to Σ :

$$S_{\mu\nu}n^{\nu} = 0.$$

(f) Let $K_{\mu\nu}^{\pm}$ be the extrinsic curvature tensor of Σ on each side of Σ . Show that:

$$[K_{\mu\nu}] = \frac{1}{2}\gamma^{\rho}_{\mu}\gamma^{\sigma}_{\nu}[\partial_n g_{\rho\sigma}].$$

Finally then, show that in the presence of the surface density when using coordinates continuously defined across the surface, Einstein's equations give the jump conditions:

$$[g_{\mu\nu}] = 0, \quad [K_{\mu\nu}] - [K]\gamma_{\mu\nu} = -8\pi G\varepsilon S_{\mu\nu}$$

where $K = g^{\mu\nu}K_{\mu\nu}$.

Problem 7.14: Maximally Symmetric Spaces. Let us study Minkowski space ($k = 0$), de-Sitter space ($k > 0$), and anti-de Sitter space ($k < 0$) by the line element:

$$-d\tau^2 = -(1 - kr^2)dt^2 + \frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2$$

where we have replaced the cosmological constant with a generic parameter k . For a vector field ψ with components ψ^{μ} , let $\hat{\psi} = \psi^{\mu}\partial_{\mu}$. $\hat{\psi}$ is often referred to interchangeably with ψ .

(a) Let ξ^{μ} be a Killing vector of our spacetime. Show that the conditions $L_{\xi}g_{\mu\nu} = 0$ in these coordinates require:

$$\begin{aligned} \partial_t \xi^t &= \frac{kr}{1 - kr^2} \xi^r, & \partial_r \xi^t &= \frac{\partial_t \xi^r}{(1 - kr^2)^2}, & \partial_{\theta} \xi^t &= \frac{r^2 \partial_t \xi^{\theta}}{1 - kr^2}, & \partial_{\varphi} \xi^t &= \frac{r^2 \sin^2 \theta}{1 - kr^2} \partial_t \xi^{\varphi}, \\ \partial_r \xi^r &= -\frac{kr \xi^r}{1 - kr^2}, & \partial_r \xi^{\theta} &= -\frac{\partial_{\theta} \xi^r}{r^2(1 - kr^2)}, & \partial_r \xi^{\varphi} &= -\frac{\partial_{\varphi} \xi^r}{r^2 \sin^2 \theta(1 - kr^2)}, \\ \partial_{\theta} \xi^{\theta} &= -\frac{\xi^r}{r}, & \partial_{\theta} \xi^{\varphi} &= -\frac{\partial_{\varphi} \xi^{\theta}}{\sin^2 \theta}, & \partial_{\varphi} \xi^{\varphi} &= -\frac{\xi^r}{r} - \frac{\cos \theta}{\sin \theta} \xi^{\theta}. \end{aligned}$$

(b) Solve these conditions as differential equations. Show that the vector space of solutions to these conditions is 10 dimensional and that it is spanned by the vector fields:

$$\begin{aligned} \hat{H} &= -\partial_t \\ \hat{P}_1 &= \frac{\sqrt{kr}}{\sqrt{1 - kr^2}} \sinh(\sqrt{kt}) \sin \theta \cos \varphi \partial_t + \sqrt{1 - kr^2} \cosh(\sqrt{kt}) \sin \theta \cos \varphi \partial_r \\ &\quad + \frac{\sqrt{1 - kr^2}}{r} \cosh(\sqrt{kt}) \cos \theta \cos \varphi \partial_{\theta} - \frac{\sqrt{1 - kr^2}}{r \sin \theta} \cosh(\sqrt{kt}) \sin \varphi \partial_{\varphi} \end{aligned}$$

$$\begin{aligned}
\hat{P}_2 &= \frac{\sqrt{kr}}{\sqrt{1-kr^2}} \sinh(\sqrt{kt}) \sin \theta \sin \varphi \partial_t + \sqrt{1-kr^2} \cosh(\sqrt{kt}) \sin \theta \sin \varphi \partial_r \\
&\quad + \frac{\sqrt{1-kr^2}}{r} \cosh(\sqrt{kt}) \cos \theta \sin \varphi \partial_\theta + \frac{\sqrt{1-kr^2}}{r \sin \theta} \cosh(\sqrt{kt}) \cos \varphi \partial_\varphi \\
\hat{P}_3 &= \frac{\sqrt{kr}}{\sqrt{1-kr^2}} \sinh(\sqrt{kt}) \cos \theta \partial_t + \sqrt{1-kr^2} \cosh(\sqrt{kt}) \cos \theta \partial_r - \frac{\sqrt{1-kr^2}}{r} \cosh(\sqrt{kt}) \sin \theta \partial_\theta \\
\hat{J}_1 &= -\sin \varphi \partial_\theta - \cos \varphi \frac{\cos \theta}{\sin \theta} \partial_\varphi \\
\hat{J}_2 &= \cos \varphi \partial_\theta - \sin \varphi \frac{\cos \theta}{\sin \theta} \partial_\varphi \\
\hat{J}_3 &= \partial_\varphi \\
\hat{K}_1 &= \frac{r \cosh(\sqrt{kt})}{\sqrt{1-kr^2}} \sin \theta \cos \varphi \partial_t + \sqrt{1-kr^2} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \sin \theta \cos \varphi \partial_r \\
&\quad + \frac{\sqrt{1-kr^2}}{r} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \cos \theta \cos \varphi \partial_\theta - \frac{\sqrt{1-kr^2}}{r \sin \theta} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \sin \varphi \partial_\varphi \\
\hat{K}_2 &= \frac{r \cosh(\sqrt{kt})}{\sqrt{1-kr^2}} \sin \theta \cos \varphi \partial_t + \sqrt{1-kr^2} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \sin \theta \cos \varphi \partial_r \\
&\quad + \frac{\sqrt{1-kr^2}}{r} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \cos \theta \sin \varphi \partial_\theta + \frac{\sqrt{1-kr^2}}{r \sin \theta} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \cos \varphi \partial_\varphi \\
\hat{K}_3 &= \frac{r \cosh(\sqrt{kt})}{\sqrt{1-kr^2}} \cos \theta \partial_t + \sqrt{1-kr^2} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \cos \theta \partial_r - \frac{\sqrt{1-kr^2}}{r} \frac{\sinh(\sqrt{kt})}{\sqrt{k}} \sin \theta \partial_\theta.
\end{aligned}$$

Show that in the Minkowski limit $k \rightarrow 0$, $-\hat{H}$, $\hat{P}_a$, $\hat{J}_a$, and $\hat{K}_a$ precisely correspond to generators of time translations, space translations, rotations, and boosts, with their indices referring to Cartesian coordinates (x, y, z) .

- (c) The 10 symmetry generators of our spacetime form a Lie algebra. Show precisely that their Lie brackets are:

$$\begin{aligned}
\hat{H} \angle \hat{P}_a &= k \hat{K}_a, & \hat{H} \angle \hat{J}_a &= 0, & \hat{H} \angle \hat{K}_a &= \hat{P}_a \\
\hat{P}_a \angle \hat{P}_b &= k \epsilon_{ab}^c \hat{J}_c, & \hat{P}_a \angle \hat{J}_b &= \epsilon_{ab}^c \hat{P}_c, & \hat{P}_a \angle \hat{K}_b &= \hat{H} \delta_{ab} \\
\hat{J}_a \angle \hat{J}_b &= \epsilon_{ab}^c \hat{J}_c, & \hat{J}_a \angle \hat{K}_b &= \epsilon_{ab}^c \hat{K}_c, & \hat{K}_a \angle \hat{K}_b &= -\epsilon_{ab}^c \hat{K}_c
\end{aligned}$$

where ϵ_{ab}^c is used to indicate the antisymmetric symbol $[abc]$ and does not include any metric dependence. Compare these to the Poincare algebra.

7.8 Arnowitt-Deser-Misner Formalism

Now that we have the action for general relativity, we can find the Hamiltonian for gravity. The Hamiltonian formalism explicitly gives time evolution of fields from one equal time slice to another, and so to develop the Hamiltonian for general relativity we need to explicitly choose a time-slicing. Let $t(X)$ be a scalar valued function on spacetime with $\frac{\partial t}{\partial x^0}$ everywhere positive and $\frac{\partial t}{\partial x^\mu}$ a timelike vector. Then, we can think of $t(X)$ as the “time” (according to *some* observer, precisely who we will discuss later) and the set of all points X in spacetime for which $t(X)$ takes a particular value t we call the time slice $\mathbb{S}(t)$. Because $\nabla_\mu t$ is timelike, $\mathbb{S}(t)$ is a spacelike three-dimensional hypersurface (space at fixed time). We will use coordinates y^a for $\mathbb{S}(t)$. Typically, it is convenient to define our x^μ coordinates so that $x^0 = t$ and $x^a = y^a$. Assume we have done so unless stated explicitly otherwise. Then, define again the lapse function L , shift vector N_a , and spatial metric γ_{ab} precisely as before:

$$g_{00} = -L^2 + N^2, \quad g_{0a} = N_a, \quad g_{ab} = \gamma_{ab} \quad (7.8.1)$$

where $N^2 = N^a N_a$, $N^a = \gamma^{ab} N_b$, and $\gamma^{ac} \gamma_{cb} = \delta_b^a$. γ_{ab} is by construction the metric tensor on $\mathbb{S}(t)$. The future oriented unit normal vector n^μ to $\mathbb{S}(t)$ is given by:

$$n^0 = \frac{1}{L}, \quad n^a = -\frac{N^a}{L} \implies n_0 = -L, \quad n_a = 0. \quad (7.8.2)$$

The spatial metric can be lifted to a tensor $\gamma_{\mu\nu}$ on spacetime $\mathbb{T}$ by defining it to agree with the spatial metric when contracted with vectors on $\mathbb{S}(t)$ and to vanish when contracted with vectors orthogonal to $\mathbb{S}(t)$. The result is given by (7.4.44):

$$g_{\mu\nu} = \gamma_{\mu\nu} - n_\mu n_\nu. \quad (7.8.3)$$

Then, the lifted spatial metric automatically satisfies:

$$\gamma^\mu{}_\rho \gamma^\rho{}_\nu = \gamma^\mu{}_\nu \quad (7.8.4)$$

and thus $\gamma^\mu{}_\nu$ acts as a projector of vectors in spacetime into purely spatial vectors. Automatically $\gamma^{\mu\nu}$ satisfies (1) it vanishes whenever any upper index is 0 and (2) it coincides with the already defined spatial tensor when all indices are lower. Any other tensor on $\mathbb{S}(t)$ can be lifted to a tensor on $\mathbb{T}$ by defining the lifted version to satisfy these two properties. The first of these guarantees the tensor is orthogonal to the normal vector n^μ and the second guarantees it matches its own definition on $\mathbb{S}$ alone.

The extrinsic curvature tensor $K_{\mu\nu}$ of the time slice is defined exactly as in (7.7.26) by:

$$K_{\mu\nu} = K_{\nu\mu} = \gamma^\rho{}_\mu \nabla_\nu n_\rho = \nabla_\mu n_\nu + n_\mu n^\rho \nabla_\rho n_\nu \quad (7.8.5)$$

which is symmetric automatically, though not obviously so when looking at this definition. Because $\gamma^\mu{}_\nu n^\nu = 0$, the extrinsic curvature tensor automatically satisfies $K^\mu{}_\nu n^\nu = 0$ and so has:

$$K^{0\mu} = 0 \quad (7.8.6)$$

by using the component expression for n_μ . Thus, $K_{\mu\nu}$ is actually determined fully by the spatial components K_{ab} only, given by:

$$K_{ab} = \nabla_a n_b + n_a n^\rho \nabla_\rho n_b = \partial_a n_b - \Gamma^\rho{}_{ab} n_\rho = L \Gamma^0{}_{ab} \quad (7.8.7)$$

which is plainly symmetric. Explicitly:

$$K_{ab} = L \frac{1}{2} g^{0\rho} (\partial_a g_{\rho b} + \partial_b g_{\rho a} - \partial_\rho g_{ab}) \quad (7.8.8)$$

$$= \frac{L}{2} g^{00} (\partial_a g_{0b} + \partial_b g_{0a} - \partial_0 g_{ab}) + \frac{L}{2} g^{0c} (\partial_a g_{cb} + \partial_b g_{ca} - \partial_c g_{ab}) \quad (7.8.9)$$

$$= \frac{1}{2L} (\dot{\gamma}_{ab} - \partial_a N_b - \partial_b N_a) + \frac{N^c}{2L} (\partial_a \gamma_{cb} + \partial_b \gamma_{ca} - \partial_c \gamma_{ab}). \quad (7.8.10)$$

There is no reason to believe that the covariant derivative of a vector tangent to $\mathbb{S}(t)$ would also be tangent to $\mathbb{S}(t)$. Let us confirm this by calculation. For $\vec{e}_a$ the spatial coordinate basis vectors, the spatial covariant derivatives are given by:

$$\nabla_b \vec{e}_a = \Gamma^\rho{}_{ab} \vec{e}_\rho = \Gamma^0{}_{ab} \vec{e}_0 + \Gamma^c{}_{ab} \vec{e}_c. \quad (7.8.11)$$

The $\vec{e}_0$ is not tangent to $\mathbb{S}(t)$. However, we can define an induced spatial covariant derivative $\mathscr{D}$ by projecting out the component of ordinary covariant differentiation which is orthogonal to $\mathbb{S}(t)$. That is, the combination $\nabla_b \vec{e}_a$ can be decomposed into a piece $(\nabla_b \vec{e}_a)_\parallel$ which is tangent to $\mathbb{S}(t)$ and a piece which is orthogonal

$(\nabla_b \vec{e}_a)_\perp$:

$$\nabla_b \vec{e}_a = (\nabla_b \vec{e}_a)_\parallel + (\nabla_b \vec{e}_a)_\perp. \quad (7.8.12)$$

Then, we define:

$$\mathcal{D}_b \vec{e}_a = (\nabla_b \vec{e}_a)_\parallel. \quad (7.8.13)$$

Because $(\nabla_b \vec{e}_a)_\parallel$ is tangent to $\mathbb{S}(t)$, it can be written as a linear combination of the spatial basis vectors for some **spatial connection coefficients** C^c_{ab} :

$$\mathcal{D}_b \vec{e}_a = C^c_{ab} \vec{e}_c. \quad (7.8.14)$$

With a little calculation:

$$\vec{e}_c \cdot \nabla_b \vec{e}_a = \vec{e}_c \cdot (\nabla_b \vec{e}_a)_\parallel + 0 \quad (7.8.15)$$

$$\implies \vec{e}_c \cdot \nabla_b \vec{e}_a = \vec{e}_c \cdot C^d_{ab} \vec{e}_d = \gamma_{cd} C^d_{ab} \quad (7.8.16)$$

$$\implies C^c_{ab} = \gamma^{cd} \vec{e}_d \cdot \nabla_b \vec{e}_a. \quad (7.8.17)$$

Then, using the Christoffel symbols of our ordinary covariant differentiation:

$$C^c_{ab} = \gamma^{cd} \vec{e}_d \cdot \Gamma^\rho_{ab} \vec{e}_\rho = \gamma^{cd} \Gamma^\rho_{ab} g_{\rho d} \quad (7.8.18)$$

$$= \gamma^{cd} \Gamma^0_{ab} g_{0d} + \gamma^{cd} \Gamma^e_{ab} g_{ed} = \Gamma^0_{ab} N^c + \Gamma^c_{ab} \quad (7.8.19)$$

$$= \Gamma^0_{ab} N^c + \frac{1}{2} g^{c\sigma} (\partial_a g_{\sigma b} + \partial_b g_{\sigma a} - \partial_\sigma g_{ab}) \quad (7.8.20)$$

$$= \Gamma^0_{ab} N^c + \frac{1}{2} g^{c0} (\partial_a g_{0b} + \partial_b g_{0a} - \partial_0 g_{ab}) + \frac{1}{2} g^{cd} (\partial_a g_{db} + \partial_b g_{da} - \partial_d g_{ab}) \quad (7.8.21)$$

$$= K_{ab} \frac{N^c}{L} + \frac{N^c}{2L^2} (\partial_a N_b + \partial_b N_a - \dot{\gamma}^a) + \frac{1}{2} \gamma^{cd} (\partial_a \gamma_{db} + \partial_b \gamma_{da} - \partial_d \gamma_{ab}) - \frac{N^c N^d}{2L^2} (\partial_a \gamma_{db} + \partial_b \gamma_{da} - \partial_d \gamma_{ab}) \quad (7.8.22)$$

$$= K_{ab} \frac{N^c}{L} - K_{ab} \frac{N^c}{L} + \frac{1}{2} \gamma^{cd} (\partial_a \gamma_{db} + \partial_b \gamma_{da} - \partial_d \gamma_{ab}). \quad (7.8.23)$$

Thus, the induced spatial connection coefficients are:

$$C^c_{ab} = \frac{1}{2} \gamma^{cd} (\partial_a \gamma_{db} + \partial_b \gamma_{da} - \partial_d \gamma_{ab}) \quad (7.8.24)$$

which is precisely the Levi-Civita connection on the time slice! With these connection coefficients, automatically the spatial covariant derivative of any spatial tensor ϕ^a is given by:

$$\mathcal{D}_b \phi^a = \partial_b \phi^a + C^d_{cb} \hat{G}^c_d \phi^a. \quad (7.8.25)$$

By thinking of the shift vector as a spatial vector then, we can write the extrinsic curvature more simply as:

$$K_{ab} = \frac{1}{2L} (\dot{\gamma}_{ab} - \partial_a N_b - \partial_b N_a) + \frac{N_c}{L} C^c_{ab} \quad (7.8.26)$$

$$\implies K_{ab} = \frac{1}{2L} (\dot{\gamma}_{ab} - \mathcal{D}_a N_b - \mathcal{D}_b N_a). \quad (7.8.27)$$

We can lift spatial covariant derivatives on spatial tensors to be spacetime tensors by the usual lifting procedure. Let f^a be a spatial vector field and let f^μ be its lifted version. Then by definition:

$$f^0 = \mathcal{D}^0 f^0 = \mathcal{D}^0 f^a = \mathcal{D}^a f^0 = 0, \quad \mathcal{D}^b f^a = \gamma^{bc} \mathcal{D}_c f^a \quad (7.8.28)$$

where $\mathcal{D}_c f^a$ is already defined by using the spatial connection coefficients. Because the spatial connection is defined simply by projecting onto only the spatial components, we should expect that this lifting is equivalent to taking the ordinary covariant derivative and then projecting spatially on each component. Let us confirm this. Consider that projection, meaning $\gamma^{\nu\sigma} \gamma^\mu_\rho \nabla_\sigma f^\rho$. Because $\gamma^{0\mu} = 0$, we have:

$$\gamma^{0\sigma} \gamma^0_\rho \nabla_\sigma f^\rho = \mathcal{D}^0 f^0 \quad (7.8.29)$$

$$\gamma^{0\sigma} \gamma^a_\rho \nabla_\sigma f^\rho = \mathcal{D}^0 f^a \quad (7.8.30)$$

$$\gamma^{a\sigma} \gamma^0_\rho \nabla_\sigma f^\rho = \mathcal{D}^a f^0. \quad (7.8.31)$$

The double spatial combination is the only interesting one:

$$\gamma^{b\sigma} \gamma^a_\rho \nabla_\sigma f^\rho = \gamma^{bd} \gamma^a_0 \nabla_d f^0 + \gamma^{bd} \gamma^a_c \nabla_d f^c \quad (7.8.32)$$

$$= \gamma^{bd} N^a (\partial_d f^0 + \Gamma^0_{cd} f^c) + \gamma^{bd} \delta^a_c \nabla_d f^c \quad (7.8.33)$$

$$= \gamma^{bd} N^a \frac{K_{cd}}{L} f^c + \gamma^{bd} (\partial_d f^a + \Gamma^a_{d\rho} f^\rho) \quad (7.8.34)$$

$$= -\frac{N^a}{L} K^b_c f^c + \gamma^{bc} \left(\partial_c f^a + C^a_{cd} f^d - \frac{N^a}{L} K_{cd} f^d \right) \quad (7.8.35)$$

$$= \gamma^{bc} \mathcal{D}_c f^a = \mathcal{D}^b f^a. \quad (7.8.36)$$

Therefore, identically as a tensor equation:

$$\mathcal{D}_\nu f^\mu = \gamma^\mu_\rho \gamma^\sigma_\nu \nabla_\sigma f^\rho \quad (7.8.37)$$

for all spatial vector fields lifted onto spacetime. The same process repeats itself for each spatial index, so that any spatial tensor field $\phi^{a_1 \dots a_m}_{b_1 \dots b_n}$ which is lifted to a spacetime tensor field $\phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n}$ then has spatial covariant derivatives given by:

$$\boxed{\mathcal{D}_\mu \phi^{\rho_1 \dots \rho_m}_{\sigma_1 \dots \sigma_n} = \gamma^\nu_\mu \gamma^{\rho_1}_{\alpha_1} \dots \gamma^{\rho_m}_{\alpha_m} \gamma^{\beta_1}_{\sigma_1} \dots \gamma^{\beta_n}_{\sigma_n} \nabla_\nu \phi^{\alpha_1 \dots \alpha_m}_{\beta_1 \dots \beta_n}.} \quad (7.8.38)$$

Because $\mathcal{D}_a$ is the Levi-Civita connection corresponding to γ_{ab} , it automatically satisfies metric compatibility with the spatial metric:

$$\mathcal{D}_c \gamma_{ab} = 0 \quad (7.8.39)$$

and so factors of γ_{ab} commute with $\mathcal{D}_c$. This even remains true of the lifted tensors by using that $\gamma_{\mu\nu} n^\nu = 0$:

$$\mathcal{D}_\rho \gamma_{\mu\nu} = \gamma^\sigma_\rho \gamma^\alpha_\mu \gamma^\beta_\nu \nabla_\sigma \gamma_{\alpha\beta} \quad (7.8.40)$$

$$= \gamma^\sigma_\rho \gamma^\alpha_\mu \gamma^\beta_\nu \nabla_\sigma (g_{\alpha\beta} + n_\alpha n_\beta) \quad (7.8.41)$$

$$= \gamma^\sigma_\rho \gamma^\alpha_\mu \gamma^\beta_\nu (n_\alpha \nabla_\sigma n_\beta + n_\beta \nabla_\sigma n_\alpha) \quad (7.8.42)$$

$$= 0. \quad (7.8.43)$$

Thus for all spatial tensor fields ϕ , $\mathcal{D}_\rho(\gamma_{\mu\nu}\phi) = \gamma_{\mu\nu}\mathcal{D}_\rho\phi$. Importantly, $\mathcal{D}_\rho\phi$ is only defined for ϕ which are (lifted versions of) spatial tensor fields.

Let $\mathcal{R}^d_{acb}$ be the spatial Riemann curvature tensor, so that for any spatial vector field:

$$[\mathcal{D}_c, \mathcal{D}_b]f^d = \mathcal{R}^d_{acb}f^a. \quad (7.8.44)$$

Lifting all tensors to spacetime indices gives automatically:

$$[\mathcal{D}_\sigma, \mathcal{D}_\nu]f^\rho = \mathcal{R}^\rho_{\mu\sigma\nu}f^\mu. \quad (7.8.45)$$

It is important to note that this only holds for all vector fields f^μ which are lifted versions of purely spatial vector fields f^a . We can make this purely generic by considering a generic spacetime vector field ξ^μ from which we can define a spatial vector field ξ^a which when lifted back to a spacetime vector field is $\gamma^\mu_\nu \xi^\nu$. Thus, for all ξ^μ :

$$[\mathcal{D}_\sigma, \mathcal{D}_\nu](\gamma^\rho_\mu \xi^\mu) = \mathcal{R}^\rho_{\mu\sigma\nu} \gamma^\mu_\lambda \xi^\lambda. \quad (7.8.46)$$

Using the (7.4.44):

$$\nabla_\alpha \gamma^\rho_\beta = \nabla_\alpha (\delta^\rho_\beta + n^\rho n_\beta) = \nabla_\alpha n^\rho n_\beta + n^\rho \nabla_\alpha n_\beta. \quad (7.8.47)$$

Then, with a bit of computational effort we find:

$$\mathcal{D}_\sigma \mathcal{D}_\nu (\gamma^\rho_\mu \xi^\mu) = \gamma^\rho_\lambda \gamma^\alpha_\sigma \gamma^\beta_\nu \nabla_\alpha \mathcal{D}_\beta (\gamma^\lambda_\mu \xi^\mu) = \gamma^\rho_\lambda \gamma^\alpha_\sigma \gamma^\beta_\nu \nabla_\alpha (\gamma^\lambda_\tau \gamma^\omega_\beta \nabla_\omega (\gamma^\tau_\mu \xi^\mu)) \quad (7.8.48)$$

$$= \gamma^\rho_\lambda \gamma^\alpha_\sigma \gamma^\beta_\nu \nabla_\alpha \nabla_\beta (\gamma^\lambda_\mu \xi^\mu) - K^\rho_\sigma K_{\mu\nu} \xi^\mu + \gamma^\rho_\lambda K_{\sigma\nu} \nabla_n (\gamma^\lambda_\mu \xi^\mu). \quad (7.8.49)$$

Returning this to the commutator we have:

$$[\mathcal{D}_\sigma, \mathcal{D}_\nu](\gamma^\rho_\mu \xi^\mu) = \gamma^\rho_\lambda \gamma^\alpha_\sigma \gamma^\beta_\nu [\nabla_\alpha, \nabla_\beta](\gamma^\lambda_\mu \xi^\mu) - K^\rho_\sigma K_{\mu\nu} \xi^\mu + K^\rho_\nu K_{\mu\sigma} \xi^\mu \quad (7.8.50)$$

$$\implies \mathcal{R}^\rho_{\mu\sigma\nu} \gamma^\mu_\lambda \xi^\lambda = \gamma^\rho_\lambda \gamma^\alpha_\sigma \gamma^\beta_\nu R^\lambda_{\tau\alpha\beta} \gamma^\tau_\mu \xi^\mu - K^\rho_\sigma K_{\mu\nu} \xi^\mu + K^\rho_\nu K_{\mu\sigma} \xi^\mu. \quad (7.8.51)$$

Because this holds for all ξ^μ , we finally have that the lifted spatial Riemann tensor $\mathcal{R}_{\dots}$ is related to the spatial projection of the full spacetime Riemann tensor $R_{\dots}$ by:

$$\boxed{\gamma^\rho_\lambda \gamma^\tau_\mu \gamma^\alpha_\sigma \gamma^\beta_\nu R^\lambda_{\tau\alpha\beta} = \mathcal{R}^\rho_{\mu\sigma\nu} + K^\rho_\sigma K_{\mu\nu} - K^\rho_\nu K_{\mu\sigma}.} \quad (7.8.52)$$

Now that we have a good handle on the 3+1 (space+time) decomposition properties of tensorial quantities, let us begin to try to rewrite the Einstein-Hilbert action in this decomposed form. The spacetime volume

element $d\mathbb{T} = \sqrt{-\det g}d^4x = \sqrt{-\det g}dtd^3y$ is our first target. Using the definition of the determinant:

$$\det g = [\mu\nu\rho\sigma]g_{\mu 0}g_{\nu 1}g_{\rho 2}g_{\sigma 3} = [0\nu\rho\sigma]g_{00}g_{\nu 1}g_{\rho 2}g_{\sigma 3} + [a\nu\rho\sigma]g_{0a}g_{1\nu}g_{2\rho}g_{3\sigma} \quad (7.8.53)$$

$$= [abc]g_{00}g_{1a}g_{2b}g_{3c} - [0a\rho\sigma]g_{0a}g_{01}g_{2\rho}g_{3\sigma} + [ab\rho\sigma]g_{0a}g_{1b}g_{2\rho}g_{3\sigma} \quad (7.8.54)$$

$$= (-L^2 + N^2) \det \gamma - [abc]N_a N_1 \gamma_{2b} \gamma_{3c} + [0ab\sigma]N_a \gamma_{1b} g_{20} g_{3\sigma} + [abc\sigma]N_a \gamma_{1b} \gamma_{2c} g_{3\sigma} \quad (7.8.55)$$

$$= (-L^2 + N^2) \det \gamma - [abc]N_a N_1 \gamma_{2b} \gamma_{3c} + [abc]N_a N_2 \gamma_{1b} \gamma_{3c} - [abc]N_a N_3 \gamma_{1b} \gamma_{2c} \quad (7.8.56)$$

$$= (-L^2 + N^2) \det \gamma - N_1 N^d [abc] \gamma_{ad} \gamma_{2b} \gamma_{3c} - N_2 N^d [abc] \gamma_{ad} \gamma_{3b} \gamma_{1c} - N_3 N^d [abc] \gamma_{ad} \gamma_{1b} \gamma_{2c} \quad (7.8.57)$$

$$= -L^2 \det \gamma + N^2 \det \gamma - N_1 N^d [d23] \det \gamma - N_2 N^d [d31] \det \gamma - N_3 N^d [d12] \det \gamma \quad (7.8.58)$$

$$= -L^2 \det \gamma + N^2 \det \gamma - (N_1 N^1 + N_2 N^2 + N_3 N^3) \det \gamma \quad (7.8.59)$$

$$\Rightarrow \sqrt{-\det g} = L \sqrt{\det \gamma}. \quad (7.8.60)$$

Therefore, the spacetime measure can be written:

$$\boxed{d\mathbb{T} = L dt d\mathbb{S}} \quad (7.8.61)$$

where the spatial measure is:

$$\boxed{d\mathbb{S} = \sqrt{\det \gamma} d^3y}. \quad (7.8.62)$$

Next let us turn our attention to the Ricci scalar piece of the Lagrangian density. Contracting ρ with σ and a factor of $g^{\mu\nu}$ with (7.8.52):

$$g^{\mu\nu} \gamma^\rho_\lambda \gamma^\tau_\mu \gamma^\alpha_\rho \gamma^\beta_\nu R^\lambda_{\tau\alpha\beta} = \mathcal{R} + K^2 - K^\rho_\sigma K^\sigma_\rho \quad (7.8.63)$$

$$\Rightarrow \gamma^{\alpha\lambda} \gamma^{\tau\beta} R_{\lambda\tau\alpha\beta} = \mathcal{R} + K^2 - K^{ab} K_{ab} \quad (7.8.64)$$

$$\Rightarrow (g^{\alpha\lambda} + n^\alpha n^\lambda)(g^{\beta\tau} + n^\beta n^\tau) R_{\lambda\tau\alpha\beta} = \mathcal{R} + K^2 - K^{ab} K_{ab} \quad (7.8.65)$$

$$\Rightarrow R^{\alpha\beta}_{\alpha\beta} + R^\alpha_{\tau\alpha\beta} n^\tau n^\beta + R_{\lambda\beta}^\beta n^\lambda n^\alpha + R_{\lambda\tau\alpha\beta} n^\lambda n^\tau n^\alpha n^\beta = \mathcal{R} + K^2 - K^{ab} K_{ab} \quad (7.8.66)$$

$$\Rightarrow R + 2R_{\mu\nu} n^\mu n^\nu = \mathcal{R} + K^2 - K^{ab} K_{ab}. \quad (7.8.67)$$

Using the definition of the Riemann tensor:

$$R_{\mu\nu} n^\mu n^\nu = n^\nu [\nabla_\rho, \nabla_\nu] n^\rho = n^\nu \nabla_\rho \nabla_\nu n^\rho - n^\nu \nabla_\nu \nabla_\rho n^\rho \quad (7.8.68)$$

$$= \nabla_\rho (n^\nu \nabla_\nu n^\rho) - \nabla_\rho n^\nu \nabla_\nu n^\rho - \nabla_\nu (n^\nu \nabla_\rho n^\rho) + \nabla_\nu n^\nu \nabla_\rho n^\rho \quad (7.8.69)$$

$$= \nabla_\rho (n^\nu \nabla_\nu n^\rho - n^\rho \nabla_\nu n^\nu) - (K^\nu_\rho - n_\rho n^\alpha \nabla_\alpha n^\nu) (K^\rho_\nu - n_\nu n^\beta \nabla_\beta n^\rho) + (K^\mu_\mu - n^\mu n^\nu \nabla_\nu n_\mu)^2 \quad (7.8.70)$$

$$= \nabla_\rho (n^\nu \nabla_\nu n^\rho - n^\rho \nabla_\nu n^\nu) - K^{ab} K_{ab} + 0 + 0 - n_\rho n^\alpha \nabla_\alpha n^\nu n_\nu n^\beta \nabla_\beta n^\rho + (K - 0)^2 \quad (7.8.71)$$

$$= \nabla_\rho (n^\nu \nabla_\nu n^\rho - n^\rho \nabla_\nu n^\nu) - K^{ab} K_{ab} + K^2. \quad (7.8.72)$$

Thus, the spacetime Ricci scalar is related to the spatial Ricci scalar by:

$$\boxed{R = K^{ab} K_{ab} - K^2 + \mathcal{R} + \nabla_\rho (2n^\rho \nabla_\nu n^\nu - 2n^\nu \nabla_\nu n^\rho)}. \quad (7.8.73)$$

In our time slicing, the spacetime region $\mathbb{M}$ is divided into a family of time slices $\mathbb{S}$ at each time t between some initial and final time, so that a spacetime volume integral becomes:

$$\int_{\mathbb{M}} f(X) d\mathbb{T} = \int_{t_0}^{t_f} \int_{\mathbb{S}(t)} f(X) L d\mathbb{S} dt. \quad (7.8.74)$$

The boundary $\partial\mathbb{M}$ then has three components, the initial time slice $\mathbb{S}_0$, the final time slice $\mathbb{S}_f$, and the cylindrical shell given by the spatial boundary $\partial\mathbb{S}(t)$ at each time between t_0 and t_f . Thus, a boundary integral becomes:

$$\int_{\partial\mathbb{M}} f^\mu(X) d\Sigma_\mu = \int_{\mathbb{S}_0} f^\mu(X) d\Sigma_\mu + \int_{\mathbb{S}_f} f^\mu(X) d\Sigma_\mu + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} f^\mu(X) d\Sigma_\mu. \quad (7.8.75)$$

To avoid ambiguity with the future oriented normal vector n^μ to each time slice, the metric $\gamma_{\mu\nu}$ on each time slice, and the time slice extrinsic curvature tensor $K_{\mu\nu}$, when discussing boundary integrals in this formalism we use n'^μ to mean the oriented normal vector to $\partial\mathbb{M}$, $\gamma'_{\mu\nu}$ to mean the metric on $\partial\mathbb{M}$, and $K'_{\mu\nu}$ to mean the extrinsic curvature tensor of $\partial\mathbb{M}$.

On $\mathbb{S}_f$, the outward pointing normal vector n'^μ coincides with n^μ and so $d\Sigma_\mu = -n_\mu d\mathbb{S}$. On $\mathbb{S}_0$, the outward pointing normal vector n'^μ points opposite to n^μ and so $d\Sigma_\mu = n_\mu d\mathbb{S}$. On the cylindrical shell,

the outward pointing normal vector n'^μ will be a spatial radial vector r^μ . On the shell, we use coordinates $y'^1 = t, y'^2 = \theta^1, y'^3 = \theta^2$. Let σ_{ij} be the induced metric on the spatial boundary $\partial\mathbb{S}$ in terms of the two spatial boundary coordinates θ^i . Then, by repeating precisely the same steps which lead from (7.8.53) to (7.8.60) but for three dimensions:

$$\sqrt{|\det \gamma'|} = \sqrt{-\det \gamma'} = L\sqrt{\det \sigma}. \quad (7.8.76)$$

Thus, taking $d\mathbb{A}$ to be the invariant surface area measure on $\partial\mathbb{S}$:

$$d\mathbb{A} = \sqrt{\det \sigma} d^2\theta \quad (7.8.77)$$

we have that the hypersurface measure $d\Sigma_\mu$ on the cylindrical shell becomes:

$$d\Sigma_\mu = r_\mu \sqrt{|\det \gamma'|} dy'^1 dy'^2 dy'^3 = L r_\mu \sqrt{\det \sigma} dt d\theta^1 d\theta^2 = L r_\mu dt d\mathbb{A}. \quad (7.8.78)$$

So, the boundary integrals can be written as:

$$\int_{\partial\mathbb{M}} f^\mu d\Sigma_\mu = \int_{\mathbb{S}_f} (-f^\mu n_\mu) d\mathbb{S} + \int_{\mathbb{S}_0} f^\mu n_\mu d\mathbb{S} + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} f^\mu r_\mu L d\mathbb{A} dt. \quad (7.8.79)$$

In order to evaluate the boundary term in the Einstein-Hilbert action in our 3+1 decomposition, we need to decompose the extrinsic curvature scalar K' on $\partial\mathbb{M}$. By definition of $K'_{\mu\nu}$, automatically $K' = \nabla_\mu n'^\mu$. On $\mathbb{S}_f$ then $K' = \nabla_\mu n'^\mu = \nabla_\mu n^\mu = K$. On $\mathbb{S}_0$ then $K' = \nabla_\mu n'^\mu = -\nabla_\mu n^\mu = -K$. On the cylindrical shell, $K' = \nabla_\mu r^\mu$. Because r^μ is a spatial vector (it points radially out of $\partial\mathbb{S}$), it satisfies $r^\mu n_\mu = 0$ and has a sensible spatial covariant derivative $\mathcal{D}_a r^b$. Then, we can define the extrinsic curvature tensor κ_{ij} of $\partial\mathbb{S}$ viewed as a surface within $\mathbb{S}$ precisely analogously to the definition of $K_{\mu\nu}$. The extrinsic curvature scalar κ then is given by:

$$\kappa = \mathcal{D}_a r^a. \quad (7.8.80)$$

Because of this:

$$\nabla_\mu r^\mu = g^{\mu\nu} \nabla_\mu r_\nu = (\gamma^{\mu\nu} - n^\mu n^\nu) \nabla_\mu r_\nu \quad (7.8.81)$$

$$= \gamma^\mu{}_\rho \gamma^\rho{}_\nu \nabla_\mu r^\nu - n^\mu \nabla_n r_\mu \quad (7.8.82)$$

$$= \mathcal{D}_\rho r^\rho - \nabla_n (n^\mu r_\mu) + r_\mu \nabla_n n^\mu \quad (7.8.83)$$

$$= \kappa + r_\mu \nabla_n n^\mu. \quad (7.8.84)$$

With all of our ingredients, let us finally decompose the Einstein-Hilbert action:

$$S_{\text{EH}} = \int_{\mathbb{M}} \frac{R - 2\Lambda}{16\pi G} d\mathbb{T} + \int_{\partial\mathbb{M}} \frac{\varepsilon'(K' - K'_0)}{8\pi G} d\Sigma \quad (7.8.85)$$

$$= \int_{\mathbb{M}} \frac{K^{ab} K_{ab} - K^2 + \mathcal{R} - 2\Lambda + \nabla_\mu (2n^\mu \nabla_\nu n^\nu - 2\nabla_n n^\mu)}{16\pi G} d\mathbb{T} + \int_{\mathbb{S}_f} \frac{(-1)(K - K_0)}{8\pi G} d\mathbb{S} \\ + \int_{\mathbb{S}_0} \frac{(-1)(-K + K_0)}{8\pi G} d\mathbb{S} + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} \frac{\kappa + r_\mu \nabla_n n^\mu - K'_0}{8\pi G} L d\mathbb{A} dt \quad (7.8.86)$$

$$= \int_{t_0}^{t_f} \int_{\mathbb{S}} \frac{K^{ab} K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} dt + \int_{\partial\mathbb{M}} \frac{n^\mu \nabla_\nu n^\nu - \nabla_n n^\mu}{8\pi G} d\Sigma_\mu \\ - \int_{\mathbb{S}_f} \frac{K - K_0}{8\pi G} d\mathbb{S} + \int_{\mathbb{S}_0} \frac{K - K_0}{8\pi G} d\mathbb{S} + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} \frac{\kappa + r_\mu \nabla_n n^\mu - K'_0}{8\pi G} L d\mathbb{A} dt \quad (7.8.87)$$

$$= \int_{t_0}^{t_f} \int_{\mathbb{S}} \frac{K^{ab} K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} dt + \int_{\mathbb{S}_f} \frac{n^\mu K - \nabla_n n^\mu}{8\pi G} (-n_\mu) d\mathbb{S} + \int_{\mathbb{S}_0} \frac{n^\mu K - \nabla_n n^\mu}{8\pi G} n_\mu d\mathbb{S} \\ + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}} \frac{n^\mu K - \nabla_n n^\mu}{8\pi G} r_\mu d\Sigma - \int_{\mathbb{S}_f} \frac{K - K_0}{8\pi G} d\mathbb{S} + \int_{\mathbb{S}_0} \frac{K - K_0}{8\pi G} d\mathbb{S} + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} \frac{\kappa + r_\mu \nabla_n n^\mu - K'_0}{8\pi G} d\Sigma \quad (7.8.88)$$

$$= \int_{t_0}^{t_f} \int_{\mathbb{S}} \frac{K^{ab} K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} dt + \int_{\mathbb{S}_f} \frac{K_0}{8\pi G} d\mathbb{S} - \int_{\mathbb{S}_0} \frac{K_0}{8\pi G} d\mathbb{S} + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}(t)} \frac{\kappa - K'_0}{8\pi G} L d\mathbb{A} dt. \quad (7.8.89)$$

It is now clear what is the most natural way to define K'_0 , the extrinsic curvature of the spacetime boundary surface when embedded in vacuum. We define the embedding to be so that the time slices are not extrinsically

curved. Thus $K_0 = 0$ on the end-caps and $K'_0 = \kappa_0$, the spatial extrinsic curvature of the spatial boundary surface $\partial\mathbb{S}$ on the shell. This is quite natural, as the reason we ever chose to introduce the K_0 term was to cancel off the divergent but trivial contribution of the spatial boundary. As that is all we wish to cancel, it is all we subtract. Together then, we have that in 3+1 decomposition, known as the Arnowitt-Deser-Misner (ADM) formalism, the Einstein-Hilbert action becomes:

$$S_{\text{EH}} = \int_{t_0}^{t_f} \int_{\mathbb{S}} \frac{K^{ab}K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} dt + \int_{t_0}^{t_f} \int_{\partial\mathbb{S}} \frac{\kappa - \kappa_0}{8\pi G} L d\mathbb{A} dt. \quad (7.8.90)$$

To include interactions of the metric with other fields ϕ , we simply add the action $S_\phi[g, \phi]$ for those fields. We can also write their action as an integral over space and then time:

$$S_\phi[g, \phi] = \int_{\mathbb{M}} \mathfrak{L}_\phi(g, \phi, \nabla\phi) d\mathbb{T} = \int_{t_0}^{t_f} \int_{\mathbb{S}} \mathfrak{L}_\phi(g, \phi, \nabla\phi) L d\mathbb{S} dt = \int_{t_0}^{t_f} \mathcal{L}_\phi dt \quad (7.8.91)$$

$$\implies \mathcal{L}_\phi = \int_{\mathbb{S}} \mathfrak{L}_\phi(g, \phi, \nabla\phi) L d\mathbb{S}. \quad (7.8.92)$$

Now that we have written the action explicitly as a time integral, we can immediately identify the **ADM Lagrangian**:

$$\mathcal{L} = \int_{\mathbb{S}} \frac{K^{ab}K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} + \int_{\partial\mathbb{S}} \frac{\kappa - \kappa_0}{8\pi G} L d\mathbb{A} + \mathcal{L}_\phi. \quad (7.8.93)$$

Using this Lagrangian, we can pass to a Hamiltonian in the standard way through the Legendre transformation.

The Einstein-Hilbert pieces of the ADM Lagrangian, meaning everything except the contribution from $\mathcal{L}_\phi$, have no dependence on $\dot{L}$ or $\dot{N}^a$. Therefore, gravity in isolation produces vanishing conjugate momenta to both the lapse function and the shift vector, causing them to act as Lagrange multipliers rather than genuine phase space variables. This is exactly analogous to the fact that the scalar potential in electromagnetism has vanishing conjugate momentum and becomes a Lagrange multiplier which enforces Gauss' law, and consequently enforces local charge conservation. We will show shortly that the lapse function and shift vector as Lagrange multipliers enforce the local conservation of energy and linear momentum (which are the analogs of charge in gravity). The time derivatives of the lapse function and shift vector can appear in $\mathcal{L}_\phi$, because they appear in the connection coefficients. However, because $\mathcal{L}_\phi$ is the Lagrangian for the other fields, the resulting variation of the total Lagrangian with respect to $\dot{L}$ and $\dot{N}^a$ will give that their canonical momenta are some functions of the fields ϕ^n and their conjugate momenta φ_n (here we use generic field indices from the middle of the alphabet to avoid confusion with spatial indices from the start of the alphabet). Thus, in the presence or absence of external fields, the conjugate momenta to L and N_a satisfy phase space constraints in terms of the other quantities. One can in principle compute the full Legendre transformation for generic $\mathcal{L}_\phi$, however the expression is obnoxiously complicated, and generally is much simpler to work directly with whatever $\mathcal{L}_\phi$ happens to be physically irrelevant. For electromagnetism, fluids, or point particles, the Lagrangian density happens to depend on the metric but not actually on the connection coefficients (by chance). This causes their dependence on L and N^a to be particularly simple.

To begin the Legendre transformation, consider the conjugate momenta φ_n to the fields ϕ^n

$$\varphi_n = \frac{\delta\mathcal{L}}{\delta\dot{\phi}^n} = \frac{\delta\mathcal{L}_\phi}{\delta\dot{\phi}^n} = L\sqrt{\det\gamma} \frac{\partial\mathfrak{L}_\phi}{\partial\nabla_0\phi^n}. \quad (7.8.94)$$

If we were considering only the ϕ^n fields to be dynamical, the resulting Hamiltonian would be:

$$\mathcal{H}_\phi = \int \varphi_n \dot{\phi}^n d^3y - \mathcal{L}_\phi = \int \left(\varphi_n \dot{\phi}^n - \mathfrak{L}_\phi L \sqrt{\det\gamma} \right) d^3y = \int \mathcal{H}_0 d^3y \quad (7.8.95)$$

$$\mathcal{H}_\phi = \varphi_n \dot{\phi}^n - \mathfrak{L}_\phi L \sqrt{\det\gamma} \quad (7.8.96)$$

where in the last line we defined the Hamiltonian coordinate density by the spatial integrand of the Hamiltonian. For electromagnetism, fluids, point particles (but not in full generality), the Hamiltonian coordinate density happens to take a conveniently simple dependence on L , N^a , and γ_{ab} . In particular, it takes the form:

$$\mathcal{H}_\phi = LH_\phi - N^a P_{\phi a} \quad (7.8.97)$$

where H_ϕ and $P_{\phi a}$ are independent of L and N^a . H_ϕ is known as the synchronized Hamiltonian density of the fields ϕ and $P_{\phi a}$ viewed as a spatial vector is known as the synchronized linear momentum density of the fields ϕ .

Next we need the conjugate momentum to the metric and so we need to vary the Lagrangian with respect to the time derivatives of the metric. By hypothesis, we are considering specialized systems for which $\mathfrak{L}_\phi$ does not depend on the metric derivatives, and so only the Einstein-Hilbert piece of the action contributes to the Legendre transformation for the metric. The conjugate momentum to L and N^a then vanish identically:

$$p_L = \frac{\delta \mathcal{L}}{\delta \dot{L}} = 0, \quad p_{N^a} = \frac{\delta \mathcal{L}}{\delta \dot{N}^a} = 0 \quad (7.8.98)$$

and so L and N_a are not genuine dynamical degrees of freedom. Instead, they provide phase space constraints as Lagrange multipliers as their Euler-Lagrange equations simply become:

$$\frac{\delta \mathcal{L}}{\delta L} \stackrel{!}{=} 0, \quad \frac{\delta \mathcal{L}}{\delta N^a} \stackrel{!}{=} 0. \quad (7.8.99)$$

The metric γ_{ab} does have a well-defined conjugate momentum p^{ab} and so is genuinely dynamical. $\mathcal{L}$ depends on $\dot{\gamma}_{ab}$ only through the extrinsic curvature tensor K_{ab} :

$$p^{ab} = \frac{\delta \mathcal{L}}{\delta \dot{\gamma}_{ab}} = \frac{1}{8\pi G} \left(K^{cd} \frac{\partial K_{cd}}{\partial \dot{\gamma}_{ab}} - K \gamma^{cd} \frac{\partial K_{cd}}{\partial \dot{\gamma}_{ab}} \right) L \sqrt{\det \gamma}. \quad (7.8.100)$$

Using that $\dot{\gamma}_{ab}$ is symmetric and the definition of the extrinsic curvature:

$$\frac{\partial \dot{\gamma}_{cd}}{\partial \dot{\gamma}_{ab}} = \frac{1}{2} (\delta_c^a \delta_d^b + \delta_d^a \delta_c^b) \quad (7.8.101)$$

$$K_{ab} = \frac{1}{2L} (\dot{\gamma}_{ab} - \mathcal{D}_a N_b - \mathcal{D}_b N_a) \implies \frac{\partial K_{cd}}{\partial \dot{\gamma}_{ab}} = \frac{1}{4L} (\delta_c^a \delta_d^b + \delta_d^a \delta_c^b) \quad (7.8.102)$$

$$\implies p^{ab} = \frac{\sqrt{\det \gamma}}{16\pi G} (K^{ab} - K \gamma^{ab}). \quad (7.8.103)$$

Importantly, p^{ab} is **NOT** a proper tensor, due to the factor of $\sqrt{\det \gamma}$. Instead, it is called a **tensor density** as under a transformation of spatial coordinates, it transforms automatically according to:

$$p'^{ab} = \det \left(\frac{\partial y}{\partial y'} \right) \frac{\partial y'^a}{\partial y^c} \frac{\partial y'^b}{\partial y^d} p^{cd}. \quad (7.8.104)$$

Because p^{ab} is not a true tensor, its covariant derivative is not automatically defined. However, $\frac{p^{ab}}{\sqrt{\det \gamma}}$ is a true tensor and so does have an already defined covariant derivative. The convenient definition of the covariant derivative of p^{ab} is:

$$\mathcal{D}_c p^{ab} = \sqrt{\det \gamma} \mathcal{D}_c \left(\frac{p^{ab}}{\sqrt{\det \gamma}} \right) \quad (7.8.105)$$

as then this quantity is also a tensor density. Let $p = p^{ab} \gamma_{ab}$ be a shorthand for the trace of p^{ab} . Then, taking the trace of the expression for p^{ab} :

$$p = \frac{\sqrt{\det \gamma}}{16\pi G} (K - 3K) = -\frac{\sqrt{\det \gamma}}{8\pi G} K \quad (7.8.106)$$

$$\implies K^{ab} = \frac{16\pi G}{\sqrt{\det \gamma}} \left(p^{ab} - \frac{p}{2} \gamma^{ab} \right) \quad (7.8.107)$$

$$\implies \dot{\gamma}_{ab} = \mathcal{D}_a N_b + \mathcal{D}_b N_a + \frac{32\pi GL}{\sqrt{\det \gamma}} \left(p_{ab} - \frac{p}{2} \gamma_{ab} \right) \quad (7.8.108)$$

Therefore, the full Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{S}} (p^{ab} \dot{\gamma}_{ab} + \varphi_n \dot{\phi}^n) d^3 y - \mathcal{L} \quad (7.8.109)$$

$$= \int_{\mathbb{S}} \left(2p^{ab} \mathcal{D}_a N_b + \frac{32\pi GL}{\sqrt{\det \gamma}} \left(p^{ab} p_{ab} - \frac{p^2}{2} \right) + \frac{K^2 - K^{ab} K_{ab} + 2\Lambda - \mathcal{R}}{16\pi G} L \sqrt{\det \gamma} + \mathcal{H}_0 \right) d^3 y + \int_{\partial \mathbb{S}} \frac{\kappa_0 - \kappa}{8\pi G} L d\mathbb{A} \quad (7.8.110)$$

$$= \int_{\mathbb{S}} \left(\frac{16\pi GL}{\sqrt{\det \gamma}} \left(p^{ab} p_{ab} - \frac{p^2}{2} \right) + 2p^{ab} \mathcal{D}_b N_a + \frac{2\Lambda - \mathcal{R}}{16\pi G} L \sqrt{\det \gamma} + \mathcal{H}_0 \right) d^3 y + \int_{\partial \mathbb{S}} \frac{\kappa_0 - \kappa}{8\pi G} L d\mathbb{A}. \quad (7.8.111)$$

Now using Stokes' theorem:

$$\int_{\mathbb{S}} p^{ab} \mathcal{D}_b N_a d^3 y = \int_{\mathbb{S}} \frac{p^{ab}}{\sqrt{\det \gamma}} \mathcal{D}_b N_a d\mathbb{S} = \int_{\mathbb{S}} \left(\mathcal{D}_b \left(\frac{p^{ab}}{\sqrt{\det \gamma}} N_a \right) - N_a \mathcal{D}_b \left(\frac{p^{ab}}{\sqrt{\det \gamma}} \right) \right) d\mathbb{S} \quad (7.8.112)$$

$$= \int_{\partial\mathbb{S}} \frac{p^{ab}}{\sqrt{\det \gamma}} N_a r_b d\mathbb{A} - \int_{\mathbb{S}} N_a \mathcal{D}_b p^{ab} d^3 y. \quad (7.8.113)$$

Thus, the ADM Hamiltonian can be written as:

$$\mathcal{H}[\gamma, p, \phi, \varphi, L, N] = \int_{\mathbb{S}} (LH - N^a P_a) d^3 y + \mathcal{H}_{\partial\mathbb{S}} \quad (7.8.114)$$

where the synchronized Hamiltonian density H and synchronized linear momentum density P^a are:

$$H = \frac{16\pi G}{\sqrt{\det \gamma}} \left(p^{ab} p_{ab} - \frac{p^2}{2} \right) + \frac{2\Lambda - \mathcal{R}}{16\pi G} \sqrt{\det \gamma} + H_\phi, \quad P_a = 2\mathcal{D}^b p_{ab} + P_{\phi a} \quad (7.8.115)$$

and the spatial boundary contribution to the Hamiltonian is:

$$\mathcal{H}_{\partial\mathbb{S}} = \int_{\partial\mathbb{S}} \left(\frac{\kappa_0 - \kappa}{8\pi G} L + \frac{2p_{ab} r^b}{\sqrt{\det \gamma}} N^a \right) d\mathbb{A}. \quad (7.8.116)$$

The spatial metric γ_{ab} and its conjugate momenta satisfy the canonical brackets:

$$\{\gamma_{ab}(y), \gamma_{cd}(y')\} = 0, \quad \{\gamma_{ab}(y), p^{cd}(y')\} = \frac{\delta_a^c \delta_b^d + \delta_b^c \delta_a^d}{2} \delta(y - y'), \quad \{p^{ab}(y), p^{cd}(y')\} = 0. \quad (7.8.117)$$

The lapse function and shift vector have vanishing conjugate momenta, and so for interior variations Hamilton's equations give the constraints:

$$\frac{\delta \mathcal{H}}{\delta L} = H \stackrel{!}{=} 0, \quad \frac{\delta \mathcal{H}}{\delta N^a} = -P_a \stackrel{!}{=} 0. \quad (7.8.118)$$

Thus, the on-shell value of the ADM Hamiltonian is given simply by the boundary term:

$$\mathcal{H}|_{\text{on-shell}} = \mathcal{H}_{\partial\mathbb{S}}. \quad (7.8.119)$$

Many sources are not careful about boundary terms and incorrectly claim that on-shell the ADM Hamiltonian is 0.

The constraints $H = 0$ and $P_a = 0$ are enforced by the Lagrange multipliers and are present due to L and N^a lacking conjugate momenta. This is precisely analogous to the electromagnetic case in which Gauss' law appears as a constraint enforced by the Lagrange multiplier that is the scalar potential due to its lack of a conjugate momenta. In the electromagnetic case Gauss' law is a first-class constraint and thus generates the gauge transformations of the theory. Let us now study the gravitational constraint algebra. Using the explicit formulas for H and P_a we can compute their Poisson brackets. Doing so is algebraically very tedious. In order to do so efficiently, for either smooth spatial scalar functions A or smooth spatial vector functions A^a which decay sufficiently quickly at large spatial distances, define the linear functionals:

$$H[A] = \int_{\mathbb{S}} H A d^3 y, \quad P[A] = \int_{\mathbb{S}} P_a A^a d^3 y. \quad (7.8.120)$$

For pure gravity (meaning no other fields than the metric), Poisson brackets of these functionals can be computed using (7.8.117). The particular functional derivatives are:

$$\frac{\delta H[A]}{\delta \gamma_{ab}} = -\frac{HA}{2} \gamma^{ab} + \frac{A\mathcal{R}^{ab} + A(2\Lambda - \mathcal{R})\gamma^{ab} - \mathcal{D}^a \mathcal{D}^b A + \gamma^{ab} \mathcal{D}^2 A}{16\pi G} \sqrt{\det \gamma} + \frac{32\pi G}{\sqrt{\det \gamma}} A \left(p^{ac} p_c^b - \frac{p}{2} \gamma^{ab} \right) \quad (7.8.121)$$

$$\frac{\delta H[A]}{\delta p^{ab}} = \frac{32\pi G}{\sqrt{\det \gamma}} \left(p_{ab} - \frac{p}{2} \gamma_{ab} \right) A \quad (7.8.122)$$

$$\frac{\delta P[A]}{\delta \gamma_{ab}} = \mathcal{D}_c (p^{ab} A^c) - p^{ac} \mathcal{D}_c A^b - p^{bc} \mathcal{D}_c A^a \quad (7.8.123)$$

$$\frac{\delta P[A]}{\delta p^{ab}} = -\mathcal{D}_a A_b - \mathcal{D}_b A_a. \quad (7.8.124)$$

Using these, the Poisson bracket algebra of constraints gives (after significant labor):

$$\{H[A], H[B]\} = P[B\partial A - A\partial B] = \int_{\mathbb{S}} P^a (B\partial_a A - A\partial_b B) d^3 y \quad (7.8.125)$$

$$\{H[A], P[B]\} = H[(B \cdot \partial)A] = \int_{\mathbb{S}} H B^a \partial_a A d^3 y \quad (7.8.126)$$

$$\{P[A], P[B]\} = P[(B \cdot \partial)A - (A \cdot \partial)B] = \int_{\mathbb{S}} P_a (B^b \partial_b A^a - A^b \partial_b B^a) d^3 y. \quad (7.8.127)$$

These Poisson brackets are typically maintained in the presence of other fields provided they are described by a coordinate invariant Lagrangian density (and can be checked explicitly in cases of physical interest). The Poisson brackets of these constraints are all proportional to each other and the Hamiltonian is of the form of these constraints up to a boundary term that Poisson commutes with everything on the spatial interior, therefore all of constraints have weakly-vanishing Poisson brackets with each other, making them first class.

Thus, $H[A]$ and $P[B]$ generate all of our first class constraints and thus the gauge transformations of general relativity. As argued in section 7.1, these gauge transformations should be gauge diffeomorphisms and should be symmetries due to the local covariant conservation of the energy-momentum tensor. Let us now explain how this is in fact true. As constructed in section 1.4, the Poisson bracket $\{f, g\}$ for two quantities f and g gives the Poisson representation of the Lie bracket of f under transformations generated by g . By (7.1.67), the Lie derivative $L_\xi \psi$ is precisely the Lie bracket $\psi \angle \xi$. Thus, under a gauge diffeomorphism $x'^\mu = x^\mu + \varepsilon \xi^\mu(x) + \mathcal{O}(\varepsilon^2)$ for a smooth vector field $\xi^\mu(x)$, by the definition of the Lie derivative:

$$L_\xi g_{\mu\nu} = \xi^\rho \partial_\rho g_{\mu\nu} + g_{\mu\rho} \partial_\nu \xi^\rho + g_{\nu\rho} \partial_\mu \xi^\rho. \quad (7.8.128)$$

Using $g_{00} = -L^2 + N^2$, $g_{0a} = N_a$, $g_{ab} = \gamma_{ab}$, in components this gives explicitly:

$$L_\xi(L) = \xi^\rho \partial_\rho L + L \xi^0 - L N^a \partial_a \xi^0 \quad (7.8.129)$$

$$L_\xi N^a = \xi^\rho \partial_\rho N^a + N^a (\xi^0 - N^b \partial_b \xi^0) + \xi^a - N^b \partial_b \xi^a - L^2 \gamma^{ab} \partial_b \xi^0 \quad (7.8.130)$$

$$L_\xi \gamma_{ab} = \xi^\rho \partial_\rho \gamma_{ab} + N_a \partial_b \xi^0 + N_b \partial_a \xi^0 + \gamma_{ac} \partial_b \xi^c + \gamma_{bc} \partial_a \xi^c. \quad (7.8.131)$$

Under a general transformation generated by our constraints $H[A]$ and $P[B]$ we have (using (7.8.108), (7.8.121)-(7.8.124)):

$$\{\gamma_{ab}, H[A] + P[B]\} = \frac{A}{L} \dot{\gamma}_{ab} - \frac{A}{L} (\mathcal{D}_a N_b + \mathcal{D}_b N_a) - \mathcal{D}_a B_b - \mathcal{D}_b B_a. \quad (7.8.132)$$

Requiring this to match (7.8.131) gives the identification:

$$\xi^0 = \frac{A}{L}, \quad \xi^a = -\frac{A}{L} N^a - B^a. \quad (7.8.133)$$

Therefore, $H[A]$ generates a diffeomorphism by $A(x)n^\mu(x)$ in the normal direction to space and $P[B]$ generates a (possibly time dependent) spatial diffeomorphism $-B^a$. With this identifications, the transformation properties of L , N^a , and a generic functional F of γ_{ab} and p^{ab} under the diffeomorphism becomes:

$$L_\xi(L) = \dot{A} - N^a \partial_a A - B^a \partial_a L \quad (7.8.134)$$

$$L_\xi N^a = -\dot{B}^a + N^b \partial_b B^a - B^b \partial_b N^a - L \gamma^{ab} \partial_b A + \gamma^{ab} A \partial_b L \quad (7.8.135)$$

$$L_\xi F = \{F, H[A] + P[B]\}. \quad (7.8.136)$$

The Poisson bracket algebra of constraints thus simply expresses the extent to which diffeomorphisms fail to commute with each other on-shell. These are the gauge diffeomorphism version of (2.8.132), viewing L and N^a as Lagrange multipliers (and being careful about the transformation properties of their spatial coordinate dependence and behavior under rescaling the time coordinate).

The ADM Hamiltonian $\mathcal{H}$ is precisely $H[L] - P[N]$ plus a boundary term. Because $\mathcal{H}$ is the generator time evolution and $H[L]$ generates diffeomorphisms by n^μ , we have that the coefficient of L in the boundary term is the local generator of diffeomorphisms on the boundary in the n^μ direction. Similarly, because $-P[N]$ generates a diffeomorphism by N^a , the coefficient of $-N^a$ in the boundary is the local generator of diffeomorphisms on the boundary in the direction of N^a . Hence, we define:

$$H^{\partial\mathbb{S}} = \frac{\kappa_0 - \kappa}{8\pi G} \sqrt{\det \sigma}, \quad P_a^{\partial\mathbb{S}} = -\frac{2p_{ab}r^b}{\sqrt{\det \gamma}} \sqrt{\det \sigma} \quad (7.8.137)$$

where σ is the metric on the spatial boundary and θ^i are the coordinates on the spatial boundary, so that the on-shell value of the ADM Hamiltonian (and thus the **total energy**) of the system becomes:

$$E = \int_{\partial\mathbb{S}} (H^{\partial\mathbb{S}} L - P_a^{\partial\mathbb{S}} N^a) d^2 \theta. \quad (7.8.138)$$

Similarly, if A^a is a spatial vector-field, then the **total linear momentum** of the system from translations

along A^a is:

$$P[A] = \int_{\partial\mathbb{S}} P_a^{\partial\mathbb{S}} A^a d^2\theta. \quad (7.8.139)$$

For everything but cosmology, we can treat $\Lambda = 0$ and spacetime as asymptotically Minkowski space. Then, it is natural to choose our coordinates so that the metric $g_{\mu\nu}$ asymptotically limits to $\eta_{\mu\nu}$ in usual Cartesian coordinates (t, x, y, z) . In such coordinates, L becomes 1 on the spatial boundary and N^a becomes 0. As well, it then becomes possible to consider an overall uniform translation of spatial infinity. Thus, the ADM energy and ADM linear momentum become:

$$E = \int_{\partial\mathbb{S}} \frac{\kappa_0 - \kappa}{8\pi G} d\mathbb{A}, \quad P_a = \int_{\partial\mathbb{S}} \frac{-2p_{ab}}{\sqrt{\det\gamma}} d\mathbb{A}^b. \quad (7.8.140)$$

The constraints $H[A] = 0$ and $P[B] = 0$ are the gravitational Gauss' laws on the spatial interior. The ADM energy and linear momentum are the gravitational versions of the integral form of Gauss' law. In electromagnetism, the integral form of Gauss' law expresses the total electric charge q in a region of space by the integral of the normal component of the electric field across the boundary of that region. In gravity, the equivalents of electric charge are energy and linear momentum and the ADM energy and momentum express the total energy and momentum of a gravitating system in a region of space in terms of integrals of the normal components of the gravitational field across the boundary of that region.

Theorem 7.6: Arnowitt-Deser-Misner Theorem

By decomposing the spacetime metric $g_{\mu\nu}$ into the lapse function L , shift vector N^a , and spatial metric according to:

$$L = \frac{1}{\sqrt{-g^{00}}}, \quad N^a = -\frac{g^{0a}}{g^{00}}, \quad \gamma_{ab} = g_{ab} \quad (7.8.141)$$

the spacetime $\mathbb{T}$ can be considered as a one parameter family of spatial manifolds $\mathbb{S}(t)$ with metric $\gamma_{ab}(t, y)$ and spatial coordinates y^a . The Einstein-Hilbert action then produces the ADM Lagrangian:

$$\mathcal{L} = \int_{\mathbb{S}} \frac{K^{ab}K_{ab} - K^2 + \mathcal{R} - 2\Lambda}{16\pi G} L d\mathbb{S} + \int_{\partial\mathbb{S}} \frac{\kappa - \kappa_0}{8\pi G} L d\mathbb{A} \quad (7.8.142)$$

where K_{ab} is the extrinsic curvature tensor of space:

$$K_{ab} = \frac{1}{2L} (\dot{\gamma}_{ab} - \mathcal{D}_a N_b - \mathcal{D}_b N_a) \quad (7.8.143)$$

and $\mathcal{D}_a$ is the spatial covariant derivative using the Levi-Civita connection corresponding to γ_{ab} . Further, $\mathcal{R}$ is the Ricci scalar of $\mathbb{S}(t)$, κ is the extrinsic curvature scalar of the spatial boundary in the physical spacetime and κ_0 is the extrinsic curvature scalar of the spatial boundary when embedded in Minkowski space. The Legendre transform then produces the ADM Hamiltonian:

$$\mathcal{H}[\gamma, p, L, N] = \int_{\mathbb{S}} (LH - N^a P_a) d^3y + \int_{\partial\mathbb{S}} \left(\frac{\kappa_0 - \kappa}{8\pi G} L + \frac{2p_{ab}r^b}{\sqrt{\det\gamma}} N^a \right) d\mathbb{A} \quad (7.8.144)$$

where the synchronized Hamiltonian density H and synchronized linear momentum density P^a are:

$$H = \frac{16\pi G}{\sqrt{\det\gamma}} \left(p^{ab}p_{ab} - \frac{p^2}{2} \right) + \frac{2\Lambda - \mathcal{R}}{16\pi G} \sqrt{\det\gamma} + H_\phi, \quad P_a = 2\mathcal{D}^b p_{ab} + P_{\phi a} \quad (7.8.145)$$

and p^{ab} is the conjugate momentum to the spatial metric. The lapse function and shift vector act as Lagrange multipliers, producing the first-class constraints:

$$H[A] = \int_{\mathbb{S}} H A d^3y \stackrel{!}{=} 0, \quad P[B] = \int_{\mathbb{S}} P_a B^a d^3y \stackrel{!}{=} 0 \quad (7.8.146)$$

for all compactly supported smooth scalar functions A and tensor fields B^a . These constraints satisfy the constraint algebra:

$$\{H[A], H[B]\} = P[B\partial A - A\partial B] = \int_{\mathbb{S}} P^a (B\partial_a A - A\partial_b B) d^3y \quad (7.8.147)$$

$$\{H[A], P[B]\} = H[(B \cdot \partial)A] = \int_{\mathbb{S}} H B^a \partial_a A d^3y \quad (7.8.148)$$

$$\{P[A], P[B]\} = P[(B \cdot \partial)A - (A \cdot \partial)B] = \int_{\mathbb{S}} P_a (B^b \partial_b A^a - A^b \partial_b B^a) d^3 y. \quad (7.8.149)$$

On-shell, they generate diffeomorphisms as the gauge transformations of the theory. If the spacetime is asymptotically Minkowski space at large spatial distances, then using coordinates which asymptotically approach Minkowski Cartesian coordinates, the total energy and total linear momentum of a gravitationally interacting system are given by:

$$E = \int_{\partial \mathbb{S}} \frac{\kappa_0 - \kappa}{8\pi G} d\mathbb{A}, \quad P_a = \int_{\partial \mathbb{S}} \frac{-2p_{ab}}{\sqrt{\det \gamma}} d\mathbb{A}^b. \quad (7.8.150)$$

We have not been especially precise about what it means for a spacetime to be asymptotically flat (asymptotically Minkowski space). In particular, one needs $g_{\mu\nu} \rightarrow \eta_{\mu\nu}$ at large spacelike distances sufficiently quickly for the ADM energy and momentum to converge. One also probably wants them to be unambiguous in an appropriate sense. As total energy and momentum in an asymptotically flat space, you should expect that they transform together as a four-vector under Lorentz transformations of that flat Minkowski space. As well, you might expect that they act as generators of global translations of quantities at spacelike infinity. Certainly asymptotic Minkowski space is Poincare symmetric. However, there are generically more coordinate transformations which preserve the asymptotic Minkowski metric than there would be for a simple globally flat Minkowski metric. These additional transformations are called Bondi–Metzner–Sachs (BMS) transformations. The full symmetry group of asymptotic Minkowski space is called the BMS group. It contains Poincare transformations (meaning transformations which satisfy the Poincare algebra), but it contains many distinct Poincare transformations which are mixed under different BMS transformations. The physically correct required fall off rates for the metric toward Minkowski space are currently somewhat controversial/not perfectly well-understood, and so there is ambiguity in the present understanding of exactly how big the BMS group is. Wald [122] says that the ADM momentum transforms properly as a four-vector and that it is conserved in a generic spacetime, but I haven't understood or checked the details yet.

Exercises

Problem 7.15: Constraint Algebra Details. Using the Poisson brackets (7.8.117), show (7.8.147)–(7.8.149) by explicit calculation.

Problem 7.16: ★ Schwarzschild Solution. Consider a stationary point mass of mass m in an otherwise completely source-free vacuum spacetime.

- (a) By following the arguments leading to (7.7.71), justify that for proper choice of coordinates the proper time element of the resulting spacetime due to this point mass can be written in the form:

$$-d\tau^2 = -T(r)dt^2 + S(r)dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2$$

where $T(r)$ and $S(r)$ are some yet-undetermined functions of r only and the point $r = 0$ is defined as the location of the mass.

- (b) Show that the off-diagonal elements of the Ricci tensor vanish and that Einstein's equations require that for all $r > 0$:

$$\begin{aligned} \frac{T'}{rS} - \frac{S'T'}{4S^2} - \frac{T'^2}{4ST} + \frac{T''}{2S} &= 0 \\ \frac{S'}{rS} + \frac{S'T'}{4ST} + \frac{T'^2}{4T^2} - \frac{T''}{2T} &= 0 \\ 1 - \frac{1}{S} + \frac{rS'}{2S^2} - \frac{rT'}{2ST} &= 0. \end{aligned}$$

- (c) Because of the presence of the mass, the metric need not be well-behaved at $r = 0$. Show that the most general solutions for $T(r)$ and $S(r)$ are:

$$T(r) = B \left(1 + \frac{A}{r} \right), \quad S(r) = \frac{1}{1 + \frac{A}{r}}$$

for some constants A and B . Assume that we define the time coordinate as that at large spatial distances it asymptotically becomes Minkowski time. Show that in these coordinates, $B = 1$.

- (d) We can consider the spatial boundary as $r = R$ for some large constant R . Show that n^μ , κ , and κ_0 are given by:

$$n^\mu = \left(0, \sqrt{1 + \frac{A}{R}}, 0, 0\right)^\mu, \quad \kappa = \frac{2}{R} \sqrt{1 + \frac{A}{R}}, \quad \kappa_0 = \frac{2}{R}.$$

Using these, compute the ADM energy and momentum of our solution over all spacetime ($R \rightarrow \infty$). Show that:

$$E = -\frac{A}{2G}, \quad P_a = 0.$$

Thus conclude that the total mass of our spacetime is precisely:

$$m = -\frac{A}{2G}$$

and that the metric due to a stationary point mass m , known as the Schwarzschild metric, has proper time element:

$$-d\tau^2 = -\left(1 - \frac{2Gm}{r}\right) dt^2 + \frac{dr^2}{1 - \frac{2Gm}{r}} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2.$$

- (e) The Schwarzschild metric looks like it possesses two singularities. At the point $r \rightarrow 0$, $g_{00} \rightarrow \infty$ and $g_{11} \rightarrow -\infty$. As well, on the shell $r \rightarrow 2Gm$, $g_{00} \rightarrow 0$ and $g_{11} \rightarrow \pm\infty$. The singular behavior of the metric at $r = 0$ cannot be removed by any coordinate transformation. It is a genuine property of the physical system originating from the fact there is a point mass there. However, the apparently singular behavior at $r = 2Gm$ can be completely removed by going to the right coordinates. Define the Lemaître coordinates $(\sigma, \rho, \theta, \varphi)$ where θ and φ are unchanged and:

$$\sigma = t + 2\sqrt{2Gmr} + 2Gm \ln \left| \frac{\sqrt{r} - \sqrt{2Gm}}{\sqrt{r} + \sqrt{2Gm}} \right|,$$

$$\rho = t + 2\sqrt{2Gmr} \left(1 + \frac{r}{6Gm}\right) + 2Gm \ln \left| \frac{\sqrt{r} - \sqrt{2Gm}}{\sqrt{r} + \sqrt{2Gm}} \right|.$$

Show that:

$$d\sigma = dt + \sqrt{\frac{2Gm}{r}} \frac{dr}{1 - \frac{2Gm}{r}}, \quad d\rho = dt + \sqrt{\frac{r}{2Gm}} \frac{dr}{1 - \frac{2Gm}{r}}$$

and that the point $r = 0$ is equivalently $\rho = \sigma$. Show further that in these coordinates:

$$-d\tau^2 = -d\sigma^2 + \left(\frac{4Gm}{3(\rho - \sigma)}\right)^{\frac{2}{3}} d\rho^2 + \left(\frac{9Gm}{2}\right)^{\frac{2}{3}} (\rho - \sigma)^{\frac{4}{3}} (d\theta^2 + \sin^2 \theta d\varphi^2)$$

which is plainly well-behaved everywhere but at the location of the point mass. Note: although we derived the Schwarzschild solution as the metric formed by a stationary point mass, there is a theorem known as **Birkhoff's Theorem** which states that any source-free spherically symmetric solution to Einstein's equations must be static and asymptotically flat. An immediate consequence of this is that the spacetime outside of any spherically symmetric body, if not spoiled by any other sources, must be the Schwarzschild metric with m equal to the body's mass.

Problem 7.17: ★ Schwarzschild Black Hole. Consider a point mass m moving under the influence of gravity due to a stationary point mass M . Assume that m is much smaller than M so that we can treat the metric as simply that produced by M (this is known as the test body limit).

- (a) Show that in Schwarzschild coordinates, the Lagrangian and Hamiltonian of the test body become:

$$\mathcal{L} = -m \sqrt{1 - \frac{2GM}{r} + \frac{\dot{r}^2}{1 - \frac{2GM}{r}} + r^2 \dot{\theta}^2 + r^2 \sin^2 \theta \dot{\varphi}^2}$$

$$\mathcal{H} = \sqrt{1 - \frac{2GM}{r}} \sqrt{m^2 + \left(1 - \frac{2GM}{r}\right) p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\varphi^2}{r^2 \sin^2 \theta}}.$$

- (b) Show that it is possible to choose the spherical coordinates so that the motion of the test-body is solely in the spatial plane $\theta = \frac{\pi}{2}$. Let E and L be the energy and angular momentum of the test body in these

coordinates. Show that the motion of the body is then determined by:

$$\left(\frac{dr}{dt}\right)^2 = \left(1 - \frac{2GM}{r}\right)^2 - \frac{1}{E^2} \left(m^2 + \frac{L^2}{r^2}\right) \left(1 - \frac{2GM}{r}\right)^3, \quad \frac{d\varphi}{dt} = \frac{L}{Er^2} \left(1 - \frac{2GM}{r}\right)$$

- (c) Explain that the t coordinate corresponds to the time as measured by a spatially stationary observer arbitrarily far away (“at infinity”). Assume that the initial conditions are such that eventually r approaches the value $2GM$. Show that it takes an infinitely long time, as measured by the observer at infinity, for m to reach $r = 2GM$. Therefore, to an observer at infinity, anything that falls to $r \leq 2GM$ will leave a permanent image at $r = 2GM$.
- (d) Consider the mass m to be initially moving radially outward from M with only the minimum amount of energy necessary to escape to arbitrarily far away. Show that with these initial conditions:

$$E = m, \quad L = 0.$$

Then, show that the coordinate velocity of m remains purely radial and is given by:

$$\frac{dr}{dt} = \left(1 - \frac{2GM}{r}\right) \sqrt{\frac{2GM}{r}}.$$

Let R be the value of r at which the outward radial motion begins. Let ds_R be the proper distance element for radial displacements at $r = R$ and let $d\tau_R$ be the proper time element for a spatially stationary observer at $r = R$. Show that:

$$ds_R = \frac{dr}{\sqrt{1 - \frac{2GM}{R}}}, \quad d\tau_R = \sqrt{1 - \frac{2GM}{R}} dt.$$

Let v be the velocity of m when $r = R$ as measured by a spatially stationary observer at the same value of r . Show that:

$$v = \frac{ds_R}{d\tau_R} = \sqrt{\frac{2GM}{R}}.$$

Thus, the proper escape velocity formula is coincidentally exactly unchanged from the Newtonian formula. A **black hole** is a region of spacetime from which the escape velocity at its boundary is the speed of light, thus preventing anything from leaving its interior. Show that the Schwarzschild solution contains a black hole around the origin defined by the region $r \leq 2GM$. Thus, the radius (as defined by surface area) $2GM$, known as the **Schwarzschild radius** characterizes the size of the black hole. The boundary of the black hole $r = 2GM$ is known as the **event horizon**.

Problem 7.18: ★ Precession of Mercury. Consider again a test mass m moving in a Schwarzschild metric of mass M and recall the results of the previous problem.

- (a) Let $s = \frac{1}{r}$. Show that viewed as a function of φ , $s(\varphi)$ satisfies:

$$\left(\frac{ds}{d\varphi}\right)^2 = \frac{E^2 - m^2}{L^2} + \frac{2GMm^2}{L^2} s - s^2 + 2GMs^3$$

$$\frac{d^2s}{d\varphi^2} + s - \frac{GMm^2}{L^2} - 3GMs^2 = 0$$

thus this is the general relativistic form of the Binet equation. Show that this is equivalent to the trajectory followed by a Newtonian test body of mass m under the influence of the potential:

$$U(r) = -\frac{GMm}{r} - \frac{GML^2}{mr^3}.$$

- (b) Show that the orbit is bound for $E < m$ and unbound for $E \geq m$.
- (c) Consider a bound orbit which is safely far away from the event horizon $r = 2GM$ so that $2GMs$ is always small. Show that in the limit that the $3GMs^2$ term in the Binet equation is totally neglected, the resulting orbit is:

$$s = \frac{1}{\ell}(1 + \varepsilon \cos \varphi)$$

where ℓ and ε are given by:

$$\ell = \frac{L^2}{GMm^2}, \quad \varepsilon = \sqrt{1 + \frac{E^2 - m^2}{L^2} \ell^2}.$$

- (d) Let ℓ and ε be defined as previously. Define the dimensionless quantities $u(\varphi) = \ell s(\varphi)$ and $h = \frac{2GM}{\ell}$. Show that the exact trajectory of a bound orbit is now characterized by:

$$\left(\frac{du}{d\varphi}\right)^2 = \varepsilon^2 - (u-1)^2 + hu^3, \quad \varepsilon < 1.$$

Explain that for orbits of large average radius compared to the Schwarzschild radius of the spacetime, h is a small parameter.

- (e) Let $\Delta\phi$ be the change in orbital angle as the trajectory goes from its maximum radius to a minimum and then back to a maximum. Explain that in order for the orbit to close, $\Delta\phi$ must be 2π . Let $\sigma = \Delta\phi - 2\pi$ be the precession of the orbit. Show by direct integration that to lowest order in h :

$$\sigma = \frac{6\pi GM}{\ell} + \mathcal{O}\left(\frac{2GM}{\ell}\right)^2.$$

This precession is observable for the planet Mercury. Mercury precesses both due to effects of the other planets as well as due to general relativistic corrections to Newton's laws. Einstein correctly explained the precession of Mercury, which already had been in tension with Newtonian predictions, leading to one of the earliest precision tests of general relativity.

Problem 7.19: ★ Bending of Light by Gravity. Consider the Maxwell Lagrangian density in a curved spacetime with no current source.

- (a) Show that the equation of motion for the vector potential becomes:

$$\nabla_\nu \mathcal{F}^{\mu\nu} = 0.$$

- (b) Assume that the effect of the electromagnetic field on the spacetime can be neglected and that the field is propagating in an otherwise source free ($T_{\mu\nu} = 0$) region. Explain that it is possible to select covariant Lorenz gauge, meaning $\nabla_\mu A^\mu = 0$, and that in this gauge A^μ satisfies:

$$\nabla^2 A^\mu = 0.$$

- (c) In flat spacetime the above equation of motion becomes simply the d'Alembert wave equation, the solutions of which are spanned by plane-waves with a lightlike wavenumber 4-vector and polarization orthogonal to that wavenumber (due to Lorenz gauge). A plane-wave is characterized by the form $\xi^\mu e^{i\varphi}$ where ξ^μ is a constant vector and $\varphi(x)$ is a scalar field that depends linearly on x . In curved spacetime, the naive concept of plane-waves cannot be maintained covariantly without modification (depending linearly on coordinates, for example, is not a coordinate invariant concept, nor is a uniform constant vector). These plane waves can be composed to form wavepackets which propagate in flat spacetime like massless particles. The curved spacetime analog is a solution:

$$A^\mu = \text{Re}(\xi^\mu e^{i\varphi})$$

where the separation into amplitude (ξ^μ) and phase (φ) is determined by the criterion that the phase should vary with position much more rapidly than the amplitude, as this is a covariant generalization of requiring ξ^μ to be constant on the scale on which φ changes. This is enforced mathematically by 2 criteria. Let ε be a unitless power-counting parameter. We expand both the amplitude and phase in terms of ε , beginning the amplitude expansion at ε^0 and the phase expansion at ε^1 . This ensures that $\nabla\varphi$ is always much larger than $\nabla\xi$ for small ε . That is:

$$\varphi(x) = \frac{1}{\varepsilon} \varphi_0(x) + \varphi_1(x) + \mathcal{O}(\varepsilon), \quad \xi^\mu(x) = \xi_0^\mu(x) + \varepsilon \xi_1^\mu(x) + \mathcal{O}(\varepsilon^2).$$

We further enforce that each piece of $\varphi(x)$ evolve more quickly than each piece of $\xi^\mu(x)$ by organizing expressions by numbers of derivatives on φ , and requiring cancellation at each order in that number. This expansion is known as the **eikonal approximation**. Show that the Lorenz gauge conditions require:

$$\xi_0^\mu k_\mu = 0, \quad \nabla_\mu \xi_0^\mu = 0, \quad \xi_1^\mu k_\mu = -\xi_0^\mu \nabla_\mu \varphi_1$$

where we have defined $k_\mu = \nabla_\mu \varphi_0$ as the local wavenumber vector. Explain why this definition of the

wavenumber makes sense.

- (d) Show in the above expansion that Maxwell's equations in Lorenz gauge require:

$$k^2 = 0, \quad k^\nu \nabla_\nu k_\mu = 0, \quad k_\nu \nabla^\nu \xi_0^\mu = 0, \quad k_\nu \nabla^\nu \varphi_1 = \frac{i}{2} \nabla^\nu k_\nu.$$

Show that these equations correspond to requiring (1) the wavenumber to be lightlike, (2) the trajectory defined by $\frac{dx^\mu}{d\lambda} = k^\mu(x)$ to be a geodesic, (3,4) the magnitude of the wave to decay at rate $\frac{1}{2} \nabla^\nu k_\nu$ along the geodesic.

- (e) Explain how the results of this question demonstrate that even in curved spacetime, light rays propagate like massless particles following lightlike geodesics, with the tangent vector to the geodesic given by the wavenumber of the light wave.

Problem 7.20: ★ Deflection of Light by Schwarzschild. Using the result of the previous problem, model a light ray passing by a Schwarzschild source of mass M by the trajectory of a massless particle. Let the incoming direction of the light from very far away be in the x direction and let b be the impact parameter of the light, meaning the minimum value of r the light would ever reach relative to the source if M were 0.

- (a) Let $s = \frac{1}{r}$. Show that $L = Eb$ and that the trajectory now satisfies:

$$\left(\frac{ds}{d\varphi}\right)^2 = \frac{1}{b^2} - s^2 + 2GMs^3.$$

- (b) Define the dimensionless quantities $u = bs$ and $h = \frac{2GM}{b}$. Explain that h is small for light which misses the source significantly compared to the Schwarzschild radius. Let χ , the deflection angle, be the angle between the incoming and outgoing light ray. Let $\Delta\varphi$ be the difference in φ between when the light makes its closest approach to the source and when the light has gone arbitrarily far away. Show that:

$$\chi = 2\Delta\varphi - \pi, \quad \Delta\varphi = \int_0^{u_{\max}} \frac{du}{\sqrt{1 - u^2 + hu^3}}$$

where $u_{\max}$ is the maximum value attained by u during the trajectory.

- (c) Show that the deflection angle is given by:

$$\chi = \frac{4GM}{b} + \mathcal{O}\left(\frac{2GM}{b}\right)^2.$$

Show (by referencing the results of Coulomb scattering) that this angle is twice the naive result one would get by assuming Newton's laws of motion and gravity to apply to massless particles moving at the speed of light. Thus, the experimentally confirmed fact that general relativity gives the correct deflection angle serves as another test to demonstrate the improvement of Einstein over Newton.

Problem 7.21: ★ Kerr-Schild Solutions. In this question we study a particular class of solutions to the source-free Einstein's equations which happen to be intimately related to black holes.

- (a) Consider the Schwarzschild solution of mass m and call its time coordinate t_S . Introduce the coordinates t, x, y, z by treating r, θ, φ as standard spherical coordinates and shifting the time in a radially dependent way:

$$t = t_S + f(r), \quad x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta$$

for some function $f(r)$. Show that the line element can be put in the form:

$$-d\tau^2 = -dt^2 + dx^2 + dy^2 + dz^2 + (v_\mu dx^\mu)^2$$

for some vector field v_μ by some appropriate choice of $f(r)$. In particular, show that we should take:

$$f(r) = 2Gm \ln \left(\frac{r - 2Gm}{2Gm} \right)$$

and that then the metric becomes:

$$g_{\mu\nu} = \eta_{\mu\nu} - 2\phi \ell_\mu \ell_\nu$$

where ϕ is a scalar field and ℓ_μ is a lightlike vector field given by:

$$\phi = -\frac{Gm}{r}, \quad \ell_\mu = (1, \sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)_\mu.$$

Verify that the integral curves of the vector-field ℓ^μ are affinely parameterized geodesics (meaning curves

satisfying $\frac{dx^\mu}{d\lambda} = \ell^\mu(x(\lambda))$ are affinely parameterized geodesics). Spacetimes for which the metric can be put in the form $g_{\mu\nu} = \eta_{\mu\nu} - 2\phi\ell_\mu\ell_\nu$ for some scalar field ϕ and some lightlike affinely geodesic vector field ℓ_μ are called Kerr-Schild spacetimes and this form of the metric is called Kerr-Schild form. The coordinates in which the metric takes Kerr-Schild form are called Kerr-Schild coordinates. Note that for the Schwarzschild solution, ϕ is precisely the Newtonian gravitational scalar potential of a point mass of mass m .

- (b) Suppose we have a Kerr-Schild spacetime in Kerr-Schild coordinates. Show that the inverse metric is given by:

$$g^{\mu\nu} = \eta^{\mu\nu} + 2\phi\ell^\mu\ell^\nu$$

where $\ell^\mu = \eta^{\mu\nu}\ell_\nu = g^{\mu\nu}\ell_\nu$ and that the curvature terms in Einstein's equations simplify to:

$$R^\mu{}_\nu - \frac{1}{2}R\delta^\mu_\nu = \partial^2(\phi\ell^\mu\ell_\nu) - \partial_\nu(\ell^\mu\partial_\rho(\phi\ell^\rho)) - \partial^\mu(\ell_\nu\partial_\rho(\phi\ell^\rho)) + \delta^\mu_\nu\partial_\rho(\ell^\rho\partial_\sigma(\phi\ell^\sigma))$$

where $\partial^\mu = \eta^{\mu\nu}\partial_\nu$ and $\partial^2 = \eta^{\mu\nu}\partial_\mu\partial_\nu$. Notice that this is linear in ϕ !

- (c) Show that in Kerr-Schild coordinates, ℓ_μ is a lightlike affinely geodesic vector field for Minkowski space (meaning using $\eta_{\mu\nu}$ as the metric instead of $g_{\mu\nu}$). Because ℓ_μ has this simple structure and Einstein's equations become linear in ϕ , Kerr-Schild solutions are an extremely tractable special case of general relativity. It happens, for reasons I do not understand, that stationary black holes are Kerr-Schild spacetimes.

Problem 7.22: ★ The Kerr Solution and the Newman-Janis Shift.

- (a) Consider the Cartesian-like coordinate system T, X, Y, Z and consider the spherical-like coordinates $T, \mathcal{R}, \Theta, \Phi$ related to T, X, Y, Z by:

$$X + iY = (\mathcal{R} + ia)e^{i\Phi}\sin\Theta, \quad Z = \mathcal{R}\cos\Theta$$

for a positive constant a . Show that in the $a \rightarrow 0$ limit $\mathcal{R}, \Theta, \Phi$ are related to X, Y, Z as standard spherical coordinates.

- (b) Consider the vector ℓ_μ defined in the T, X, Y, Z coordinate system by:

$$\ell_\mu = (1, \cos\Phi\sin\Theta, \sin\Phi\sin\Theta, \cos\Theta)_\mu.$$

Show by direct computation that in Minkowski spacetime this vector field generates flows which are lightlike affinely parameterized geodesics.

- (c) Consider the scalar field ϕ defined by:

$$\phi = \text{Re} \left(\frac{-Gm}{\sqrt{X^2 + Y^2 + (Z - ia)^2}} \right).$$

Note that ϕ is like a complexly translated Newtonian potential of a point mass of mass m . Show that the Kerr-Schild form of the metric:

$$g_{\mu\nu} = \eta_{\mu\nu} - 2\phi\ell_\mu\ell_\nu$$

is a solution to the vacuum Einstein's equations everywhere where the functions involved are non-singular (this is known as the Kerr solution). Note that in the $a \rightarrow 0$ limit it smoothly becomes the Schwarzschild solution in Kerr-Schild coordinates. The complex translation which relates the Kerr solution to the Schwarzschild solution is known as the Newman-Janis shift.

- (d) Using the Kerr-Schild coordinate representation, and by considering (7.8.150), compute the ADM energy and linear momentum of the Kerr solution. Then, by taking L, N^a in (7.8.150) to correspond to a rotation about the z -axis, compute the ADM angular momentum of the Kerr solution. Show that:

$$E = m, \quad \vec{P} = 0, \quad \vec{J} = ma\vec{e}_z.$$

Thus, the Kerr solution has mass m and angular momentum ma , which is about the z axis.

- (e) Define a new spherical-like coordinate system, known as Boyer-Lindquist coordinates, t, r, θ, φ related to $T, \mathcal{R}, \Theta, \Phi$ by:

$$T = t + u(r), \quad \mathcal{R} = r, \quad \Theta = \theta, \quad \Phi = \varphi + v(r)$$

for some functions $u(r)$ and $v(r)$. Show that these functions can be chosen so that all nondiagonal elements of the metric vanish except g_{03} . In particular, show that these functions should be taken to be:

$$u(r) = Gm \ln \left(\frac{r^2 - 2Gmr + a^2}{2Gm} \right) + \frac{G^2m^2}{\sqrt{G^2m^2 - a^2}} \ln \left(\frac{r - Gm - \sqrt{G^2m^2 - a^2}}{r - Gm + \sqrt{G^2m^2 - a^2}} \right),$$

$$v(r) = \frac{a}{2\sqrt{G^2m^2 - a^2}} \ln \left(\frac{r - Gm - \sqrt{G^2m^2 - a^2}}{r - Gm + \sqrt{G^2m^2 - a^2}} \right).$$

Thus, show that the line element in these coordinates becomes:

$$\begin{aligned} -d\tau^2 = & - \left(1 - \frac{2Gmr}{r^2 + a^2 \cos^2 \theta} \right) dt^2 + \frac{r^2 + a^2 \cos^2 \theta}{r^2 - 2Gmr + a^2} dr^2 + (r^2 + a^2 \cos^2 \theta) d\theta^2 \\ & + \left(r^2 + a^2 + \frac{2Gma^2r}{r^2 + a^2 \cos^2 \theta} \sin^2 \theta \right) \sin^2 \theta d\varphi^2 - \frac{4Gmar \sin^2 \theta}{r^2 + a^2 \cos^2 \theta} dt d\varphi. \end{aligned}$$

The Boyer-Lindquist coordinates are typically the most useful for calculations in Kerr spacetime.

- (f) The metric in Boyer-Lindquist coordinates has a singularity at $r^2 - 2Gmr + a^2 = 0$. This coordinate singularity can be removed by a coordinate transformation, but the surface of this coordinate singularity has a physical meaning. Let Σ be the set of points so that $r^2 - 2Gmr + a^2 = 0$. Show that Σ consists of two parts, an outer part (with the greater value of r) Σ_+ and an inner part Σ_- . Show that Σ_+ is topologically a 2-sphere $\times \mathbb{R}$ (representing the time direction) and thus at each time separates spacetime into an inside and an outside. Show as well that Σ_+ is a lightlike surface and thus acts as an event horizon. Consequently, explain that the Kerr solution represents a stationary spinning black hole. Very advanced uniqueness theorems of general relativity prove that the Kerr solution is the unique uncharged stationary spinning black hole solution to Einstein's equation [15].
- (g) Using the relationship between r, θ, φ and X, Y, Z show that the surface of points such that $r = 0$ is a disk at $Z = 0$ in the X, Y plane with radius a . Show that the metric is singular at $X^2 + Y^2 = a^2$. This singularity cannot be removed by coordinate transformation and is the Kerr equivalent of the point singularity at the center of the Schwarzschild metric. Attempting to calculate what happens to an observer experiencing such a truly singular metric behavior gives nonsensical results. Consequently, there is a common belief, known as the Cosmic Censorship Hypothesis, that all unremovable singularities that occur in general relativity are hidden inside of an event horizon. Show that in order for this to be true of the Kerr solution, the spin $S = ma$ of the black hole must satisfy:

$$S \leq Gm^2.$$

A black hole for which $S = Gm^2$ is called extremal.

Problem 7.23: ★ Geodesics in Kerr and the Carter Constant. Consider a test mass of mass m moving in a Kerr metric of mass M .

- (a) Show that in Boyer-Lindquist coordinates the Lagrangian and Hamiltonian of the test body become:

$$\begin{aligned} \mathcal{L} = & -m \sqrt{1 - \frac{2GMr}{\Sigma} + \frac{4GMar \sin^2 \theta}{\Sigma} \dot{\varphi} - \frac{\Sigma}{\Delta} \dot{r}^2 - \Sigma \dot{\theta}^2 - \left(r^2 + a^2 + \frac{2GMa^2r \sin^2 \theta}{\Sigma} \right) \dot{\varphi}^2 \sin^2 \theta} \\ \mathcal{H} = & \sqrt{1 - \frac{2GMr}{\Sigma} + \frac{4a^2G^2M^2r^4 \sin^2 \theta}{\Sigma((r^2 + a^2)^2 - a^2\Delta \sin^2 \theta)}} \sqrt{m^2 + \frac{\Delta}{\Sigma} p_r^2 + \frac{p_\theta^2}{\Sigma} + \frac{\Sigma p_\varphi^2}{(r^2 + a^2)^2 - a^2\Delta \sin^2 \theta}} \\ & + \frac{2GMar}{(r^2 + a^2)^2 - a^2\Delta \sin^2 \theta} p_r \end{aligned}$$

where:

$$\Sigma = r^2 + a^2 \cos^2 \theta, \quad \Delta = r^2 - 2Gmr + a^2$$

- (b) Let E be the energy of the test particle, L be the angular momentum about the z -axis (conjugate to φ) of the test particle. The Kerr spacetime is not spherically symmetric, and so there is no fully conserved angular momentum vector of the test particle. However, the Kerr spacetime does happen to have a special additional symmetry. Show that in Boyer-Lindquist coordinates the Hamilton-Jacobi equation admits a separable solution (and hence Kerr geodesics are integrable). That is, show that the Hamilton-Jacobi canonical action can be written in the form:

$$S_c(t, r, \theta, \varphi) = T(t) + R(r) + \Theta(\theta) + \Phi(\varphi)$$

for some to-be-determined functions $T(t), R(r), \Theta(\theta)$, and $\Phi(\varphi)$. Use this to show that the Carter constant defined by:

$$Q = p_\theta^2 + \frac{\cos^2 \theta}{\sin^2 \theta} L^2 + a^2(m^2 - E^2) \cos^2 \theta + (L - aE)^2$$

of the test particle is conserved during its geodesic motion. Show that Q becomes the squared-magnitude of angular momentum in the $a \rightarrow 0$ (Schwarzschild) limit. While integrable, the Kerr geodesics cannot be expressed in terms of elementary functions.

Problem 7.24: ★ Exact Gravitational Waves. For many experimental purposes, such as the study of gravitational waves, a perturbative approach to Einstein's theory is very useful. In order to perform that perturbative treatment, an efficient exact organization of the problem is helpful first.

- (a) Define the “inverse metric tensor density” $\mathfrak{g}^{\mu\nu}$ by:

$$\mathfrak{g}^{\mu\nu} = g^{\mu\nu} \sqrt{-\det g}.$$

Show that the Ricci tensor contribution to Einstein's equations can be expressed exactly as:

$$\begin{aligned} 2|\det g| \left(R^{\mu\nu} - \frac{1}{2} R g^{\mu\nu} \right) = & \mathfrak{g}^{\rho\sigma} \partial_{\rho\sigma}^2 \mathfrak{g}^{\mu\nu} + \mathfrak{g}^{\mu\nu} \partial_{\rho\sigma}^2 \mathfrak{g}^{\rho\sigma} - \mathfrak{g}^{\mu\sigma} \partial_{\rho\sigma}^2 \mathfrak{g}^{\rho\nu} - \mathfrak{g}^{\nu\sigma} \partial_{\rho\sigma}^2 \mathfrak{g}^{\rho\mu} \\ & - \partial_{\sigma} \mathfrak{g}^{\mu\rho} \partial_{\rho} \mathfrak{g}^{\nu\sigma} + \partial_{\rho} \mathfrak{g}^{\rho\sigma} \partial_{\sigma} \mathfrak{g}^{\mu\nu} - g_{\alpha\beta} g^{\rho\sigma} \partial_{\rho} \mathfrak{g}^{\mu\alpha} \partial_{\sigma} \mathfrak{g}^{\nu\beta} \\ & + g^{\mu\beta} g_{\rho\alpha} \partial_{\sigma} \mathfrak{g}^{\nu\alpha} \partial_{\beta} \mathfrak{g}^{\rho\sigma} + g^{\nu\beta} g_{\rho\alpha} \partial_{\sigma} \mathfrak{g}^{\mu\alpha} \partial_{\beta} \mathfrak{g}^{\rho\sigma} - \frac{1}{2} g^{\mu\nu} g_{\rho\alpha} \partial_{\sigma} \mathfrak{g}^{\alpha\beta} \partial_{\beta} \mathfrak{g}^{\rho\sigma} \\ & - \frac{1}{8} (2g^{\mu\tau} g^{\nu\omega} - g^{\mu\nu} g^{\tau\omega}) (2g_{\alpha\rho} g_{\beta\sigma} - g_{\alpha\beta} g_{\rho\sigma}) \partial_{\tau} \mathfrak{g}^{\alpha\beta} \partial_{\omega} \mathfrak{g}^{\rho\sigma}. \end{aligned}$$

The inverse metric tensor density is useful to introduce primarily because it makes this above expression *relatively* simple, compared to the alternative of expressing it in terms of the metric $g_{\mu\nu}$ directly.

- (b) For studying gravitational waves, it is generally easiest to use “harmonic coordinates”, also known as de Donder gauge. Harmonic coordinates x^{μ} are coordinates which treated as scalar functions satisfy the wave equation $\nabla^2 x^{\mu} = 0$. Note that standard Cartesian coordinates satisfy the wave equation in Minkowski space, and so in some sense this is a generalization of Cartesian coordinates. Show that de Donder gauge can be equivalently written as:

$$\nabla^2 x^{\mu} = -g^{\alpha\beta} \Gamma^{\mu}_{\alpha\beta} = \frac{\partial_{\nu} \mathfrak{g}^{\mu\nu}}{\sqrt{-\det g}} \stackrel{!}{=} 0.$$

Explain how it is possible to construct harmonic coordinates in a finite size neighborhood of a point of choice if the spacetime is such that the wave equation has a well defined Green's functions in the neighborhood of the point. Thus, in quite general spacetimes we can comfortably believe in our ability to go to harmonic coordinates.

- (c) Let $\kappa = \sqrt{32\pi G}$. Then, define the exact graviton field $h^{\mu\nu}$ by:

$$\mathfrak{g}^{\mu\nu} = \eta^{\mu\nu} + \kappa h^{\mu\nu}.$$

This κ is a useful constant to introduce because the $\sqrt{G}$ dependence leads to it being the simplest way to organize the perturbation series for gravity in terms of G and the factor of 32π leads to the simplest coefficients in the action when the Einstein-Hilbert action is rewritten in terms of $h^{\mu\nu}$. Note that $h^{\mu\nu}$ captures the deviation of the metric from Minkowski space. Show that the harmonic coordinate condition requires exactly that:

$$\partial_{\nu} h^{\mu\nu} = 0$$

and show that in harmonic coordinates in terms of $h^{\mu\nu}$, Einstein's equations exactly become:

$$\begin{aligned} -\partial^2 h^{\mu\nu} = & \kappa \left(-\frac{T^{\mu\nu}}{2} |\det \mathfrak{g}| + h^{\rho\sigma} \partial_{\rho\sigma}^2 h^{\mu\nu} - \partial_{\sigma} h^{\mu\rho} \partial_{\rho} h^{\nu\sigma} - g_{\alpha\beta} g^{\rho\sigma} \partial_{\rho} h^{\mu\alpha} \partial_{\sigma} h^{\nu\beta} \right. \\ & + g^{\mu\beta} g_{\rho\alpha} \partial_{\sigma} h^{\nu\alpha} \partial_{\beta} h^{\rho\sigma} + g^{\nu\beta} g_{\rho\alpha} \partial_{\sigma} h^{\mu\alpha} \partial_{\beta} h^{\rho\sigma} - \frac{1}{2} g^{\mu\nu} g_{\rho\alpha} \partial_{\sigma} h^{\alpha\beta} \partial_{\beta} h^{\rho\sigma} \\ & \left. - \frac{1}{8} (2g^{\mu\tau} g^{\nu\omega} - g^{\mu\nu} g^{\tau\omega}) (2g_{\alpha\rho} g_{\beta\sigma} - g_{\alpha\beta} g_{\rho\sigma}) \partial_{\tau} h^{\alpha\beta} \partial_{\omega} h^{\rho\sigma} \right) \end{aligned}$$

where $\partial^2 = \eta^{\rho\sigma} \partial_{\rho} \partial_{\sigma}$.

Problem 7.25: ★ Perturbative Gravitational Waves. Consider a perturbation series for $h^{\mu\nu}$ and $T^{\mu\nu}$ in powers of κ (the gravitational coupling):

$$h^{\mu\nu} = h_{(0)}^{\mu\nu} + \kappa h_{(1)}^{\mu\nu} + \kappa^2 h_{(2)}^{\mu\nu} + \mathcal{O}(\kappa^3)$$

$$T^{\mu\nu} = T_{(0)}^{\mu\nu} + \kappa T_{(1)}^{\mu\nu} + \kappa^2 T_{(2)}^{\mu\nu} + \mathcal{O}(\kappa^3).$$

- (a) Show from Einstein's equations in de Donder gauge that $h_{(0)}^{\mu\nu}$ satisfies $\partial_\nu h_{(0)}^{\mu\nu} = 0$ and the Minkowski space wave equation:

$$\partial^2 h_{(0)}^{\mu\nu} = 0.$$

- (b) Show from Einstein's equations in de Donder gauge that $h_{(1)}^{\mu\nu}$ satisfies $\partial_\nu h_{(1)}^{\mu\nu} = 0$ and the Minkowski space wave equation with a source:

$$\partial^2 h_{(1)}^{\mu\nu} = \frac{\tau_{(0)}^{\mu\nu}}{2}$$

where $\tau_{(0)}^{\mu\nu}$ is called effectively total energy-momentum tensor and is given by $\tau_{(0)}^{\mu\nu} = T_{(0)}^{\mu\nu} + \tau_{g(0)}^{\mu\nu}$ and $\tau_{g(0)}^{\mu\nu}$ is called the effective gravitational energy-momentum tensor. Show that $\tau_{g(0)}^{\mu\nu}$ is given by:

$$\begin{aligned} \tau_{g(0)}^{\mu\nu} = & -2h_{(0)}^{\rho\sigma}\partial_{\rho\sigma}^2 h_{(0)}^{\mu\nu} + 2\partial_\sigma h_{(0)}^{\mu\rho}\partial_\rho h_{(0)}^{\nu\sigma} + 2\partial^\rho h_{(0)}^{\mu\sigma}\partial_\rho h_{(0)\sigma}^\nu - 2\partial_\sigma h_{(0)\rho}^\nu\partial^\mu h_{(0)}^{\rho\sigma} - 2\partial_\sigma h_{(0)\rho}^\mu\partial^\nu h_{(0)}^{\rho\sigma} \\ & + \eta^{\mu\nu}\partial_\rho h_{(0)}^{\alpha\beta}\partial_\beta h_{(0)\alpha}^\rho + \frac{1}{4}(2\eta^{\mu\tau}\eta^{\nu\omega} - \eta^{\mu\nu}\eta^{\tau\omega})(2\eta_{\alpha\rho}\eta_{\beta\sigma} - \eta_{\alpha\beta}\eta_{\rho\sigma})\partial_\tau h_{(0)}^{\alpha\beta}\partial_\omega h_{(0)}^{\rho\sigma} \end{aligned}$$

where indices have been raised and lowered using the Minkowski metric (as will be done throughout this question). Explain why $\tau_{g(0)}^{\mu\nu}$ can be thought of like the effective energy-momentum tensor due to the free gravitational wave $h_{(0)}^{\mu\nu}$.

- (c) From the diffeomorphism symmetry $x'^\mu = x^\mu + \xi^\mu(x)$ of Einstein's theory, using a perturbative expansion for $\xi^\mu(x)$ in terms of κ :

$$\xi^\mu = \xi_{(0)}^\mu + \kappa \xi_{(1)}^\mu + \mathcal{O}(\kappa^2),$$

show that in order for $g'^{\mu\nu}$ to have the form $\eta^{\mu\nu} + \kappa h'^{\mu\nu}$ with $h'^{\mu\nu}$ having a well-defined Taylor series expansion in terms of κ , $\xi_{(0)}^\mu$ must correspond to a Poincare transformation. Then, assuming we are in our desired frame (so that we make no further Poincare transformations), show that $h_{(0)}^{\mu\nu}$ has the gauge transformation property:

$$h_{\mu\nu}'^{(0)} = h_{\mu\nu}^{(0)} + \partial_\mu \xi_\nu^{(1)} + \partial_\nu \xi_\mu^{(1)} - \eta_{\mu\nu} \partial \cdot \xi^{(1)}.$$

- (d) Show that in order for $h_{(0)}^{\mu\nu}$ to also be in de Donder gauge, $\xi_{(1)}^\mu$ must satisfy:

$$\partial^2 \xi_{(1)}^\mu = 0.$$

Show further that the given expression for $\tau_{g(0)}^{\mu\nu}$ is NOT gauge invariant under these transformations. There is no instantaneous gauge-invariant expression for the energy-momentum tensor of a gravitational wave. However, there is a gauge invariant expression for the time and space averaged energy-momentum tensor of such a wave.

- (e) Show that the general solution for $h_{(0)}^{\mu\nu}(x)$ can be written in the form:

$$h_{(0)}^{\mu\nu}(x) = 2\text{Re} \int \tilde{h}^{\mu\nu}(k) e^{ik \cdot x} \delta_+(k^2) \frac{d^4 k}{(2\pi)^{\frac{3}{2}}}$$

where $\delta_+(k^2) = \delta(k^2) \vartheta(k^0)$ and $\tilde{h}^{\mu\nu}(k)$ is some arbitrary complex function defined for values of k^μ for which $k^0 = \sqrt{(k^1)^2 + (k^2)^2 + (k^3)^2}$. Show that de Donder gauge requires $k_\nu \tilde{h}^{\mu\nu} = 0$. Show that $\xi_{(1)}^\mu$ can be put into the same form (if it maintains de Donder gauge):

$$\xi_{(1)}^\mu(x) = 2\text{Re} \int \tilde{\xi}^\mu(k) e^{ik \cdot x} \delta_+(k^2) \frac{d^4 k}{(2\pi)^{\frac{3}{2}}}$$

and that the gauge transformation property of $h_{\mu\nu}^{(0)}$ results in the field amplitude $\tilde{h}^{\mu\nu}$ transforming according to:

$$\tilde{h}'_{\mu\nu} = \tilde{h}_{\mu\nu} + ik_\mu \tilde{\xi}_\nu + ik_\nu \tilde{\xi}_\mu - i\eta_{\mu\nu} k \cdot \tilde{\xi}.$$

(de Donder gauge is not a complete gauge fixing, any choice of $\tilde{\xi}_\mu$ maintains it.)

- (f) Let v^μ be a constant timelike unit vector ($v \cdot v = -1$, using the Minkowski metric). Show that by appropriate choice of $\tilde{\xi}^\mu(k)$ it is possible to go to a de Donder gauge in which $h'^{\mu\nu}$ is traceless

$(\eta_{\mu\nu}h'^{\mu\nu} = 0)$. Show that one such choice is:

$$\tilde{\xi}^\mu = \frac{\eta_{\rho\sigma}\tilde{h}^{\rho\sigma}}{2ik \cdot v} v^\mu.$$

- (g) Assuming we are now in a traceless de Donder gauge, show further that it is possible to implement another gauge transformation so that tracelessness is preserved and additionally $h'_{\mu\nu}v^\nu = 0$. In particular, show that $\tilde{\xi}^\mu$ should be chosen to be:

$$\tilde{\xi}_\mu = \frac{-i}{k \cdot v} \left(\tilde{h}_{\mu\nu}v^\nu - \frac{k_\mu \tilde{h}_{\rho\sigma}v^\rho v^\sigma}{2k \cdot v} \right).$$

All of our gauge conditions now imply:

$$\partial_\nu h^{\mu\nu} = 0, \quad \eta_{\mu\nu}h^{\mu\nu} = 0, \quad h^{\mu\nu}v_\nu = 0.$$

A graviton field $h^{\mu\nu}$ satisfying these conditions for some v^μ is said to be in transverse-traceless gauge.

- (h) Show that in transverse-traceless gauge, $\tilde{h}^{\mu\nu}$ can be decomposed into the form:

$$\tilde{h}^{\mu\nu}(k) = h_+(k)\mathcal{E}_+^\mu\mathcal{E}_+^\nu + h_-(k)\mathcal{E}_-^\mu\mathcal{E}_-^\nu$$

for some complex functions $h_\pm(k)$ and where the polarization vectors $\mathcal{E}_\pm^\mu$ are precisely the electromagnetic polarization vectors from problem 4.44. In particular, show that there exists a Lorentz frame in which $v^\mu = (1, 0, 0, 0)^\mu$, $k^\mu = (\omega, 0, 0, \omega)^\mu$ for some positive constant ω , and that in that frame we can take:

$$\mathcal{E}_\pm^\mu = \left(0, \frac{1}{\sqrt{2}}, \frac{\pm i}{\sqrt{2}}, 0 \right)^\mu.$$

Thus, while electromagnetic waves propagate as linear combinations of helicity 1 and helicity -1 vector fields, gravitational waves propagate as linear combinations of helicity 2 and helicity -2 tensor fields (the helicity has magnitude 2 due to the product of 2 polarization vectors of the same helicity). Altogether then, in transverse-traceless gauge a generic gravitational wave takes the form:

$$h_{(0)}^{\mu\nu} = 2\text{Re} \int (h_+(k)\mathcal{E}_+^\mu\mathcal{E}_+^\nu + h_-(k)\mathcal{E}_-^\mu\mathcal{E}_-^\nu) e^{ik \cdot x} \delta_+(k^2) \frac{d^4k}{(2\pi)^{\frac{3}{2}}}.$$

- (i) Let $t^{\mu\nu}$ be the time and space averaged effective energy-momentum tensor of a gravitational wave, and denote that averaging by the symbol $\mathbb{T}$ (which we have previously often used for time-averaging alone). Suppose a function $f(t)$ has Fourier components only with angular frequency all above a certain angular frequency ω_0 ; show that if that function is averaged over a time interval several times the duration of $\frac{2\pi}{\omega_0}$, the result will be 0. Similarly, show that the time-average of the total time-derivative of a periodic function is 0. Using these rules, show that the time and space averaged behavior of $\tau_{g(0)}^{\mu\nu}$, when averaged over time and length scales large compared to the periods and wavelengths of modes in $h_{(0)}^{\mu\nu}$, gives:

$$t^{\mu\nu} = \mathbb{T}(\tau_{g(0)}^{\mu\nu}) = \mathbb{T}(\partial^\mu h_{(0)}^{\rho\sigma} \partial^\nu h_{(0)\rho\sigma}).$$

Show further that under small gauge transformations which preserve de Donder gauge, this expression is gauge invariant.

- (j) Consider a gravitational plane wave of a particular wavenumber k_μ :

$$h_{(0)}^{\mu\nu} = \text{Re}((h_+\mathcal{E}_+^\mu\mathcal{E}_+^\nu + h_-\mathcal{E}_-^\mu\mathcal{E}_-^\nu)e^{ik \cdot x})$$

where here h_+ and h_- are simply two complex coefficients. Show that its time and space averaged effective energy-momentum tensor is:

$$t^{\mu\nu} = \frac{1}{2}k^\mu k^\nu (|h_+|^2 + |h_-|^2).$$

Problem 7.26: ★ Measuring a Gravitational Wave. Gravitational waves from distant astronomical source have been measured on Earth. This was first accomplished by the LIGO and Virgo collaborations. Let us consider a simplified model of gravitational wave measurement. Consider a light detector that at spatial coordinates $(0, 0, 0)$ that fires a laser light in the direction of a mirror at $(0, 0, L)$. The light then reflects off of the mirror and returns to the detector after a total time of $2L$ in the absence of a gravitational wave. In the presence of a gravitational wave, this time will be changed. The detector's ability to measure the time between emission and detection thus gives a measurement of the average proper distance between the detector and the mirror during the propagation of the light.

- (a) Explain that if the incoming gravitational wave has a much longer period than the time between

emission and detection at the detector, then the proper distance s between the detector and mirror can be treated as constant during the propagation.

- (b) Consider a metric perturbation that is a transverse-traceless gauge gravitational wave. Show that the worldlines of the detector and mirror are unperturbed to first order in κ .
- (c) Suppose the light is emitted at the detector at coordinates $(\tau, 0, 0, 0)^\mu$ and let $v^\mu = (1, 0, 0, 0)^\mu$ be the initial four-velocity of the detector and mirror. Let $\iota^\mu = (0, 0, 0, 1)^\mu$ be the displacement between the detector and the mirror. Show that the proper distance to the mirror at $(\tau, 0, 0, L)^\mu$ to first order in κ is:

$$s = L + \kappa \text{Im} \int (h_+(\mathcal{E}_+ \cdot \iota)^2 + h_-(\mathcal{E}_- \cdot \iota)^2) \frac{1 - e^{iL\iota \cdot k}}{k \cdot \iota} e^{i\tau k \cdot v} \delta_+(k^2) \frac{d^4 k}{(2\pi)^{\frac{3}{2}}} + \mathcal{O}(\kappa^2).$$

Thus explain that the τ dependence of s (which can be measured by sending many light pulses over time) allows one to detect incoming gravitational waves. Real detectors, instead of being purely linear, are L-shaped, with a mirror that causes the right angle and another mirror that causes the reflection back. Having these L-shaped detectors (and multiple of them) allows significantly improved extraction about directional information of the gravitational waves.

Problem 7.27: ★ Robertson-Walker Metric. In the simplest cosmological model of our universe, under extremely long range averaging, the universe is treated as spatially homogeneous and isotropic at fixed time.

- (a) Consider a metric $g_{\mu\nu}$ and decompose it into its ADM pieces L , N_a , γ_{ab} . Explain that in order for γ_{ab} to be homogeneous and isotropic at fixed time t_0 it must have 3 Killing vectors which at a point of interest in local Cartesian coordinates act like translations and 3 Killing vectors which at a point of interest in local Cartesian coordinates act like rotations. Then, under the assumptions of homogeneity and isotropy, show that γ_{ab} is maximally symmetric as a spatial metric and so the spatial line element can be written in the form:

$$ds^2 = \gamma_{ab} dx^a dx^b = \frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2$$

for some constant k using the spherical-like coordinates r, θ, φ . Explain why the definition of these spherical like coordinates may be time dependent.

- (b) Consider the proper distance between nearby spatial locations at two different times. Show that homogeneity and isotropy require that for some function $A(t_1, t_0)$:

$$ds(t_1) = A(t_1, t_0) ds(t_0).$$

Show further then that it is possible to use coordinates (t, r, θ, φ) where r, θ, φ are valid at all times so that the spatial metric at a generic time can be written as:

$$\gamma_{11} = \frac{a^2(t)}{1 - kr^2}, \quad \gamma_{12} = \gamma_{13} = 0, \quad \gamma_{22} = a^2(t)r^2, \quad g_{23} = 0, \quad g_{33} = a^2(t)r^2 \sin^2 \theta.$$

This function $a(t)$ is called the scale factor. Show that $A(t_1, t_0) = \frac{a(t_1)}{a(t_0)}$ and explain that $a(t)$ represents the factor by which spatial distances between the same spatial coordinates have expanded at the time t relative to the same distance at the time at which $a = 1$. Show that k measures the spatial curvature of the universe at the time at which $a = 1$.

- (c) Show that the Killing vectors of γ_{ab} are:

$$\begin{aligned} \hat{P}_1 &= \sqrt{1 - kr^2} \sin \theta \cos \varphi \partial_r + \frac{\sqrt{1 - kr^2}}{r} \cos \theta \cos \varphi \partial_\theta - \frac{\sqrt{1 - kr^2}}{r \sin \theta} \sin \varphi \partial_\varphi \\ \hat{P}_2 &= \sqrt{1 - kr^2} \sin \theta \sin \varphi \partial_r + \frac{\sqrt{1 - kr^2}}{r} \cos \theta \sin \varphi \partial_\theta + \frac{\sqrt{1 - kr^2}}{r \sin \theta} \cos \varphi \partial_\varphi \\ \hat{P}_3 &= \sqrt{1 - kr^2} \cos \theta \partial_r - \frac{\sqrt{1 - kr^2}}{r} \sin \theta \partial_\theta \\ \hat{J}_1 &= -\sin \varphi \partial_\theta - \cos \varphi \frac{\cos \theta}{\sin \theta} \partial_\varphi \\ \hat{J}_2 &= \cos \varphi \partial_\theta - \sin \varphi \frac{\cos \theta}{\sin \theta} \partial_\varphi \\ \hat{J}_3 &= \partial_\varphi. \end{aligned}$$

- (d) Explain that in order for the full spacetime to be homogeneous and isotropic $\hat{P}_1, \hat{P}_2, \hat{P}_3, \hat{J}_1, \hat{J}_2, \hat{J}_3$ must

be symmetries of the full metric $g_{\mu\nu}$ as well. Show that these require the metric to take the form:

$$g_{00} = -L(t)^2, \quad g_{01} = g_{02} = g_{03} = 0, \quad g_{ab} = \gamma_{ab} \text{ (as previously).}$$

Show further that it is possible to choose the time coordinate so that $L(t) = 1$ and thus altogether conclude that the generic line element of a homogeneous and isotropic spacetime has the form:

$$-d\tau^2 = -dt^2 + a^2(t) \left(\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2 \right).$$

This is known as the Robertson-Walker metric. The time coordinate t here with respect to which equal time slices are homogeneous and isotropic is called the cosmological time.

Problem 7.28: ★ Cosmology and the Friedmann equation. Consider a homogeneous and isotropic spacetime meant to model the large scale behavior of our universe. From the Robertson-Walker metric, the only dynamical variable characterizing such a spacetime is the scale factor $a(t)$. Einstein's equations then will give an equation for $a(t)$.

- (a) Compute the Ricci tensor of the Robertson-Walker metric. Show that it is diagonal and that the diagonal entries are:

$$R_{00} = -\frac{3\ddot{a}}{a}, \quad R_{11} = \frac{2k + 2\dot{a}^2 + a\ddot{a}}{1 - kr^2}, \quad R_{22} = r^2(1 - kr^2)R_{11}, \quad R_{33} = R_{22} \sin^2 \theta.$$

- (b) Let $\mathcal{E}(t)$ be the average energy density of the universe at cosmological time t . Show that the 00 component of Einstein's equations imply the scale factor evolves according to:

$$\left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \mathcal{E} - \frac{k}{a^2}.$$

This equation of motion is known as the Friedmann equation. A metric with scale factor satisfying the Friedmann equation is called a Friedmann-Lemaître-Robertson-Walker metric. For the rest of this question, suppose that the scale factor is defined so that at the present time it takes the value 1.

- (c) Consider matter which is sufficiently nonrelativistic so as to be treated at large scales as effectively stationary. Let $\mathcal{E}_m^{(0)}$ be the energy density of such matter in the present. Show that $\mathcal{E}_m(t)$, the energy density of that matter at a general time, is given by:

$$\mathcal{E}_m(t) = \frac{\mathcal{E}_m^{(0)}}{a^3(t)}$$

by using that mass is conserved in nonrelativistic systems. Hint: think about how the total volume of the system depends on time.

- (d) Consider electromagnetic waves propagating in space. Because we are only studying the large scale averaged out behavior of such electromagnetic radiation in cosmology, we are interested in the spatially averaged energy density of electromagnetic waves. Consider a vector potential which is a linear combination (for simplicity of calculation, include finitely many terms in the sum) of plane waves of different wavenumbers. Show that the spatially averaged energy density of the full electromagnetic field is the linear combination of the spatially averaged energy densities of each plane wave. Thus, we can consider the spatially averaged energy density per wavenumber. Next, consider an electromagnetic plane wave of wavenumber $\vec{k}$ and use the results of problem 4.44 to show that for each wavenumber and helicity, the electromagnetic wave is identically a harmonic oscillator. Then, show that for a harmonic oscillator the energy of the oscillator is $E = \omega J$ where ω is the angular frequency of the oscillator and J is adiabatically invariant. Using this and the dispersion relation $\omega = |\vec{k}|$ for electromagnetic waves, show that the energy density $\mathcal{E}_r(t)$ of electromagnetic radiation at a general time is given by:

$$\mathcal{E}_r(t) = \frac{\mathcal{E}_r^{(0)}}{a^4(t)}$$

where $\mathcal{E}_r^{(0)}$ is the energy density of electromagnetic radiation in the present, assuming that the rate of expansion is much slower than the rate of oscillation of the wave (which is very well-satisfied in life).

- (e) Consider the universe to have a nonzero cosmological constant Λ . Show that the energy density due to the cosmological constant is:

$$\mathcal{E}_\Lambda(t) = \mathcal{E}_\Lambda^{(0)} = \frac{\Lambda}{8\pi G}.$$

- (f) Using the results of the previous parts and assuming there is negligible exchange of energy between matter and radiation, show that the Friedmann equation can be written as:

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3} \left(\frac{\mathcal{E}_m^{(0)}}{a^3} + \frac{\mathcal{E}_r^{(0)}}{a^4} + \mathcal{E}_\Lambda^{(0)} \right) - \frac{k}{a^2}.$$

This is the absolute simplest cosmological model. Let H_0 , called the Hubble parameter, be the value of $\dot{a}$ at the present time. Show that there is a critical energy density $\mathcal{E}_{\text{crit}}$ so that the sign of the curvature of the universe is determined by whether the present energy density is above or below this critical amount (the sign of k matches the sign of $\mathcal{E}^{(0)} - \mathcal{E}_{\text{crit}}$). Show that $\mathcal{E}_{\text{crit}}$ is given by:

$$\mathcal{E}_{\text{crit}} = \frac{3H_0^2}{8\pi G}.$$

- (g) Define a normalized time coordinate $t' = H_0 t$ to use for the rest of this question (equivalently, define the units of the time coordinate so that H_0 has the numerical value 1). Define the relative densities $\Omega_m, \Omega_r, \Omega_\Lambda$ by the ratio of the respective present energy densities to the critical energy density:

$$\Omega_m = \frac{\mathcal{E}_m^{(0)}}{\mathcal{E}_{\text{crit}}}, \quad \Omega_r = \frac{\mathcal{E}_r^{(0)}}{\mathcal{E}_{\text{crit}}}, \quad \Omega_\Lambda = \frac{\mathcal{E}_\Lambda^{(0)}}{\mathcal{E}_{\text{crit}}}.$$

Show that in terms of the normalized time and relative densities, the Friedmann equation can be written even more simply as:

$$\dot{a}^2 = 1 - \Omega_\Lambda - \Omega_m - \Omega_r + \Omega_\Lambda a^2 + \frac{\Omega_m}{a} + \frac{\Omega_r}{a^2}.$$

- (h) Suppose light was emitted from a distant source long ago at cosmological time t_{emit} . Define the redshift z of the observed light as the difference in the emitted and observed frequency of the light, divided by the observed frequency:

$$z = \frac{\omega_{\text{emitted}} - \omega_{\text{observed}}}{\omega_{\text{observed}}}.$$

Show that z is related to the scale factor by:

$$z = \frac{1}{1 + a(t_{\text{emit}})}.$$

The electromagnetic spectrum given off by stars is understood using Planck's law (5.12.122) (which we derive from fundamental principles in Part II). Using Planck's law as the theoretical emitted spectrum and comparing with the observed spectrum of various stars, the redshift of light from each of those stars can be calculated. In turn, this gives a measurement of the scale factor at the time the light from those stars was emitted, which then using the numerical solution to the Friedmann equation can be inverted to identify the time since that light was emitted, thus giving a measure of distance. This method allows us to measure the distances to other galaxies. Based on these measurements and their implications for the Friedmann equation, it is possible also to measure the values $H_0, \Omega_m, \Omega_r, \Omega_\Lambda$. There is currently enormous experimental tension on the correct value of H_0 , but it is of the order of $2.2 \times 10^{-18} \text{s}^{-1}$ (and so the universe is expanding, because it is positive). Astonishingly, the experimental value of $\Omega_m + \Omega_r + \Omega_\Lambda$ is consistent with 1, and so the universe seems to be flat on extremely large scales.

- (i) With the information in the previous parts, show that at sufficiently earlier times, a becomes arbitrarily small and so radiation dominates the time evolution of the universal expansion rate in the early universe. Show that in the radiation dominated phase of the Friedmann equation, the scale factor has the approximate time dependence:

$$a(t) \approx \sqrt{2\sqrt{\Omega_r}(t - t_0)}$$

for some constant t_0 and thus there is a time at which the universe shrinks to a point ($a(t_0) = 0$) in this model. The moment at which the universe contracts to a point if the time evolution is run backward is called the Big Bang. Knowing the values of the parameters of the Friedmann equation thus gives a way to calculate the time since the Big Bang (about 13.7 billion years). Sometimes the time since the Big Bang is called the age of the universe, however, the Friedmann equation is derived from Einstein's equations, which are only the lowest order possible theory of gravity and based on modern high energy physics it is understood that at sufficiently high energies Einstein's equations are necessarily modified. These and other possible modifications to the theory become increasingly important in the

early universe, and so the validity of the Friedmann equation as a model breaks down sufficiently far in the past. Because of this, the Big Bang should more correctly be understood as the time at which the universe was so much more compressed than today that we cannot extrapolate time evolution backward past it using any theory we know of, rather than the point at which existence literally began.

- (j) With the information in the previous parts, show that at sufficiently late times, a becomes arbitrarily large if the cosmological constant is positive (which it seems to be by experiment) and so the cosmological constant dominates the time evolution of the universal expansion rate in the late universe. Show that in the cosmological constant dominated phase of the Friedmann equation, the scale factor has the approximate time dependence:

$$a(t) \approx e^{\sqrt{\Omega_\Lambda}(t-t_1)}$$

for some constant t_1 . Far out, everything's going very far out.

7.9 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 7.4: Aristotle's Force Revisited** demonstrates that any autonomous motion of a particle on a pseudo-Riemannian manifold can be described by a geometric variational principle given by a sum of the geodesic distance and the usual contribution from a vector potential.
- **Problem 7.12: Familiar energy-momentum tensors in curved spacetime** explicitly confirms that the energy-momentum tensor which appears in Einstein's equations coincides with the energy-momentum tensor we have previously found for various theories of interest, as required by the Belinfante-Rosenfeld theorem.
- **Problem 7.16: Schwarzschild Solution** and
- **Problem 7.17: Schwarzschild Black Hole** and
- **Problem 7.18: Precession of Mercury** and
- **Problem 7.19: Bending of Light by Gravity** and
- **Problem 7.20: Deflection of Light by Schwarzschild** establish basic physically observable and properties of spherically symmetric gravitating bodies, including nonspinning black holes. These questions describe the simplest ways in which general relativity has been experimentally shown to supersede Newton's theory of gravity.
- **Problem 7.21: Kerr-Schild Solutions** and
- **Problem 7.22: The Kerr Solution and the Newman-Janis Shift** and
- **Problem 7.23: Geodesics in Kerr and the Carter Constant** study the basic physical properties of stationary spinning black holes and their extraordinary mathematical structure.
- **Problem 7.24: Exact Gravitational Waves** and
- **Problem 7.25: Perturbative Gravitational Waves** and
- **Problem 7.26: Measuring a Gravitational Wave** describe the absolute basics of gravitational wave physics, which is currently an extremely active area of research which provides high precision tests of general relativity.
- **Problem 7.27: Robertson-Walker Metric** and
- **Problem 7.28: Cosmology and the Friedmann equation** describe the basics of cosmology and the distant past and distant future of our universe.

In this chapter we developed the theory of general relativity. This theory finally gave us an experimentally consistent theory of gravity consistent with the principles of relativity, specifically, the causality structure implied by Lorentz transformation symmetry and the universal invariance of the speed of light. General relativity provides a highly technical and sophisticated theory which remains in perfect agreement with experiment to the present day. General relativity has many properties which are directly analogous to electromagnetism. In electromagnetism, the vector potential has a gauge transformation symmetry and couples to the electric current. The gauge transformation symmetry is interdependent with the local conservation of the electric current by Noether's theorem. In general relativity, the spacetime metric has diffeomorphism symmetry, which is a kind of gauge transformation symmetry, and couples to the energy-momentum tensor. The diffeomorphism symmetry is interdependent with the local conservation of energy-momentum by Noether's theorem.

In section 7.1, we deduced that the appropriate relativistic generalization of the Newtonian concept of gravity coupling to mass is for gravity to couple to energy-momentum and that the necessary resulting symmetry from that coupling is local spacetime translational symmetry, or equivalently diffeomorphism symmetry. We then detailed the basic mathematical properties of diffeomorphisms and found that the appropriate dynamical degrees of freedom for general relativity are captured in the metric tensor of the spacetime. In section 7.2, we discussed how to define a geometrically meaningful notion of a derivative on a spacetime manifold, leading to the introduction of the connection coefficients, and we discussed the geodesic equation. In section 7.3 we discussed the motion of a point particle in general relativity under the influence of gravity and electromagnetism. In 7.4 we discuss how to define geometrically meaningful integration on a spacetime manifold and found the appropriate manifold generalization of Stokes' theorem. In section 7.5 we studied the Riemann curvature tensor and Wilson loops as capturing the curvature structure of the spacetime manifold. We found that the Riemann tensor arises quite naturally in calculations because it is contained in the commutator of two covariant derivatives. In section 7.6 we studied how to formulate our existing classical field theories, such as electromagnetism, in a curved spacetime. In doing so, we found the appropriate curved

spacetime generalization of Noether's theorem. As well, we proved the Belinfante-Rosenfeld theorem which establishes precisely how to define the energy-momentum tensor and demonstrates that it is very simply related to the metric derivative of the action. In section 7.7 we found the lowest order action consistent with diffeomorphism symmetry, known as the Einstein-Hilbert action. That action has two free parameters. We found by matching to the Newtonian limit that one of those parameters is simply the Newtonian gravitational constant. The other parameter, known as the cosmological constant, represents a uniform background energy density which affects the large scale shape of spacetime. In section 7.8 we derived the Hamiltonian formulation of general relativity, known as the ADM formalism, and found the appropriate general relativistic expressions for total energy and linear momentum of a spacetime. It is possible to follow the same arguments to define a notion of total angular momentum (however this has some serious subtleties).

This chapter is by no means a complete treatment of essential topics in general relativity. Refer to [122], [72], and [14] for strong general treatments. For more on black holes, study [88], [15], [42]. For more on gravitational waves, study [65]. There are still many more technical topics of great importance not fully covered in these works, such as the BMS group. Because general relativity is quite an advanced topic, specialized reading beyond textbook level is typically needed for answering highly specific questions.

7.10 Conclusion to Part I

Here we arrive at the end of basing physics on classical particles. As we found in chapter 4, true point particles are fundamentally problematic at a theoretical level due to not having well defined interactions with electromagnetism and experimentally troublesome due to their inability to explain the interference pattern observed in the Davisson-Germer experiment. While they cannot be exactly maintained fundamentally, point particles are an extremely useful effective theory almost all the time at every day scales. Thus, for a very large number of applications classical physics is and will always be useful.

In our studies of classical particles, we have uncovered Newton's gravity, special relativity, electromagnetism, and general relativity. We also found that although we must abandon point particles, in order to so in a way consistent with special relativity we cannot replace them with finite size rigid bodies. Instead, we must replace point particles by a continuous jiggling description. In other words, we must replace them with waves using a classical field theory. Doing so will be one of the two principle objectives of Part II. One may wonder why not try to use the continuum mechanical models we derived this chapter as our fundamental description of matter? While they are macroscopically accurate for many particle systems, they turn out to not be correct at the extremely microscopic level when discussing only a few particles. Instead, we will be more general and come up with a better microscopic theory which reduces to continuum mechanics when many particles are involved. However, there are actually many useful features of that better theory (quantum mechanics) already present within continuum mechanics, so continuum mechanics will continue to be helpful for developing intuition.

Maxwell's electromagnetism will be the most everlasting theory found so far. It is the most widely used and precisely measured interaction in physics and remains valid far beyond the regime in which we have applied it so far. However, we found that there is an unavoidable tension between our present theory of electromagnetism and statistical mechanics. Apparently, any electromagnetic system should have infinite heat capacity and be at 0 temperature, which is certainly false experimentally (look at the Sun, but only briefly). Resolving this tension will be the second of our principle objectives in Part II. We will ultimately find that in chapter 1 when we decided to base our description of physics on the Poisson representation, which is an unfaithful representation of the Lie bracket, we ended up automatically choosing the statistical properties of our systems. In Part II we will see that the faithful representation given by quantum mechanics (and when applied to fields, quantum field theory) changes the high energy behavior of the divergent integral in the ultraviolet catastrophe and leads to finite and experimentally valid results, among thousands of other nontrivial experimental checks of quantum mechanics. This requires too many new ideas to be introduced to really explain it here, but know that the ultraviolet catastrophe is an extremely important problem which will fundamentally guide our thinking in Part II.

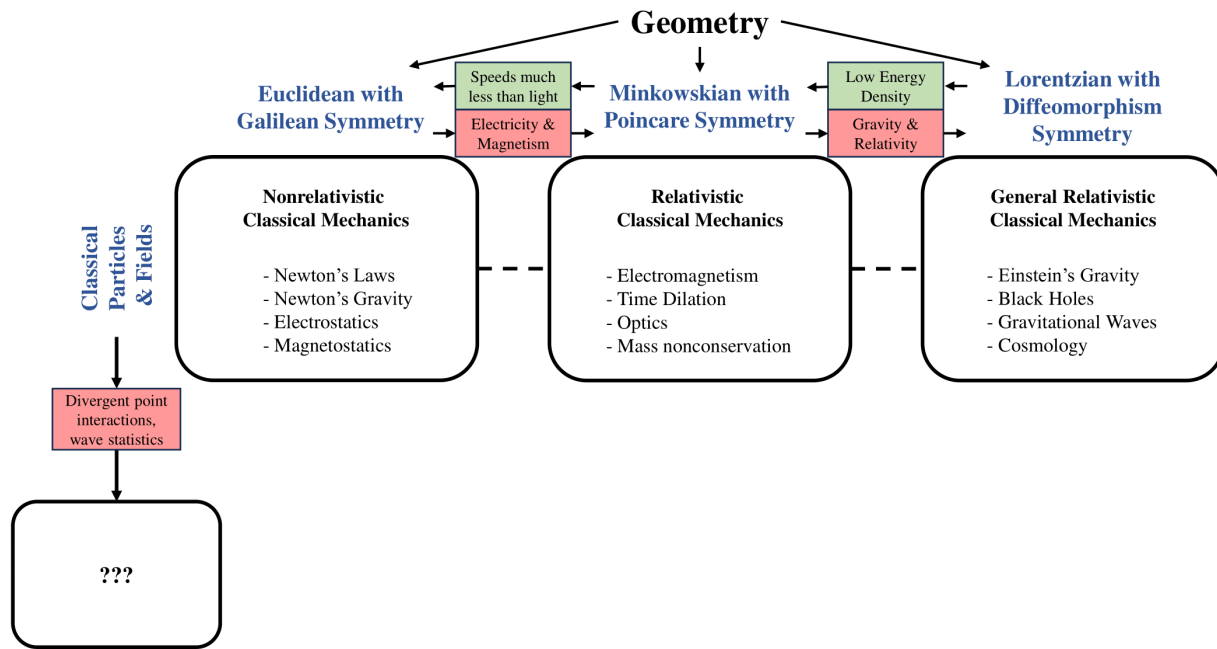


Figure 7.1: Our perspective on physics as of the end of this volume. Lorentz boost symmetry was able to solve the problem of electromagnetic coexistence but did nothing to affect the problem of point particle divergences. Diffeomorphism symmetry was able to provide for a relativistically consistent theory of gravity. However, we remain without a valid model of matter superior to point particles even though we know that point particles do not have mathematically well-defined interactions with gravity or electromagnetism. The statistical properties of classical field theory are at odds with experiment. With our knowledge so far, we cannot answer the question why does hot metal glow, because we can't even explain how metal can be hot.

Part II

Quantum Physics

Quantum Mechanics can be understood, and it can be understood by you.

Chapter 8

Single Particle Quantum Mechanics

If you feel a function $\psi(t, \vec{x})$ is abstract, imagine a whole system full of jello - beautiful green jello of the best transparency - and $\psi(t, \vec{x})$ representing some disturbance of that quantum jello from equilibrium. No position $\vec{x}$ moves. It is the jello that jiggles, shakes, and twists, always and forever. It's beautiful!

– John P. Ralston [92]

A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die.

– Max Planck [87]

If it's not in your equations, it's not in your theory.

Let's fix the point particle problem. We found that interacting point particles tend to have infinite energy, do not interact consistently with electromagnetism, and experimentally do not produce the observed macroscopic properties of matter. The most obvious solution is to try particles with a non-zero size. However, if the shape and size of a body are rigid then when one part of it moves the rest must move correspondingly. Hence, a force applied at one end of a rigid body causes the other end to move instantaneously, communicating faster than light. As such, exactly rigid bodies are inconsistent with causality in relativistic theories. Therefore neither point particles nor rigid bodies are ultimately viable for fundamental physics. All that is left is that the size and shape of matter must themselves be dynamical. That is, we need a description about how much matter is at each point in space which is allowed to change in time. Thus, there will be some field(s) $Q(t, \vec{x})$ which ultimately give the amount and configuration of matter at the location $\vec{x}$ and time t , in other words, a classical field theory of matter. Of course, given the success of the point theory of matter under certain conditions, we also need our field theory of matter to reduce to the point theory in those conditions. The description of matter by fields is called a wave theory of matter. While when we modeled a unit of matter as being a point particle we called it classical mechanics, when we model a unit of matter as being a wave we call it **single particle Quantum Mechanics**, a quite confusing name which we will clear up with time.

Before continuing onto the details, it is worth taking a moment to dispel some common misconceptions. In this chapter we cover single particle quantum mechanics, meaning we will describe a single blob of matter by a classical field (and will have it interact with stuff we already know about, like electromagnetism). Quantum mechanics is more general and powerful than covered this chapter and is the focus of this entire volume. Some readers with prior studies are likely to object to thinking about quantum mechanics like a classical field theory at all, but when considering a single particle it literally is so. They are different when considering multiple interacting particles; we will get there later. Less experienced readers are likely to be very confused about the language “quantum particle” used when describing a classical matter wave. This language is used because when our classical matter wave is only in a small region of space compared to all experimentally

relevant length scales and all parts of the wave are moving at about the same velocity, the center of mass and total momentum of that classical matter wave approximately satisfy the classical particle equations of motion (we will prove this). Under those circumstances that wave is said to be “in the classical limit” and the relevant physical consequences are generally accurately described by the point-particle theories from Part I. Remember that particle in general does **NOT** mean point-particle. We use the term particle to refer to the constituents/ingredients of our physical description, not a moving point in space. A point-particle is a specific model of matter particles which has for more than a century now been known to be **WRONG** at the level of fundamental physics.

What does the name quantum theory mean? It means anything described by the Schrödinger equation (or the related von Neumann equation) to be introduced in section 8.2. That equation is *enormously* generic. Quantum theory translated into less magical sounding words would just be called “generic Hamiltonian linear wave theory”. Readers are likely to encounter some of the following claims about quantum mechanics:

1. Electrons instantly jump between discrete atomic orbits (the Bohr model).
2. Everything in quantum mechanics is discrete. The action of any quantum system can only ever be a half-integer multiple of Planck’s constant $\hbar$ (the Bohr-Sommerfeld theory).
3. Due to the Heisenberg uncertainty principle it is impossible to know both the position and momentum of a particle at once. Knowing one makes knowing the other impossible.
4. An electron is both a wave and a point-particle at the same time except when you don’t look at it because then it is neither and except when you do look at it because then it chooses to be one or the other (wave-particle duality as it might be described in a popular science magazine).
5. When an observable is measured, the system instantaneously and fundamentally randomly collapses to an eigenstate of the operator representing that observable and the experiment records the corresponding exact eigenvalue of that eigenstate as the measured value (naive collapse postulate).
6. *Nobody really understands quantum mechanics.* – Richard Feynman [26].

These are a few among many similar common paradoxical statements about quantum mechanics. Every one of these is ridiculous and based on an incomplete understanding of both the math and physics of quantum mechanics from a century ago. These have long since been explained by much clearer and more reasonable thinking. That thinking has so far failed to propagate into lower level courses, unfortunately, or into the minds of people who just “shut up and calculate”. The era from 1900-1925 was bizarre. Problems with classical physics were known but the actual equation defining quantum mechanics (the Schrödinger equation) was not discovered until 1925. For 25 years many physicists said a great deal of wrong things now called “old quantum theory”. **Old quantum theory is NOT the basis of modern quantum mechanics** at all and learning it is mostly actively detrimental to your physics education. While it may be interesting from a historical perspective, it is not helpful for understanding quantum mechanics. Because science is iterative and gradual and it takes time to iron out inconsistencies and change minds, many scientists continued to think about and teach quantum mechanics using old quantum theory terms while presenting actual quantum mechanical equations even well after 1925. Actual quantum mechanics contradicts old quantum theory in countless fundamental ways and old quantum theory was never a coherent theory to begin with, just a loose collection of claims. The tension between those claims has caused enormous confusion for many years among students learning quantum mechanics. This confusion is rooted in history, not physics, and is not necessary for you to experience. I will briefly¹ respond to the above misconceptions, with the fullness of detail to come from reading the rest of this book.

1. In 1925 the Schrödinger equation completely replaced the “old quantum theory” Bohr model of the atom. While the Schrödinger equation does have resonances (specific frequencies it responds very strongly to), it contains no instant jumping nor a discrete response to external sources. The Schrödinger equation is fully consistent with experiment and produces atomic solutions that are smooth in space and time.

¹Here I am a victim of Brandolini’s law: the amount of energy needed to refute bullshit is an order of magnitude bigger than that needed to produce it.

2. Space, time, the action, energy, the fields, the observables, nearly everything in quantum mechanics is continuous. Quantum mechanics is actually *more* continuous than classical mechanics, because it is about waves, not discrete point particles. Some systems have discretely separated eigenvalues, but that does not correspond to having discrete physical properties. For some simple systems those eigenvalues can be calculated approximately using a mathematically souped-up version of the Bohr-Sommerfeld method that explains why that *approximation* ever gave any right answers and it explains why often it doesn't. You should completely drop the old quantum theory belief that everything is discrete.
3. The uncertainty principle is not about measurement. The unqualified "position" of a body of finite size is not uniquely defined. Nobody believes it is a deep principle that you cannot know the exact definite position of a coffee cup. It is exactly as true as saying you cannot know the exact position of an electron. There are infinitely many points on a coffee cup I could call the position and so because it is spread out in space it has no definite position. However, if I say I want to know the center of mass position of the coffee cup then that is perfectly well defined and can be known arbitrarily well. Similarly, while there are infinitely many points you could call the position of a wave, the center of mass position of that wave (such as an electron) is perfectly and exactly well defined and could be known arbitrarily well. There is no fundamental tension between defining the center of mass position of that wave to any given precision and defining the total linear momentum carried by that wave to any given precision.

When stated properly, the Heisenberg uncertainty principle is actually just a theorem of mathematics and is not about physics. A wave cannot be both a Dirac delta (meaning all located at one place) and a plane wave (meaning consisting entirely of one wavenumber) at the same time. This is as obvious as it sounds, because a Dirac delta $\delta(x)$ is not a plane wave e^{ikx} . One can do a bit better and show that the closer to being a Dirac delta a wave is, the further from being a plane wave it is, and vice versa, and give a precise bound on how close you can be to one for a given closeness to the other. There is purely mathematical a limit to how scrunched up a wave can be in space for a given range of wavenumbers it is allowed to be a linear combination of.

The uncertainty theorem only connects with physics in the classical limit (the limit that a quantum system approximately behaves like a simpler classical system). Under circumstances where a wave packet behaves approximately like a localized particle, how spread out a wave is in space (call the characteristic spatial width σ_x) has to be much smaller than our experimental length resolution w_x . (Otherwise you would see the wave having obvious finite size, so not approximately point-like.) How spread out a wave is in Fourier space (call the characteristic Fourier width σ_k) tells you about relative velocities between different parts of the wave, because as we found in chapter 4 the wavenumber can be used to compute a wave's group velocity. When a wave contains many wavenumbers, the different parts of it will move at different speeds and it will disperse in space. If the classical limit is to be a valid approximation for a given experiment, the wave packet needs to remain approximately localized in space and so we need it to also be approximately localized in Fourier space so that it doesn't spread out too much. Therefore, the classical limit requires that both σ_x and σ_k are small with respect to our experimental resolution. The uncertainty theorem gives a limit on how small σ_x and σ_k can simultaneously be, and thus sets a limit to how good of an approximation the classical theory can be to the full quantum theory.

4. The above explanation hopefully helps you develop the intuition that an electron is always described by a wave equation and that only under the circumstances of the classical limit can we approximate that wave description by a localized classical particle description. We still tend to call the electron a particle, in the sense that it is a basic constituent of the theory, but remember that does not mean it is ever a point-particle (it isn't). This real and self-consistent statement of the wave-particle duality is sometimes called the "opticommechanical analogy" and it is just the observation we made in problem 4.50 that under suitable approximations the center of a wave packet moves around like a classical particle.
5. Effectively instantaneous and effectively random collapse is a macroscopic approximate phenomenological description of the results of some measurement devices. In a real measurement process the system of interest interacts with a measurement device. Because quantum systems are very small compared to experiments which are always done in a thermal background of many degrees of freedom in which statistical mechanics is relevant, measurement of individual events in quantum mechanics has to be treated with statistical mechanics. This requires no fundamental randomness and causes the dynamical emergence on macroscopic scales of statistical behavior described by the Born rule. Collapse to an

eigenstate is a situationally appropriate approximate model of some measurements after a finite amount of time. This will be a major subject of chapter 9.

6. Feynman's quote is from 1964. Maybe when he said it almost everyone was confused. Sixty years of science have been done since then and his view, given when my grandparents were children, does not represent the present. Many essential technologies of the modern world work only because of how incredibly well we understand quantum mechanics. Do not fall victim to magical thinking. The day you do, you have turned from a scientist into a priest. *This is the 21st century. This is the century when everybody must understand quantum mechanics.* – John P. Ralston [93].

8.1 The Linear Algebra of Fields

Call the field we will use to describe matter $Q(t, \vec{x})$ and its conjugate momentum field $P(t, \vec{x})$. We don't really know at this point whether Q should be single number valued (like the scalar potential), vector valued (like the vector potential), or something else. So, for now we will proceed allowing Q to have an arbitrary unknown number of components. Still then, $Q(t, \vec{x})$ at a fixed point in time is a vector (in the math sense, meaning an element of some vector space, not in the sense of a vector in space or spacetime) valued function of position. Let us call the vector space that Q at a particular $(t, \vec{x})$ lives in $\mathbb{H}_{\text{int}}(t, \vec{x})$ so that $Q(t, \vec{x}) : \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{H}_{\text{int}}$. This $\mathbb{H}_{\text{int}}$ is called the “internal space” or space of internal degrees of freedom. We notate $\mathbb{H}_{\text{int}}(t, \vec{x})$ with the $(t, \vec{x})$ simply to indicate that because Q is defined at each $(t, \vec{x})$, there is a different “copy” of the vector space $\mathbb{H}_{\text{int}}$ at each $(t, \vec{x})$. The set of vector valued functions with addition and multiplication by constants is closed under such operations and so itself a vector space² which we will call $\mathbb{H}$. That is, $\mathbb{H}_{\text{int}}$ is the space of possible values of $Q(t, \vec{x})$ at a particular $(t, \vec{x})$ whereas $\mathbb{H}$ is the space of all configurations of the function Q at a particular time.

Recall the defining feature of the Dirac delta:

$$f(\vec{x}) = \int_{\mathbb{S}} f(\vec{x}') \delta(\vec{x} - \vec{x}') d^d \vec{x}'. \quad (8.1.1)$$

That is, any function f can be written as a linear combination (integral) over itself times the Dirac delta. If we view the function $f(\vec{x})$ as a vector in the vector space of (locally integrable) functions, then equation (8.1.1) says that any (locally integrable) function can be written as a linear combination of deltas with different centers (the center of a delta is the location of its peak) with appropriate coefficients (those coefficients being the value of the function in question at the center of the corresponding delta). As such, this means that the deltas form a basis of the vector space of (locally integrable) functions in space. We call the vector space of functions we are considering $\mathbb{H}_{\mathbb{S}}$ where $\mathbb{S}$ is for space. This motivates introducing the Dirac notation to make the linear algebra here more apparent. That is, we write the symbol $|\vec{x}\rangle$ to mean a delta with center at location $\vec{x}$ and $|f\rangle$ to mean the element $f(\vec{x})$ in the vector space of functions. Rewriting equation (8.1.1) in this notation:

$$|f\rangle = \int_{\mathbb{S}} f(\vec{x}') |\vec{x}'\rangle d^d \vec{x}'. \quad (8.1.2)$$

This simply makes the thinking more clear: $|f\rangle$ is a linear combination of the basis vectors $|\vec{x}\rangle$ and the coefficients in the expansion are $f(\vec{x})$. This notation is also very useful for writing inner products. For two real vectors $\vec{u}$ and $\vec{v}$ with components u^a and v^a in an orthonormal basis, the inner product is defined as:

$$\vec{u} \cdot \vec{v} = \sum_{a=1}^D u^a v^a. \quad (8.1.3)$$

This allows one to define $\vec{u}^T \stackrel{\text{def}}{=} \vec{u} \cdot$ as the “row vector”, “dual vector”, “covector”, or “linear functional” (depending on your favorite flavor of name) as the object which when matrix multiplied onto $\vec{v}$ returns the inner product:

$$\vec{u}^T \vec{v} \stackrel{\text{def}}{=} \vec{u} \cdot \vec{v}. \quad (8.1.4)$$

In the Dirac notation, the dual vector to $|f\rangle$ is written as $\langle f|$. Because our vector space now has a continuous basis, the sum in equation (8.1.3) becomes continuous (and so is an integral). Hence the inner

²There are many mathematically interesting technical issues here and ahead regarding Rigged Hilbert spaces, distributions, and the finer details of harmonic analysis. While important, those features will not be necessary for us to pay attention to.

product on the vector space of real valued functions is defined as:

$$f \cdot g \stackrel{\text{def}}{=} \int_{\mathbb{S}} f(\vec{x})g(\vec{x})d^d\vec{x}. \quad (8.1.5)$$

Or, in the Dirac notation:

$$\langle f|g\rangle = \int_{\mathbb{S}} f(\vec{x})g(\vec{x})d^d\vec{x}. \quad (8.1.6)$$

For complex vectors, the mathematically convenient definition of the inner product is slightly different. The complex inner product is defined by:

$$\vec{u} \cdot \vec{v} \stackrel{\text{def}}{=} \sum_{a=1}^D u_a^* v_a. \quad (8.1.7)$$

The space of complex numbers is equivalent to the plane of ordered pairs of real numbers (identifying the real and imaginary parts as the components of the ordered pair) along with a multiplication rule (the definition of complex multiplication). As such, we can think of a complex vector of complex dimension D as a real vector of dimension $2D$. We can see why this definition of the complex inner product is natural by looking at what it does to two 1 dimensional complex numbers $a + ib$ and $c + id$. Then:

$$(a + ib) \cdot (c + id) = (a - ib)(c + id) = ac + bd + i(ad - bc) = (a, b) \cdot (c, d) + i \det \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (8.1.8)$$

Thus, the real part of the complex inner product matches the real inner product of the real vectors formed from the complex numbers and the imaginary part matches the signed area of the parallelogram spanned by those real vectors. Both the real and imaginary parts of the complex inner product carry geometrically meaningful information about the vectors!

For complex valued functions f and g then we define the inner product by:

$$\langle f|g\rangle = \int_{\mathbb{S}} f^*(\vec{x})g(\vec{x})d^d\vec{x}. \quad (8.1.9)$$

Following from the definition of the inner product and $|\vec{x}\rangle$:

$$\langle \vec{x}|\vec{x}'\rangle = \int_{\mathbb{S}} \delta(\vec{x} - \vec{x}'')\delta(\vec{x}' - \vec{x}'')d^d\vec{x}'' = \delta(\vec{x} - \vec{x}') \quad (8.1.10)$$

$$\langle \vec{x}|f\rangle = \langle \vec{x}|\int_{\mathbb{S}} f(\vec{x}')|\vec{x}'\rangle d^d\vec{x}' = \int_{\mathbb{S}} f(\vec{x}')\langle \vec{x}|\vec{x}'\rangle d^d\vec{x}' = \int_{\mathbb{S}} f(\vec{x}')\delta(\vec{x} - \vec{x}')d^d\vec{x}' = f(\vec{x}) \quad (8.1.11)$$

$$\int_{\mathbb{S}} |\vec{x}\rangle\langle \vec{x}|d^d\vec{x}|f\rangle = \int_{\mathbb{S}} |\vec{x}\rangle\langle \vec{x}|f\rangle d^d\vec{x} = \int_{\mathbb{S}} |\vec{x}\rangle f(\vec{x})d^d\vec{x} = |f\rangle. \quad (8.1.12)$$

Equation (8.1.10) is what we mean by an orthonormal basis on our vector space of functions $\mathbb{H}_{\mathbb{S}}$. Equation (8.1.11) gives a way to think about the explicit function $f(\vec{x})$ just as the inner product $\langle \vec{x}|f\rangle$. Equation (8.1.12) shows that acting $\int_{\mathbb{S}} |\vec{x}\rangle\langle \vec{x}|d^d\vec{x}$ on any element of $\mathbb{H}_{\mathbb{S}}$ space returns that element. Hence, $\int_{\mathbb{S}} |\vec{x}\rangle\langle \vec{x}|d^d\vec{x}$ is the identity operator:

$$\int_{\mathbb{S}} |\vec{x}\rangle\langle \vec{x}|d^d\vec{x} = \mathbb{1}. \quad (8.1.13)$$

This is called the completeness relation.

As we said before, our field $Q(t, \vec{x})$ may have more than one component and so in general is an element of $\mathbb{H}_{\text{int}}$. We define $|Q\rangle$ to mean the element in the vector space of all field configurations $\mathbb{H}$. The vector space of field configurations allows one to pick at each point in space $\vec{x}$ at time t an element of $\mathbb{H}_{\text{int}}(t, \vec{x})$, the vector space that $Q(t, \vec{x})$ maps to. Whenever for each element of one vector space you can pick an element of another and that ordered pair is in a new combined vector space, that combined vector space is called the tensor product of the individual spaces. This is precisely the same tensor product structure introduced in section 4.9. That is, if we have a vector space $\mathbb{H}_1$ with basis elements $|a_1\rangle$ indexed by a so that a general element $|\psi_1\rangle$ of $\mathbb{H}_1$ is given by a linear combination of those elements:

$$|\psi_1\rangle = \sum_a \psi_1^a |a_1\rangle \quad (8.1.14)$$

with some components ψ_1^a and another vector space $\mathbb{H}_2$ with basis elements $|b_2\rangle$ indexed by b so that a general

element $|\psi_2\rangle$ of $\mathbb{H}_2$ is given by a linear combination of those elements:

$$|\psi_2\rangle = \sum_b \psi_2^b |b_2\rangle \quad (8.1.15)$$

with some components ψ_2^b then the tensor product space $\mathbb{H}_1 \otimes \mathbb{H}_2$ is defined by identifying basis vectors $|a_1 b_2\rangle$ written as:

$$|a_1 b_2\rangle = |a_1\rangle \otimes |b_2\rangle \quad (8.1.16)$$

and is given by the set of all linear combinations of these elements so that a general element of $|\psi\rangle$ of $\mathbb{H}_1 \otimes \mathbb{H}_2$ is given as:

$$|\psi\rangle = \sum_{a,b} \psi^{ab} |a_1 b_2\rangle \quad (8.1.17)$$

for some components ψ^{ab} . The tensor product $\otimes$ between elements of two vector spaces is defined to be linear and associative:

$$|\phi_1\rangle \otimes (\alpha|\phi_2\rangle + \beta|\psi_2\rangle) = \alpha|\phi_1\rangle \otimes |\phi_2\rangle + \beta|\phi_1\rangle \otimes |\psi_2\rangle \quad (8.1.18)$$

$$(\alpha|\phi_1\rangle + \beta|\psi_1\rangle) \otimes |\phi_2\rangle = \alpha|\phi_1\rangle \otimes |\phi_2\rangle + \beta|\psi_1\rangle \otimes |\phi_2\rangle \quad (8.1.19)$$

$$(|\phi\rangle \otimes |\psi\rangle) \otimes |\varphi\rangle = |\phi\rangle \otimes (|\psi\rangle \otimes |\varphi\rangle). \quad (8.1.20)$$

With these properties, the tensor product of two vector spaces produces the same space regardless of which bases $|a_1\rangle$ and $|b_2\rangle$ are used to construct it. Because for each $(t, \vec{x})$ we can select an element of $\mathbb{H}_{\text{int}}$, the vector space of field configurations $\mathbb{H}$ is the tensor product of our vector space of functions $\mathbb{H}_{\mathbb{S}}$ with the vector space of internal degrees of freedom $\mathbb{H}_{\text{int}}$. Thus, we write $\mathbb{H} = \mathbb{H}_{\mathbb{S}} \otimes \mathbb{H}_{\text{int}}$. This changes the completeness relation equation (8.1.13) slightly to say that instead of the left hand side equaling the identity operator on the whole vector space, it equals just the identity operator on $\mathbb{H}_{\mathbb{S}}$. At this point it is a good idea to revisit problem 4.76 to better understand tensor products.

When the field Q is real and has multiple components, $\langle Q|$ is still defined so that the inner product matches the existing definition:

$$\langle Q| \text{ defined so that for all } |Q'\rangle : \langle Q|Q'\rangle = \int_{\mathbb{S}} Q^T(\vec{x}) Q'(\vec{x}) d^d \vec{x}. \quad (8.1.21)$$

Here the transpose is taken on the internal space. For complex valued fields this generalizes exactly as before where we define:

$$\langle Q| : \langle Q|Q'\rangle = \int_{\mathbb{S}} (Q^T)^*(\vec{x}) Q'(\vec{x}) d^d \vec{x} = \int_{\mathbb{S}} Q^\dagger(\vec{x}) Q'(\vec{x}) d^d \vec{x}. \quad (8.1.22)$$

The complex conjugate of the transpose is a clunky notation but will come up often and so to avoid the mess, in the above we introduced the Hermitian conjugate or adjoint, notated with the dagger, as the conjugate transpose: $Q^\dagger = (Q^T)^*$.

With the Dirac notation, we can think of fields as vectors in an infinite dimensional vector space (there are infinitely many choices for $\vec{x}$) and so we can use results about the analytical mechanics of vectors when discussing fields. There are some significant technical details regarding extending the results of finite dimensional linear algebra to infinite dimensional vectors spaces which we will not describe in detail and which are mathematically interesting (and form the basis of the mathematical field of functional analysis). There will be some theorems and results for which we give a finite dimensional argument and then just assume the corresponding infinite dimensional result holds. This is because proving the infinite dimensional result in that case would be extremely technically challenging and for our purposes not worth the extra effort.

We are dealing with vector spaces with an inner product. Having an inner product on a vector space automatically allows one to define a norm on that vector space by the non-negative square root of the inner product of a vector with itself. Having a norm then allows one to define a distance between vectors by considering the norm of the difference of two vectors. That is, for a vector $|\psi\rangle$ in $\mathbb{H}$ we define the norm as:

$$\|\psi\| \stackrel{\text{def}}{=} \sqrt{\langle \psi | \psi \rangle}. \quad (8.1.23)$$

The norm introduces a natural notion of distance $d(u, v)$ between vectors $|u\rangle$ and $|v\rangle$:

$$d(u, v) = \|u - v\|. \quad (8.1.24)$$

We will find in the next section that we will naturally be considering fields of finite norm as our vector space of functions $\mathbb{H}_{\mathbb{S}}$. Such functions are said to be **square-integrable** because their magnitude squared has a

finite integral over all space by the definition of the norm. It turns out that a nice property of the vector space of functions with finite norm as we have defined it is that any sequence of such functions so that the distance between neighboring functions in the sequence limits to 0 itself limits to a function which also has finite norm. Thus, said space is called “complete” as it is closed under this class of limits. A vector space which both has an inner product and is complete in this sense is called a **Hilbert space**.

Theorem 8.1: Linear Algebra of Fields

A field theory with configuration fields $Q(t, \vec{x})$ of finite norm can be represented as a vector $|Q(t)\rangle$ in a Hilbert space in the Dirac notation by:

$$|Q(t)\rangle = \int_{\mathbb{S}} Q(t, \vec{x}) |\vec{x}\rangle d^d \vec{x} \quad (8.1.25)$$

where the vector $|\vec{x}\rangle$ corresponds to a Dirac delta centered at $\vec{x}$ and the inner product on the Hilbert space is given by:

$$\langle f | g \rangle = \int_{\mathbb{S}} f^\dagger(\vec{x}) g(\vec{x}) d^d \vec{x}. \quad (8.1.26)$$

The $|\vec{x}\rangle$ states satisfy the orthogonality and completeness relations:

$$\langle \vec{x} | \vec{x}' \rangle = \delta(\vec{x} - \vec{x}') \quad \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} = \mathbb{1}. \quad (8.1.27)$$

Exercises

Problem 8.1: Practice with Dirac notation. Consider a system with 1 spatial dimension and the following two vectors in the Hilbert space:

$$|\psi_1\rangle = \int_{-\infty}^{\infty} N_1 e^{-(x-\mu_1)^2/(4\sigma^2) + ik_1 x} |x\rangle dx, \quad |\psi_2\rangle = \int_{-\infty}^{\infty} N_2 e^{-(x-\mu_2)^2/(4\sigma^2) + ik_2 x} |x\rangle dx$$

for positive constants σ , N_1 , N_2 and real constants μ_1, k_1, μ_2, k_2 . Compute the following:

$$\|\psi_1\|, \quad \|\psi_2\|, \quad \langle \psi_1 | \psi_2 \rangle, \quad d(\psi_1, \psi_2).$$

Identify what values of N_1 and N_2 make $|\psi_1\rangle$ and $|\psi_2\rangle$ have norm 1. Using geometric thinking about the nature of the inner product defined in the section, try to come up with a reasonable definition of the angle θ between the vectors $|\psi_1\rangle$ and $|\psi_2\rangle$. Find a formula for that angle and compute it.

8.2 The Schrödinger Equation

The argument of this section is based on [90]. Now that we know we can simply reformulate a field theory as a vector theory in an appropriate Hilbert space, let us study the general Hamiltonian for a vector of arbitrary dimension. Let us define our vector Q (on a configuration space which is a vector space of dimension D , potentially infinite) and momentum P (giving a phase space which is a vector space of dimension $2D$). Because we would ultimately like to find a description for a wave theory of matter and matter does not seem to inescapably grow in amount with time we will suppose that our theory is stable in the sense that finite initial conditions should remain finite for all times. Consequently, this guarantees that our system has an equilibrium point (meaning a point in phase space so that if Q and P start at that location, they stay at that location for all time) [96]. Let us define Q and P so that $Q = 0, P = 0$ is such an equilibrium of our Hamiltonian (if in some coordinates this were not true, we would define new canonical coordinates equal to the old ones with the coordinate values of such an equilibrium subtracted. Subtracting constants is a canonical transformation so this is always possible to do when an equilibrium exists). Then, we can expand the Hamiltonian of the theory in a Taylor expansion near equilibrium and apply the theorem of normal modes (Theorem 1.14). Doing so, we know that in appropriately chosen coordinates our Hamiltonian can be written as:

$$\mathcal{H}(Q, P) = \sum_{k=1}^D \left(\frac{a_k}{2} Q_k^2 + \frac{b_k}{2} P_k^2 \right) + \text{Higher Order Terms} \quad (8.2.1)$$

for constants a_k and b_k with the property that $a_k b_k > 0$ for each k . Now define ω_k so that $\omega_k^2 = a_k b_k$ and so that ω_k has the same sign as both a_k and b_k . That is, $\omega_k = \sqrt{a_k b_k} \text{sgn}(a_k) = \sqrt{a_k b_k} \text{sgn}(b_k)$. Then, make the complex canonical transformation known as John's Quantum Map to new coordinates ϕ_n and momenta φ_n defined by:

$$\phi_n = \frac{1}{\sqrt{2}} \left(\left(\frac{a_n}{b_n} \right)^{\frac{1}{4}} Q_n + i \left(\frac{b_n}{a_n} \right)^{\frac{1}{4}} P_n \right) \quad (8.2.2)$$

$$\varphi_n = \frac{1}{\sqrt{2}} \left(\left(\frac{b_n}{a_n} \right)^{\frac{1}{4}} P_n + i \left(\frac{a_n}{b_n} \right)^{\frac{1}{4}} Q_n \right) = i\phi_n^* \quad (8.2.3)$$

$$\Rightarrow Q_n = \left(\frac{b_n}{a_n} \right)^{\frac{1}{4}} \frac{\phi_n - i\varphi_n}{\sqrt{2}}, \quad P_n = \left(\frac{a_n}{b_n} \right)^{\frac{1}{4}} \frac{\varphi_n - i\phi_n}{\sqrt{2}}. \quad (8.2.4)$$

Of course, one can and should check that in fact this transformation is symplectic (but you should know how to do that by now). Now writing the Hamiltonian in these new coordinates:

$$\mathcal{H} = \frac{1}{2} \sum_n (a_n Q_n^2 + b_n P_n^2) \quad (8.2.5)$$

$$= \frac{1}{2} \sum_n \text{sgn}(a_n) \left(|a_n| \left(\frac{b_n}{a_n} \right)^{\frac{1}{2}} \frac{(\phi_n - i\varphi_n)^2}{2} + |b_n| \left(\frac{a_n}{b_n} \right)^{\frac{1}{2}} \frac{(\varphi_n - i\phi_n)^2}{2} \right) \quad (8.2.6)$$

$$= \frac{1}{2} \sum_n \text{sgn}(a_n) \sqrt{a_n b_n} \frac{\phi_n^2 - 2i\phi_n \varphi_n - \varphi_n^2 + \varphi_n^2 - 2i\phi_n \varphi_n - \phi_n^2}{2} \quad (8.2.7)$$

$$= \frac{1}{i} \sum_n \omega_n \varphi_n \phi_n \quad (8.2.8)$$

By equation (8.2.3), $\varphi_n = i\phi_n^*$ and so the conjugate momentum can be written in terms of the complex conjugate. Therefore, the complex numbers ϕ_n determine the entire state. In terms of ϕ_n and ϕ_n^* :

$$\mathcal{H} = \sum_n \omega_n \phi_n^* \phi_n = \sum_n \omega_n |\phi_n|^2. \quad (8.2.9)$$

Now define a D dimensional complex Hilbert space with basis vectors $|n_\Omega\rangle$ written in components as column vectors so that $|n_\Omega\rangle$ has 0's in each entry except entry n and has entry n equal to 1. (The meaning of the subscript Ω in $|n_\Omega\rangle$ will be made clear shortly.) Then, define $|\phi\rangle$ as a vector in this Hilbert space and $\langle\phi|$ as a vector in the dual Hilbert space by:

$$|\phi\rangle = \sum_n \phi_n |n_\Omega\rangle \quad (8.2.10)$$

$$\langle \varphi | = \sum_n \varphi_n \langle n_\Omega | = \sum_n i \phi_n^* \langle n_\Omega | = i \langle \phi |. \quad (8.2.11)$$

By defining the angular frequency operator we can give a basis independent expression for $\mathcal{H}$:

$$\hat{\Omega} = \sum_n \omega_n |n_\Omega\rangle \langle n_\Omega| = \hat{\Omega}^\dagger \quad (8.2.12)$$

$$\implies \mathcal{H} = \frac{1}{i} \langle \varphi | \hat{\Omega} | \phi \rangle = \langle \phi | \hat{\Omega} | \phi \rangle. \quad (8.2.13)$$

It is now natural to see why the Hilbert space of fields with finite norm is of interest to us. If $\langle \phi | \phi \rangle$ is not finite, the $\mathcal{H}$ is liable to also be nonfinite as we could make $|\phi_n|^2$ arbitrarily large for a particular n . Thus, because we are physically interested in finite energy states we also take $\langle \phi | \phi \rangle$ to be finite. Now we can see clearly what is the meaning of the subscript Ω on $|n_\Omega\rangle$. It is a notation to help remember that $|n_\Omega\rangle$ is an eigenvector of the $\hat{\Omega}$ operator:

$$\hat{\Omega} |n_\Omega\rangle = \omega_n |n_\Omega\rangle. \quad (8.2.14)$$

From our Hamiltonian, we can compute the Lagrangian:

$$\mathcal{L} = \sum_n \varphi_n \dot{\phi}_n - \mathcal{H} = i \langle \phi | \dot{\phi} \rangle - \langle \phi | \hat{\Omega} | \phi \rangle. \quad (8.2.15)$$

Hence we see that any stable Hamiltonian to quadratic order can be written in the form of equation (8.2.13) or correspondingly its Lagrangian can be written in the form of equation (8.2.15) as long as we make sufficient variable transformations to find the appropriate expression for $|\phi\rangle$. It is important to note that we started with the real configuration space vector space of dimension D , went to the real phase space vector space of dimension $2D$ and then mapped that phase space down into a complex vector space of complex dimension D . With the Lagrangian and Hamiltonian we have found, we can now create a field theory for matter in a weak field limit about equilibrium in the correct coordinates. As such, our field theory for matter is defined by whatever $|\phi\rangle$ and $\hat{\Omega}$ are.

So far in this section we have worked under the assumption that the Hamiltonian $\mathcal{H}$ for our field would have time translational symmetry (because we believe that to be a true symmetry of the universe). However, when our field interacts with external forces we know from experience it may be interesting to consider an explicitly time dependent Hamiltonian to capture at least some of those external effects. So, sometimes we will find it useful for the angular frequency operator $\hat{\Omega}$ to be explicitly time dependent. When $\hat{\Omega}(t)$ is explicitly time dependent the eigenvectors $|n_\Omega(t)\rangle$ will generally also be time dependent. This makes them usually an inconvenient basis to use for computations. Therefore, we now introduce a generic constant basis of vectors orthonormal basis vectors $|n\rangle$:

$$\langle n | n' \rangle = \delta_{nn'}. \quad (8.2.16)$$

Because these $|n\rangle$ form a basis for the Hilbert space, $|\phi\rangle$ can be written in terms of them for some coefficients ϕ_n :

$$|\phi\rangle = \sum_n \phi_n |n\rangle \quad (8.2.17)$$

$$\implies \langle n | \phi \rangle = \sum_{n'} \phi_{n'} \langle n | n' \rangle = \sum_{n'} \phi_{n'} \delta_{nn'} = \phi_n \quad (8.2.18)$$

$$\implies |\phi\rangle = \sum_n (\langle n | \phi \rangle) |n\rangle = \left(\sum_n |n\rangle \langle n| \right) |\phi\rangle \quad \forall |\phi\rangle \quad (8.2.19)$$

$$\implies \sum_n |n\rangle \langle n| = \mathbb{1}. \quad (8.2.20)$$

These ϕ_n are not the same ϕ_n used before in the $|n_\Omega\rangle$ basis. For the rest of this section whenever we write ϕ_n we will always mean ϕ_n as defined in this constant arbitrary basis. In an arbitrary basis we define the matrix elements of $\hat{\Omega}$ as:

$$\Omega_{nk}(t) = \langle n | \hat{\Omega}(t) | k \rangle. \quad (8.2.21)$$

Notice in (8.2.12) that by construction $\hat{\Omega}$ is equal to its own complex conjugate transpose (adjoint) and so is called **self-adjoint**. Because of this:

$$\Omega_{nk}^* = (\langle n | \hat{\Omega} | k \rangle)^\dagger = \langle k | \hat{\Omega}^\dagger | n \rangle = \langle k | \hat{\Omega} | n \rangle = \Omega_{kn}. \quad (8.2.22)$$

Using the completeness relation in (8.2.20) we have:

$$\langle \phi | \hat{\Omega} | \phi \rangle = \sum_n \sum_k \langle \phi | n \rangle \langle n | \hat{\Omega} | k \rangle \langle k | \phi \rangle = \sum_{nk} \Omega_{nk} \phi_n^* \phi_k. \quad (8.2.23)$$

With this our Lagrangian becomes:

$$\mathcal{L} = i \sum_n \phi_n^* \dot{\phi}_n - \sum_{nk} \Omega_{nk} \phi_n^* \phi_k. \quad (8.2.24)$$

This gives the equation of motion for the theory:

$$\frac{\partial \mathcal{L}}{\partial \phi_n^*} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_n^*} = i \dot{\phi}_n - \sum_k \Omega_{nk} \phi_k \stackrel{!}{=} 0 \quad (8.2.25)$$

$$\implies i \dot{\phi}_n = \sum_k \Omega_{nk} \phi_k. \quad (8.2.26)$$

In terms of the Dirac notation this becomes:

$$i |\dot{\phi}\rangle = \sum_n i \dot{\phi}_n |n\rangle = \sum_{nk} |n\rangle \Omega_{nk} \phi_k = \sum_{nk} |n\rangle \langle n | \hat{\Omega} | k \rangle \langle k | \phi \rangle = \hat{\Omega} | \phi \rangle \quad (8.2.27)$$

$$\implies i |\dot{\phi}\rangle = \hat{\Omega} | \phi \rangle. \quad (8.2.28)$$

The conjugate Euler-Lagrange equation gives the equation of motion for $\langle \phi |$:

$$\frac{\partial \mathcal{L}}{\partial \phi_n} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_n} = - \sum_k \phi_k^* \Omega_{kn} - i \dot{\phi}_n^* \stackrel{!}{=} 0 \implies i \dot{\phi}_n^* = - \sum_k \Omega_{kn} \phi_k^* \quad (8.2.29)$$

$$\implies i \langle \dot{\phi} | = i \sum_n \dot{\phi}_n^* \langle n | = - \sum_{nk} \Omega_{kn} \phi_k^* \langle n | = - \sum_{nk} \langle \phi | k \rangle \langle k | \hat{\Omega} | n \rangle \langle n | = - \langle \phi | \hat{\Omega} \quad (8.2.30)$$

$$\implies i \langle \dot{\phi} | = - \langle \phi | \hat{\Omega}. \quad (8.2.31)$$

We can put the whole theory into a bit of a nicer form using some properties of the equations of motion. Notice that our equation of motion always conserves the magnitude of the state vector in time:

$$\frac{d}{dt} \langle \phi | \phi \rangle = \frac{d \langle \phi |}{dt} | \phi \rangle + \langle \phi | \frac{d | \phi \rangle}{dt} = - \frac{1}{i} \langle \phi | \hat{\Omega} | \phi \rangle + \frac{1}{i} \langle \phi | \hat{\Omega} | \phi \rangle = 0. \quad (8.2.32)$$

Because this magnitude is constant, we can divide it out of the theory to simplify things. So, define the constant $\hbar$:

$$\hbar \stackrel{\text{def}}{=} \langle \phi | \phi \rangle = \sum_n |\phi_n|^2 > 0 \quad (8.2.33)$$

and the normalized state vector $|\psi\rangle$:

$$|\psi\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{\hbar}} |\phi\rangle \implies \langle \psi | \psi \rangle = 1. \quad (8.2.34)$$

$$\implies \mathcal{L} = i \hbar \langle \psi | \dot{\psi} \rangle - \hbar \langle \psi | \hat{\Omega} | \psi \rangle. \quad (8.2.35)$$

This just brings out an overall multiplier on our Lagrangian by this positive constant $\hbar$ which is some constant to be determined in our theory. Having $|\psi\rangle$ set so that $\langle \psi | \psi \rangle = 1$ is said to “normalize” $|\psi\rangle$. Now then our Hamiltonian is given by:

$$\mathcal{H} = \langle \phi | \hat{\Omega} | \phi \rangle = \langle \psi | \hbar \hat{\Omega} | \psi \rangle \quad (8.2.36)$$

and so we define the Hamiltonian operator:

$$\hat{H}(t) = \hbar \hat{\Omega}(t) \implies \hat{H}^\dagger = \hat{H}. \quad (8.2.37)$$

This gives us:

Theorem 8.2: Lagrangian for the Schrödinger equation

There exist coordinates in which a generic stable lowest order (i.e. quadratic) field theory is described by a complex field $\psi(t, \vec{x})$ satisfying:

$$\langle \psi | \psi \rangle = 1 \quad (8.2.38)$$

with Lagrangian given by:

$$\mathcal{L} = i\hbar\langle\psi|\dot{\psi}\rangle - \langle\psi|\hat{H}|\psi\rangle \quad (8.2.39)$$

where $\hbar > 0$ is a constant and $\hat{H}$ is a self-adjoint operator called the Hamiltonian operator which defines the dynamics of the theory. Correspondingly the conjugate momentum π and Hamiltonian $\mathcal{H}$ are given by:

$$\pi = \frac{\delta\mathcal{L}}{\delta\dot{\psi}} = i\hbar\psi^\dagger \quad (8.2.40)$$

$$\implies \mathcal{H} = \langle\pi|\dot{\psi}\rangle - \mathcal{L} = \langle\psi|\hat{H}|\psi\rangle = \frac{1}{i\hbar}\langle\pi|\hat{H}|\psi\rangle. \quad (8.2.41)$$

The state $|\psi\rangle$ then satisfies the Schrödinger equation:

$$\frac{\partial\mathcal{L}}{\partial\langle\psi|} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\langle\dot{\psi}|} = i\hbar\dot{\psi} - \hat{H}|\psi\rangle \stackrel{!}{=} 0 \implies i\hbar\dot{\psi} = \hat{H}|\psi\rangle \quad (8.2.42)$$

and its adjoint satisfies the adjoint Schrödinger equation:

$$\frac{\partial\mathcal{L}}{\partial|\psi\rangle} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial|\dot{\psi}\rangle} = -\langle\psi|\hat{H} - \frac{d}{dt}i\hbar\langle\dot{\psi}| \stackrel{!}{=} 0 \implies i\hbar\langle\dot{\psi}| = -\langle\psi|\hat{H}. \quad (8.2.43)$$

The equation of motion found in theorem 8.2 is called the Schrödinger equation and it is the central equation of quantum mechanics. Going forward, we will generally call $|\psi\rangle$ the wave vector or state vector and $\psi(t, \vec{x})$ the wavefunction. We will not retain the use of the symbol ϕ as used in this section past this point and will consistently stick with only using ψ .

One may object that the Lagrangian in theorem 8.2 is not real-valued, which does seem odd considering we arrived at it through canonical transformations of a system initially in real variables. However, it is actually real-valued up to a total time derivative and so can be made real-valued with an appropriate surface term. In particular:

$$\mathcal{L} = i\hbar\langle\psi|\dot{\psi}\rangle - \langle\psi|\hat{H}|\psi\rangle \quad (8.2.44)$$

$$= \frac{i}{2}\hbar\langle\psi|\dot{\psi}\rangle - \frac{i}{2}\hbar\langle\dot{\psi}|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle + \frac{d}{dt}(i\hbar\langle\psi|\psi\rangle) \quad (8.2.45)$$

$$\simeq \frac{i\hbar}{2}(\langle\psi|\dot{\psi}\rangle - \langle\dot{\psi}|\psi\rangle) - \langle\psi|\hat{H}|\psi\rangle \quad (8.2.46)$$

$$= -\hbar\text{Im}(\langle\psi|\dot{\psi}\rangle) - \langle\psi|\hat{H}|\psi\rangle \quad (8.2.47)$$

which is now manifestly real-valued.

8.2.1 Hermitian vs. Self-Adjoint

We have referred to the Hamiltonian operator as self-adjoint. However, when dealing with fields (and so infinite dimensional vector spaces) instead of finite dimensional vector spaces, being self-adjoint is a delicate property. There is a related concept known as being Hermitian, which for finite dimensional vector spaces is the same thing. For infinite dimensional vector spaces they are different (being self-adjoint is a special case of being Hermitian) and many nice theorems we would like to use only apply when the operator to which we would apply them is specifically self-adjoint. For the rest of this subsection we are going to be careful in treating the concepts of Hermitian vs. self-adjoint but after this subsection we will not be so careful.

The subtlety in dealing with infinite dimensional Hilbert spaces comes from the fact that in an infinite dimensional Hilbert space the inner product $\langle\psi_1|\psi_2\rangle$ between two vectors in the Hilbert space contains an infinite sum when expressed in components and the convergence properties of that sum can be quite delicate. Suppose we have a linear operator $\hat{O}$ on the Hilbert space $\mathbb{H}$. Colloquially this means that when $\hat{O}$ acts on a vector $|\psi_1\rangle \in \mathbb{H}$ the output is some other vector in $\mathbb{H}$. Let $|\psi_2\rangle$ be that vector:

$$|\psi_2\rangle = \hat{O}|\psi_1\rangle. \quad (8.2.48)$$

$|\psi_1\rangle$, by being a vector in the Hilbert space, is required to have finite norm. However, depending on the particular matrix elements $\mathcal{O}_{nk}$ and components ψ_{1n} , it may be the case that $|\psi_2\rangle$ does not have finite norm.

Explicitly:

$$\langle \psi_2 | \psi_2 \rangle = \langle \psi_1 | \hat{O}^\dagger \hat{O} | \psi_1 \rangle = \sum_{nmk} \langle \psi_1 | n \rangle \langle n | \hat{O}^\dagger | m \rangle \langle m | \hat{O} | k \rangle \langle k | \psi_1 \rangle = \sum_{nmk} \psi_{1n}^* \mathcal{O}_{mn}^* \mathcal{O}_{mk} \psi_{1k}. \quad (8.2.49)$$

This infinite sum may not converge. In order to rigorously define the operator $\hat{O}$ we have to in addition to its matrix elements in some basis supply a set $D(\hat{O})$ called the domain of $\hat{O}$ which is a linear subspace of the overall Hilbert space $\mathbb{H}$. This set $D(\hat{O})$ is the set of vectors $|u\rangle$ in $\mathbb{H}$ on which we define $\hat{O}|u\rangle$ to exist. Necessarily, it can only contain vectors $|u\rangle$ so that $\hat{O}|u\rangle$ has finite norm. We will basically always require that whatever operators we are working with are densely defined in the Hilbert space. An operator $\hat{O}$ is said to be densely defined if for any given vector $|v\rangle$ in $\mathbb{H}$ and $\varepsilon > 0$ there always exists a vector $|u\rangle \in D(\hat{O})$ so that the distance between $|v\rangle$ and $|u\rangle$ is less than ε . This essentially means that every vector in $\mathbb{H}$ can be arbitrarily well approximated by a vector in $D(\hat{O})$.

In order to rigorously define $\hat{O}^\dagger$, suppose we have a densely defined operator $\hat{O}$ on a domain $D(\hat{O})$. The domain $D(\hat{O}^\dagger)$ of the adjoint $\hat{O}^\dagger$ is the set of all $|v\rangle \in \mathbb{H}$ so that there exists a $|w\rangle \in \mathbb{H}$ satisfying:

$$\langle v | (\hat{O}|u\rangle) = \langle w | u \rangle \quad (8.2.50)$$

for all $|u\rangle \in D(\hat{O})$. Because $\hat{O}$ is assumed to be densely defined we can use a theorem known as the Riesz representation theorem to guarantee that such a $|w\rangle$ is unique if it exists and then we take by definition $\hat{O}^\dagger$ to act on $|v\rangle$ according to:

$$\hat{O}^\dagger |v\rangle = |w\rangle. \quad (8.2.51)$$

(The Riesz representation theorem is the formal theorem that proves that each vector $|u\rangle \in \mathbb{H}$ has a unique dual vector $\langle u|$ and vice versa. For finite dimensional vector spaces this is obvious; for the infinite dimensional case it is still true but requires a more complicated proof to show it.) Importantly, the domain of an operator and the domain of that operator's adjoint are generally not the same.

A densely defined operator $\hat{O}$ is said to be Hermitian if for all vectors $|u\rangle$ and $|v\rangle$ which are both in $D(\hat{O})$:

$$\langle u | (\hat{O}|v\rangle) = (\langle u | \hat{O}^\dagger) |v\rangle. \quad (8.2.52)$$

The parentheses are important because they control the order in which infinite sums are taken which in general may be important. In order for this equation to be well defined, by definition it means $|v\rangle$ is in $D(\hat{O}^\dagger)$. Therefore, if this equation holds for all $|v\rangle \in D(\hat{O})$ then $D(\hat{O})$ must be a subset of $D(\hat{O}^\dagger)$. A Hermitian operator $\hat{O}$ is said to be self-adjoint whenever additionally $D(\hat{O}) = D(\hat{O}^\dagger)$. Then, the above equation holds without the need for parentheses:

$$\langle u | \hat{O} | v \rangle = \langle u | \hat{O}^\dagger | v \rangle. \quad (8.2.53)$$

In physics we generally just assume the parentheses to be unnecessary as part of our bad habit of recklessly commuting limits.

8.2.2 The Spectral Theorem

It will be extremely useful to know some basic properties of self-adjoint operators. Consider a self-adjoint operator $\hat{O}$ and an eigenstate $|\psi\rangle$ of that operator with eigenvalue λ :

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle. \quad (8.2.54)$$

Then:

$$\langle \psi | \hat{O} | \psi \rangle = \lambda \langle \psi | \psi \rangle \implies \lambda = \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle} \quad (8.2.55)$$

$$\implies \lambda^* = \frac{\langle \psi | \hat{O}^\dagger | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle} = \lambda. \quad (8.2.56)$$

Hence, the eigenvalues of a self-adjoint operator are always real. As well, taking the adjoint of the eigenvector equation gives:

$$\langle \psi | \hat{O}^\dagger = \lambda^* \langle \psi | \implies \langle \psi | \hat{O} = \lambda \langle \psi | \quad (8.2.57)$$

and so the left eigenstates and right eigenstates of $\hat{O}$ are related by taking the adjoint and share the same eigenvalue. Further, consider another eigenstate $|\psi'\rangle$ of $\hat{O}$ with eigenvalue of $\lambda' \neq \lambda$:

$$\langle\psi|\hat{O}|\psi'\rangle = \left(\langle\psi|\hat{O}\right)|\psi'\rangle = \langle\psi|\left(\hat{O}|\psi'\rangle\right) \quad (8.2.58)$$

$$\implies \langle\psi|\lambda|\psi'\rangle = \langle\psi|\lambda'|\psi'\rangle \quad (8.2.59)$$

$$\implies (\lambda - \lambda')\langle\psi|\psi'\rangle = 0 \quad (8.2.60)$$

$$\implies \langle\psi|\psi'\rangle = 0. \quad (8.2.61)$$

Hence, eigenvectors of a self-adjoint operator corresponding to distinct eigenvalues are guaranteed to be orthogonal. In fact, there is a deep and general result from linear algebra which we will use regularly known as the Spectral Theorem.

Spectral Theorem: Every normal operator $\hat{O}$ on a Hilbert space $\mathbb{H}$ possesses an orthonormal basis of eigenvectors. (A normal operator is one which satisfies $[\hat{O}, \hat{O}^\dagger] = 0$.) Every operator which possesses an orthonormal basis of eigenvectors is normal.

Rigorously proving the spectral theorem for an infinite dimensional Hilbert space requires significant mathematics we are not going to touch. Here we will provide a proof which is valid for finite dimensional Hilbert spaces, but the result does hold with appropriately rigorous careful treatment for infinite dimensional Hilbert spaces. To prove the spectral theorem we will need a few smaller results first.

Lemma: Every operator has an eigenvalue. Proof:

Consider an N dimensional Hilbert space $\mathbb{H}$ and an operator $\hat{O}$. For all vectors $|\psi\rangle \in \mathbb{H}$, we can consider the $N + 1$ vectors $|\psi\rangle, \hat{O}|\psi\rangle, \dots, \hat{O}^N|\psi\rangle$. Because we have $N + 1$ vectors in an N dimensional vector space they cannot all be linearly independent. Therefore, they must be linearly dependent and so there must exist some coefficients a_n such that:

$$\sum_{n=0}^N a_n \hat{O}^n |\psi\rangle = 0. \quad (8.2.62)$$

Let m be the largest value of n for which $a_n \neq 0$. Every polynomial on the complex numbers can be factored by the fundamental theorem of algebra and so for some constants $c, \lambda_1, \dots, \lambda_m$ we have for any z :

$$a_0 + a_1 z + \dots + a_m z^m = c(z - \lambda_1) \dots (z - \lambda_m). \quad (8.2.63)$$

Returning this to our linear dependence sum we have:

$$\sum_{n=0}^m a_n \hat{O}^n |\psi\rangle = c(\hat{O} - \lambda_1 \mathbb{1}) \dots (\hat{O} - \lambda_m \mathbb{1}) |\psi\rangle = 0. \quad (8.2.64)$$

Thus, at least one of these operators $\hat{O} - \lambda_k \mathbb{1}$ for some k must send a nonzero vector to 0. Let K be such a value of k and $|v_K\rangle$ be such a nonzero vector that $\hat{O} - \lambda_K \mathbb{1}$ sends to 0. Then, automatically:

$$(\hat{O} - \lambda_K \mathbb{1})|v_K\rangle = 0 \implies \hat{O}|v_K\rangle = \lambda_K |v_K\rangle \quad (8.2.65)$$

and so λ_K is an eigenvalue of $\hat{O}$.

Lemma: Every operator has an upper triangular matrix representation. Proof:

Consider a 1 dimensional Hilbert space $\mathbb{H}$. Trivially any operator $\hat{O}$ on that space represented by a matrix is just a number and so is upper triangular. Let S_n be the statement “Every operator on a Hilbert space of dimension less than or equal to n has an upper triangular representation”. We have already proven that S_1 is true. Now suppose that for a particular n S_n is true. Then, consider a Hilbert space $\mathbb{H}$ of dimension $n + 1$ and an operator on that space $\hat{O}$. Let λ be an eigenvalue of $\hat{O}$ (which is guaranteed to exist by our previous lemma) and consider for any vector $|\psi\rangle$:

$$\hat{O}|\psi\rangle = (\hat{O} - \lambda \mathbb{1})|\psi\rangle + \lambda|\psi\rangle. \quad (8.2.66)$$

Let $|v\rangle$ be an eigenvector of $\hat{O}$ with eigenvalue λ . Any $|\psi\rangle \in \mathbb{H}$ can be written as a part parallel to $|v\rangle$ and a piece orthogonal to $|v\rangle$:

$$|\psi\rangle = A|v\rangle + |\psi_\perp\rangle, \quad \langle v|\psi_\perp\rangle = 0. \quad (8.2.67)$$

(To see this simply define $|\psi_\perp\rangle = |\psi\rangle - \frac{\langle v|\psi\rangle}{\langle v|v\rangle}|v\rangle$.) Now acting $\hat{O}$ on $|\psi\rangle$:

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle + (\hat{O} - \lambda\mathbb{1})|\psi_\perp\rangle. \quad (8.2.68)$$

The Hilbert space $\mathbb{H}_v$ of vectors orthogonal to $|v\rangle$ has dimension n . We can see that if $|\psi\rangle \in \mathbb{H}_v$, then $|\psi_\perp\rangle = |\psi\rangle$ and consequently $\hat{O}|\psi\rangle$ is also in $\mathbb{H}_v$. Therefore, $\hat{O}$ can be defined in how it acts on $\mathbb{H}_v$ as an operator on an n dimensional Hilbert space and therefore by S_n has an upper triangular representation on $\mathbb{H}_v$. Let $|u_1\rangle, \dots, |u_n\rangle$ be an orthonormal basis of $\mathbb{H}_v$ on which $\hat{O}$ has an upper triangular representation. Then, we can complete a basis of $\mathbb{H}$ adding a normalized $|v\rangle$ to the end of the list. Then, $\hat{O}$ acts on this basis in an upper triangular way automatically and so S_{n+1} is true. By induction then, S_n is true for all n .

Now let us prove the spectral theorem:

Consider a normal operator $\hat{O}$ on a Hilbert space of dimension N and an orthonormal basis $|n\rangle$ on which it is upper triangular (which is guaranteed to exist by the previous lemma). Then, because $\hat{O}$ is upper triangular:

$$\hat{O}|n\rangle = \sum_{k=1}^n \mathcal{O}_{kn}|k\rangle \quad (8.2.69)$$

for coefficients $\mathcal{O}_{kn}$. Using the completeness relation:

$$\hat{O} = \sum_{n=1}^N \sum_{k=1}^n \mathcal{O}_{kn}|k\rangle\langle n| \implies \hat{O}^\dagger = \sum_{n=1}^N \sum_{k=1}^n \mathcal{O}_{kn}^*|n\rangle\langle k|. \quad (8.2.70)$$

Because $\hat{O}$ is normal:

$$\|\hat{O}|\psi\rangle\|^2 = \langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle = \langle\psi|\hat{O}\hat{O}^\dagger|\psi\rangle = \|\hat{O}^\dagger|\psi\rangle\|^2. \quad (8.2.71)$$

We can compute both sides easily for $|\psi\rangle = |n\rangle$:

$$\|\hat{O}|n\rangle\|^2 = \sum_{k=1}^n |\mathcal{O}_{kn}|^2, \quad \|\hat{O}^\dagger|n\rangle\|^2 = \sum_{k=n}^N |\mathcal{O}_{nk}|^2 \quad (8.2.72)$$

and these two must be equal for each n . For $n = 1$ this requires:

$$|\mathcal{O}_{11}|^2 = \sum_{k=1}^N |\mathcal{O}_{1k}|^2 = |\mathcal{O}_{11}|^2 + \sum_{k=2}^N |\mathcal{O}_{1k}|^2. \quad (8.2.73)$$

This is only possible if $\mathcal{O}_{1k} = 0$ for $k > 1$. Consequently, the first row in $\hat{O}$'s upper triangle is 0 after the first entry. Using this, we have for $n = 2$:

$$|\mathcal{O}_{22}|^2 = |\mathcal{O}_{22}|^2 + \sum_{k=3}^N |\mathcal{O}_{2k}|^2 \quad (8.2.74)$$

from which we get that $\mathcal{O}_{2k} = 0$ for $k > 2$. Iterating further, we get at each n that $\mathcal{O}_{nk} = 0$ for each $k > n$. This leaves only diagonal entries in $\hat{O}$. So, if $\hat{O}$ is normal and written in a basis in which it is upper triangular then in that basis it is automatically diagonal. Because we used an orthonormal basis to diagonalize $\hat{O}$, this basis is automatically an orthonormal basis of eigenvectors, proving that every normal operator has an orthonormal basis of eigenvectors.

The other direction of the spectral theorem is easier. Suppose $\hat{O}$ has an orthonormal basis of eigenvectors. Then, in that basis:

$$\hat{O} = \sum_n \lambda_n |n\rangle\langle n| \quad (8.2.75)$$

for eigenvalues λ_n . Automatically then:

$$\hat{O}^\dagger = \sum_n \lambda_n^* |n\rangle\langle n| \quad (8.2.76)$$

$$\implies [\hat{O}^\dagger, \hat{O}] = \hat{O}^\dagger \hat{O} - \hat{O} \hat{O}^\dagger = 0. \quad (8.2.77)$$

Thus, if $\hat{O}$ has an orthonormal basis of eigenvectors then it is a normal operator. This completes our proof of the spectral theorem.

Self-adjoint operators are of course normal as $[\hat{O}, \hat{O}^\dagger] = [\hat{O}, \hat{O}] = 0$. But, there are many normal

operators which are not self-adjoint. Another important class of normal operators we will see often is the class of **unitary** operators. A unitary operator $\hat{U}$ is an operator whose adjoint is its inverse:

$$\hat{U}^{-1} = \hat{U}^\dagger. \quad (8.2.78)$$

In finite dimensional vector spaces the left inverse and right inverse of an operator are the same. In the infinite dimensional case an operator may have a left inverse but not a right inverse and vice versa. Because of this, the notation $\hat{U}^{-1}$ for an infinite dimensional Hilbert space is only defined when the operator has both a left inverse and a right inverse and when those two inverses are the same operator. Unitarity can equivalently be written as:

$$\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{1}. \quad (8.2.79)$$

Unitary operators are automatically normal becomes: $[\hat{U}, \hat{U}^\dagger] = \hat{U} \hat{U}^\dagger - \hat{U}^\dagger \hat{U} = \mathbb{1} - \mathbb{1} = 0$. There are normal operators which are neither self-adjoint nor unitary.

Because of the spectral theorem, for any normal operator $\hat{O}$ we can always guarantee that there exists a basis of eigenvectors $|n\rangle$ which is orthonormal:

$$\hat{O}|n\rangle = \lambda_n|n\rangle, \quad \langle n|n'\rangle = \delta_{nn'}. \quad (8.2.80)$$

Because this set of vectors is a basis, any vector can be expanded in terms of them for some coefficients of linear combination:

$$|\psi\rangle = \sum_n \psi_n |n\rangle. \quad (8.2.81)$$

Using orthonormality, this implies the completeness relation:

$$\sum_n |n\rangle\langle n| = \mathbb{1}. \quad (8.2.82)$$

As well, it gives a nice expression (called the spectral expansion) for the operator $\hat{O}$ in terms of its eigenbasis:

$$\hat{O}|n\rangle = \lambda_n|n\rangle \implies \hat{O}|n\rangle\langle n| = \lambda_n|n\rangle\langle n| \quad (8.2.83)$$

$$\implies \hat{O} \sum_n |n\rangle\langle n| = \sum_n \lambda_n |n\rangle\langle n| \quad (8.2.84)$$

$$\implies \hat{O} = \sum_n \lambda_n |n\rangle\langle n| \quad (8.2.85)$$

and a correspondingly simple expression for $\langle\psi|\hat{O}|\psi\rangle$:

$$\langle\psi|\hat{O}|\psi\rangle = \langle\psi| \sum_n \lambda_n |n\rangle\langle n| \psi\rangle = \sum_n \lambda_n \langle\psi|n\rangle\langle n|\psi\rangle = \sum_n \lambda_n |\psi_n|^2. \quad (8.2.86)$$

The set of eigenvalues of an operator is known as the spectrum of that operator³.

It will be useful to understand how to change between different orthonormal bases. Consider one basis labeled as $|n_1\rangle$ and another labeled as $|n_2\rangle$. Consider a vector expanded in terms of the first basis:

$$|\psi\rangle = \sum_n \psi_n |n_1\rangle \quad (8.2.87)$$

and another vector expanded in terms of the second basis but with the same expansion coefficients:

$$|\psi'\rangle = \sum_n \psi_n |n_2\rangle. \quad (8.2.88)$$

This second vector is then related to the first some change of basis from the first to the second basis in which orthonormality is preserved. Then:

$$|\psi'\rangle = \sum_n \psi_n |n_2\rangle = \sum_n \langle n_1|\psi\rangle |n_2\rangle = \left(\sum_n |n_2\rangle\langle n_1| \right) |\psi\rangle. \quad (8.2.89)$$

And so, $|\psi'\rangle$ and $|\psi\rangle$ are related by the operator $\hat{U}$:

$$\hat{U} = \sum_n |n_2\rangle\langle n_1|, \quad |\psi'\rangle = \hat{U}|\psi\rangle. \quad (8.2.90)$$

³This definition of spectrum is valid for operators on finite dimensional operators. It is not quite correct in the infinite dimensional case but does capture the correct intuition. For our purposes, the definition given here will suffice.

It immediately follows that $\hat{U}$ is unitary:

$$\hat{U}^\dagger \hat{U} = \sum_n |n_1\rangle\langle n_2| \sum_{n'} |n'_2\rangle\langle n'_1| = \sum_{nn'} |n_1\rangle\langle n_2|n'_2\rangle\langle n'_1| = \sum_{nn'} |n_1\rangle\delta_{nn'}\langle n'_1| = \sum_n |n_1\rangle\langle n_1| = \mathbb{1} \quad (8.2.91)$$

$$\hat{U}\hat{U}^\dagger = \sum_n |n_1\rangle\langle n_1| \sum_{n'} |n'_1\rangle\langle n'_2| = \sum_{nn'} |n_2\rangle\langle n_1|n'_1\rangle\langle n'_2| = \sum_{nn'} |n_2\rangle\delta_{nn'}\langle n'_2| = \sum_n |n_2\rangle\langle n_2| = \mathbb{1}. \quad (8.2.92)$$

Thus **a change of basis between orthonormal bases is represented by a unitary operator**. As well, given any orthonormal basis $|n_1\rangle$, given a unitary operator we can define a second basis $|n_2\rangle$ by $|n_2\rangle = \hat{U}|n_1\rangle$ from which it immediately follows that $|n_2\rangle$ is also an orthonormal basis:

$$\langle n_2|n'_2\rangle = \langle n_1|\hat{U}^\dagger\hat{U}|n'_1\rangle = \langle n_1|\mathbb{1}|n'_1\rangle = \delta_{nn'} \quad (8.2.93)$$

$$\sum_n |n_2\rangle\langle n_2| = \sum_n \hat{U}|n_1\rangle\langle n_1|\hat{U}^\dagger = \hat{U}\mathbb{1}\hat{U}^\dagger = \mathbb{1}. \quad (8.2.94)$$

Thus, every unitary operator is equivalent to an orthonormal change of basis.

Sometimes we will have two normal operators $\hat{A}$ and $\hat{B}$ to work with at the same time and it would be nice for calculations if we could make them both diagonal. Suppose that it is possible to find an orthonormal basis $|n\rangle$ so that in that basis both $\hat{A}$ and $\hat{B}$ are diagonal:

$$\hat{A} = \sum_n A_n |n\rangle\langle n|, \quad \hat{B} = \sum_n B_n |n\rangle\langle n|. \quad (8.2.95)$$

Then, automatically:

$$\hat{A}\hat{B} - \hat{B}\hat{A} = \sum_n (A_n B_n - B_n A_n) |n\rangle\langle n| = 0. \quad (8.2.96)$$

Therefore, if two normal operators are simultaneously diagonalizable then they commute. Conversely, assume that $|n\rangle$ is an orthonormal basis so that in that basis $\hat{A}$ is diagonal but $\hat{B}$ may not be:

$$\hat{A} = \sum_n A_n |n\rangle\langle n|, \quad \hat{B} = \sum_{nm} B_{nm} |n\rangle\langle m|. \quad (8.2.97)$$

Now let us assume that $\hat{A}$ and $\hat{B}$ commute:

$$\langle n|[\hat{A}, \hat{B}]|m\rangle = (A_n - A_m)B_{nm} \stackrel{!}{=} 0. \quad (8.2.98)$$

Therefore, for each n either $A_n = A_m$ or $B_{nm} = 0$. If A_n has no repeated eigenvalues then $A_n = A_m$ if and only if $n = m$. So, in that case this equality requires $B_{nm} = 0$ for all $n \neq m$ in which case $\hat{B}$ is diagonal. Therefore, if two normal operators commute and one of them has no repeated eigenvalues then they are simultaneously diagonalizable. If $\hat{A}$ does have repeated eigenvalues, then on each eigenspace $\hat{A}$ is proportional to the identity operator and we can redefine the eigenvectors within that space to diagonalize $\hat{B}$ on that subspace. Whatever choices we make $\hat{A}$ will remain diagonal on the space due to being proportional to the identity. Therefore, even if the operators have repeated eigenvalues, if they are normal and commute then they are simultaneously diagonalizable. Altogether then, **two normal operators commute if and only if they are simultaneously diagonalizable**.

Some important properties of self-adjoint operators to understand are that the sum of two self-adjoint operators is guaranteed to be self-adjoint but the product is not:

$$(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger = \hat{A} + \hat{B} \quad (8.2.99)$$

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A} \neq \hat{A}\hat{B} \text{ (Unless } \hat{A} \text{ and } \hat{B} \text{ commute)}. \quad (8.2.100)$$

However, the symmetrized product of $\hat{A}$ and $\hat{B}$ is self-adjoint whenever $\hat{A}$ and $\hat{B}$ are self-adjoint:

$$\text{Sym}(\hat{A}, \hat{B}) \stackrel{\text{def}}{=} \frac{\hat{A}\hat{B} + \hat{B}\hat{A}}{2} \quad (8.2.101)$$

$$\implies \text{Sym}(\hat{A}, \hat{B})^\dagger = \frac{\hat{B}^\dagger\hat{A}^\dagger + \hat{A}^\dagger\hat{B}^\dagger}{2} = \frac{\hat{B}\hat{A} + \hat{A}\hat{B}}{2} = \text{Sym}(\hat{A}, \hat{B}). \quad (8.2.102)$$

The overall factor of $\frac{1}{2}$ is put in so that when $\hat{A}$ and $\hat{B}$ commute, $\text{Sym}(\hat{A}, \hat{B})$ reduces to simply $\hat{A}\hat{B}$. It will be useful later to have defined the symmetric product of N operators as the sum of over all $N!$ orderings of the operators with a $\frac{1}{N!}$ normalization. Let $\sigma : \{1, \dots, N\} \rightarrow \{1, \dots, N\}$ be a permutation of the numbers

1, ..., N. Then, the symmetric product in general is defined as:

$$\text{Sym}(\hat{O}_1, \dots, \hat{O}_N) \stackrel{\text{def}}{=} \frac{1}{N!} \sum_{\text{All } \sigma} \hat{O}_{\sigma(1)} \hat{O}_{\sigma(2)} \dots \hat{O}_{\sigma(N)}. \quad (8.2.103)$$

This definition is convenient mathematically because it is automatically self-adjoint if all of the input operators are self-adjoint, treats no order of multiplication of the input operators preferentially, it is linear in the input operators, and reduces to the simple product of the operators in the case that all the input operators commute. In fact, this is the unique function of N operators which satisfies all of these properties simultaneously.

Finally, the commutator of self-adjoint operators is guaranteed to be anti-self-adjoint:

$$([\hat{A}, \hat{B}])^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}^\dagger \hat{A}^\dagger - \hat{A}^\dagger \hat{B}^\dagger = [\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}]. \quad (8.2.104)$$

Usually it will be nicer to express this by saying that $\frac{1}{i}[\hat{A}, \hat{B}]$ is self-adjoint:

$$\left(\frac{1}{i}[\hat{A}, \hat{B}]\right)^\dagger = \frac{1}{i}[\hat{A}, \hat{B}]. \quad (8.2.105)$$

8.2.3 Adiabatic Invariants in Quantum Mechanics

The Schrödinger Hamiltonian defines an integrable system if $\hat{H}$ has no explicit time dependence. Because the Hamiltonian operator $\hat{H}$ is self-adjoint, by the spectral theorem it possesses an orthonormal basis of eigenvectors and real eigenvalues. Consider a time independent Hamiltonian operator with eigenvectors $|n\rangle$ and eigenvalues E_n :

$$\hat{H}|n\rangle = E_n|n\rangle, \quad \langle n|n'\rangle = \delta_{nn'}, \quad \sum_n |n\rangle\langle n| = \mathbb{1}. \quad (8.2.106)$$

Then, we can express the wavefunction in terms of this basis:

$$|\psi\rangle = \sum_n \psi_n |n\rangle \implies \psi_n = \langle n|\psi\rangle \quad (8.2.107)$$

and return these results to the Schrödinger Lagrangian:

$$\mathcal{L} = \sum_n \left(i\hbar \psi_n^* \dot{\psi}_n - E_n \psi_n^* \psi_n \right). \quad (8.2.108)$$

Legendre transforming this to the Hamiltonian gives:

$$\pi_n = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_n} = i\hbar \psi_n^* \implies \mathcal{H} = \frac{1}{i\hbar} \sum_n E_n \pi_n \psi_n. \quad (8.2.109)$$

Each ψ_n then evolves quite simply as:

$$\dot{\psi}_n = \frac{\partial \mathcal{H}}{\partial \pi_n} = \frac{1}{i\hbar} E_n \psi_n \quad (8.2.110)$$

$$\implies \psi_n(t) = e^{-\frac{i}{\hbar} E_n t} \psi_n(0). \quad (8.2.111)$$

Thus, each ψ_n (and consequently π_n) is periodic with period $\tau_n = \frac{2\pi\hbar}{E_n}$ and does not interact with the other coordinates. Immediately then, the theory has adiabatic invariants:

$$J_n = \frac{1}{2\pi} \oint \pi_n d\psi_n = \frac{1}{2\pi} \int_0^{\frac{2\pi\hbar}{E_n}} i\hbar \psi_n^* \frac{d\psi_n}{dt} dt = \hbar |\psi_n(0)|^2. \quad (8.2.112)$$

Because $\hbar$ is simply a constant, the quantities $|\psi_n(0)|^2 = |\psi_n(t)|^2$ for each n are adiabatically invariant in quantum mechanics. This means that when the Schrödinger theory is interacted with by an external force (which could make $\hat{H}$ develop explicit t dependence), the $|\psi_n(t)|^2$ evolve much more slowly and stably in time than the other degrees of freedom in the theory (such as the phase of each of the $\psi_n(t)$ or the magnitudes of the components of $|\psi\rangle$ in bases other than the eigenbasis of the Hamiltonian operator). Because of this, **$|\psi_n(t)|^2$ is stable enough on experimental time scales to be directly relevant to observations.** We can also express this quantity as:

$$|\psi_n(t)|^2 = |\langle n|\psi\rangle|^2. \quad (8.2.113)$$

We call this the **intensity** of the projection of $|\psi\rangle$ on to $|n\rangle$. In general in quantum mechanics we call the quantity $|\langle \phi|\psi\rangle|^2$ the **projective intensity** of ϕ onto $|\psi\rangle$ or vice versa. In a very literal sense, these intensities

often measure the signal strength of various experimental quantities, such as the amount of incident electric charge on a screen from a quantum system.

Instead of using the word intensity, most other sources on quantum mechanics call this quantity a probability. In some cases these intensities can manifest experimentally approximately as probabilities. This is because in an experiment in which a single quantum system is measured, due to the thermal background of the experiment and interaction of the small quantum system with the measurement apparatus, the system becomes chaotic and the combination imperfect knowledge of the exact physical state of the full interacting system with the time averaging present in measurement necessitates a statistical mechanical treatment of the quantum system. In giving such a treatment, one finds that due to the adiabatic invariance of $|\psi_n|^2$, the system approximately decays to being an eigenstate of the interacting Hamiltonian operator and which eigenstate is selected is effectively random from the perspective of the experiment, with the probability of selecting state $|n\rangle$ given by $|\psi_n|^2$ at the time the measurement interaction begins. This is known as the Born rule. We will describe how it is applied in more detail in subsection 8.5.5. The details of how and why it works that way will be saved until chapter 9. While the projective intensities sometimes manifest as probabilities, that is a derived result and not their only use, so I believe for clarity of thought (and so they are not interpreted as probabilities in inappropriate contexts) they deserve their own name.

We will make several other particular language choices with regard to quantum mechanics to avoid confusion. For example, a quantum system with a state vector $|\psi\rangle$ that lives in a Hilbert space of dimension N we will always call an N dimensional quantum system (because that is the dimension of the Hilbert space) whereas one is often likely to hear it called an “ N state quantum system”. The “ N state” description is literally incorrect as there are an infinite number of different state vectors belonging to an N dimensional Hilbert space. The “ N state” description is used because any vector in the Hilbert space can be written as a linear combination of at most N linearly independent terms; it is just an inconsistent use of the term. There will never be confusion between the Hilbert space dimension of a system in question and how many spatial dimensions we are considering because we will always say spatial dimension when referring to spatial dimensions. We will also always call $\hat{H}$ the Hamiltonian operator of the system and never just the Hamiltonian. The Hamiltonian of the system is $\langle\psi|\hat{H}|\psi\rangle$ as we have established. However, it is a very common bad habit in other sources to call $\hat{H}$ simply the Hamiltonian.

Exercises

Problem 8.2: Functions of an Operator. It will often be useful for us to introduce the notion of a function of an operator. For example, $f(\hat{H})$. For an analytic function $f(x)$ and an operator $\hat{O}$, the notation $f(\hat{O})$ is defined by applying the Taylor series expansion of $f(x)$ to $\hat{O}$. That is, if:

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

for some constants a_n , then:

$$f(\hat{O}) = \sum_{n=0}^{\infty} a_n \hat{O}^n.$$

Consider an analytic function $f(x)$ and a normal operator $\hat{O}$. Let $|n\rangle$ be an orthonormal basis of eigenvectors of $\hat{O}$ and let $\mathcal{O}_n$ be the eigenvalue corresponding to $|n\rangle$. Show that:

$$f(\hat{O})|n\rangle = f(\mathcal{O}_n)|n\rangle, \quad f(\hat{O}) = \sum_n f(\mathcal{O}_n)|n\rangle\langle n|.$$

This second expression is used to define the notation $f(\hat{O})$ when f is not analytic but $\hat{O}$ is normal.

Problem 8.3: ★ Silver Bullet Solution to the Schrödinger equation. Consider a quantum system with a time independent Hamiltonian operator $\hat{H}$. Assume that you have solved the eigenvector problem for $\hat{H}$ and thus identified an orthonormal basis of eigenvectors $|n\rangle$ of $\hat{H}$ with vector $|n\rangle$ having eigenvalue E_n . Show that the solution to the Schrödinger equation for arbitrary initial conditions can be written as:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}t\hat{H}}|\psi(0)\rangle = \sum_n e^{-\frac{i}{\hbar}tE_n}|n\rangle\langle n|\psi(0)\rangle.$$

Thus, solving the dynamics of a time translationally symmetric quantum system is equivalent to solving the eigenvector/eigenvalue problem for the Hamiltonian operator. Notice that the angular frequency of oscillation of the component of $|\psi\rangle$ in the $|n\rangle$ direction is $\frac{E_n}{\hbar}$. Show as well that the total energy of the system is:

$$E = \sum_n E_n |\langle n|\psi\rangle|^2.$$

Problem 8.4: Practice Diagonalizing Hamiltonians. Consider a two dimensional Hilbert space $\mathbb{H}$ and a quantum system with Hamiltonian operator:

$$\hat{H} = \begin{pmatrix} v_z & v_x - iv_y \\ v_x + iv_y & -v_z \end{pmatrix}$$

for some real constants v_x, v_y, v_z . This notation is defined in a basis which we will label $|u_1\rangle$ and $|u_2\rangle$ defined by:

$$|u_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |u_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \langle u_1| = (1 \ 0), \quad \langle u_2| = (0 \ 1).$$

- Show that Hamiltonian operator given is self-adjoint.
- Let $v = \sqrt{v_x^2 + v_y^2 + v_z^2}$. Show that the eigenvalues of the Hamiltonian operator are $\pm v$.
- For the rest of this question it is useful to treat (v_x, v_y, v_z) as a vector in a 3 dimensional space and to introduce standard spherical coordinates so that $v_x = v \sin \theta \cos \varphi$, $v_y = v \sin \theta \sin \varphi$, $v_z = v \cos \theta$. Let $|+\rangle$ be the eigenvector of $\hat{H}$ with eigenvalue v and $|-\rangle$ be the eigenvector of $\hat{H}$ with the eigenvalue $-v$. Show that they can be chosen to be:

$$|+\rangle = \begin{pmatrix} e^{-\frac{i\varphi}{2}} \cos \frac{\theta}{2} \\ e^{\frac{i\varphi}{2}} \sin \frac{\theta}{2} \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} -e^{-\frac{i\varphi}{2}} \sin \frac{\theta}{2} \\ e^{\frac{i\varphi}{2}} \cos \frac{\theta}{2} \end{pmatrix}.$$

- Show that in the $|\pm\rangle$ basis $\hat{H}$ can be written:

$$\hat{H} = v|+\rangle\langle+| - v|-\rangle\langle-|$$

and verify the orthogonality properties and completeness relation of the $|\pm\rangle$ basis.

- Show that the solution to the Schrödinger equation for arbitrary initial conditions is:

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

where $\hat{U}(t)$ is given by:

$$\hat{U}(t) = \cos\left(\frac{vt}{\hbar}\right) \mathbb{1} - \frac{i}{v} \sin\left(\frac{vt}{\hbar}\right) \hat{H}.$$

- Show by explicit calculation that $\hat{U}$ is unitary.

Problem 8.5: Hermitian but Not Self-Adjoint. Consider a system with 1 spatial dimension on an interval of length 1 so that the Hilbert space $\mathbb{H}$ is the space of complex valued functions $\psi(x)$ of a single real variable x so that $\int_0^1 |\psi(x)|^2 dx$ exists and is finite. Define the operator $\hat{p}_1$ as the operator so that:

$$\langle x|\hat{p}_1|\psi\rangle = -i\frac{\partial\psi}{\partial x}$$

and so that the domain of $\hat{p}_1$ (meaning the set of $|\psi\rangle \in \mathbb{H}$ on which it is defined, written $D(\hat{p}_1)$) is the set of periodic functions (meaning $\psi(x) = \psi(x+1)$). Define the operator $\hat{p}_2$ as the operator so that:

$$\langle x|\hat{p}_2|\psi\rangle = -i\frac{\partial\psi}{\partial x}$$

and so that $D(\hat{p}_2)$ is the set of functions with Dirichlet boundary conditions (meaning $\psi(0) = \psi(1) = 0$).

- An operator $\hat{L}$ is said to be Hermitian if for all $|u\rangle \in D(\hat{L})$ and $|v\rangle \in D(\hat{L})$:

$$\langle u|(\hat{L}|v\rangle) = \left(\langle v|(\hat{L}|u\rangle)\right)^*.$$

Show by direct calculation that both $\hat{p}_1$ and $\hat{p}_2$ are Hermitian.

- The adjoint domain $D(\hat{L}^\dagger)$ is defined as the set of all $|v\rangle \in \mathbb{H}$ such that there exists a $|w\rangle \in \mathbb{H}$ satisfying:

$$\langle v|(\hat{L}|u\rangle) = \langle w|u\rangle$$

for all $|u\rangle \in D(\hat{L})$. Then, the adjoint $\hat{L}^\dagger$ is defined so that for such $|v\rangle$ and $|w\rangle$:

$$\hat{L}^\dagger|v\rangle = |w\rangle.$$

Show that $D(\hat{p}_1^\dagger)$ is the set of periodic functions and so is equal to $D(\hat{p}_1)$. As well, show that:

$$\langle x|\hat{p}_1^\dagger|v\rangle = -i\frac{\partial v}{\partial x}.$$

Thus, $\hat{p}_1$ is Hermitian and has the same domain as its adjoint. Because of this $\hat{p}_1$ is self-adjoint:

$$\hat{p}_1 = \hat{p}_1^\dagger.$$

Show that $D(\hat{p}_2^\dagger)$ is simply $\mathbb{H}$ and so is larger than $D(\hat{p}_2)$. Because $D(\hat{p}_2) \neq D(\hat{p}_2^\dagger)$, even though $\hat{p}_2$ is Hermitian, it is not self-adjoint.

Problem 8.6: A Hint of Decoherence. Consider a time dependent Hamiltonian operator $\hat{H}(t)$ so that at time t it has orthonormal basis of eigenvectors $|n(t)\rangle$ and eigenvalues $E_n(t)$:

$$\hat{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle.$$

Further, assume for simplicity that none of the eigenvalues of $\hat{H}(t)$ are repeated (such an operator is called nondegenerate).

(a) Take the time derivative of the eigenvalue equation. Show that:

$$\dot{E}_n = \langle n|\dot{\hat{H}}|n\rangle, \quad \langle m|\dot{n}\rangle = \frac{\langle m|\dot{\hat{H}}|n\rangle}{E_n - E_m}$$

for $m \neq n$.

(b) Let $\psi_n(t) = \langle n|\psi(t)\rangle$. Show that the Schrödinger equation gives that these components evolve in time according to:

$$\dot{\psi}_n = -i\frac{E_n}{\hbar}\psi_n + \sum_m \frac{\langle n|\dot{\hat{H}}|m\rangle}{E_n - E_m}\psi_m.$$

(c) Let $p_n(t) = |\psi_n|^2$ and $\varphi_n(t)$ be defined so that $\psi_n(t) = \sqrt{p_n(t)}e^{i\varphi_n(t)}$. Further, let $V_{nm}(t)$ and $\phi_{nm}(t)$ be real valued functions so that:

$$\langle n|\dot{\hat{H}}|m\rangle = V_{nm}e^{i\phi_{nm}}.$$

Using that $\hat{H}$ is self-adjoint, show that $V_{nm} = V_{mn}$ and $\phi_{nm} = -\phi_{mn}$. Show that $p_n(t)$ and $\varphi_n(t)$ evolve according to:

$$\begin{aligned} \dot{p}_n &= \sum_m \frac{2V_{nm}}{E_n - E_m} \sqrt{p_n p_m} \cos(\varphi_m - \varphi_n + \phi_{nm}) \\ \dot{\varphi}_n &= -\frac{E_n}{\hbar} + \sum_m \frac{V_{nm}}{E_n - E_m} \sqrt{\frac{p_m}{p_n}} \sin(\varphi_m - \varphi_n + \phi_{nm}). \end{aligned}$$

Explain how these equations show that if $\hat{H}(t)$ changes slowly with time compared to the periods $\tau_{mn} = \frac{2\pi\hbar}{|E_m - E_n|}$ then p_n is approximately constant and φ_n varies very quickly with time. Explain how this establishes further the adiabatic invariance of $|\langle n|\psi\rangle|^2$. The fact that these phases oscillate very rapidly in many physical scenarios causes them to be difficult to access experimentally while the slow evolution of the p_n causes them to be directly experimentally meaningful.

8.3 Wigner's Theorem

As we found in theorem 8.2 the Lagrangian for quantum mechanics is of a very specific form. Consequently, only a very restricted class of canonical transformations can preserve that form and thus only a limited set of transformations can be symmetries in quantum mechanics. In section 8.2 we truncated the Hamiltonian (or equivalently the Lagrangian) at quadratic order. Because of this the Hamiltonian depends directly on 1 power of $|\psi\rangle$ and 1 power of $\langle\psi|$ (such a Hamiltonian is said to be a sesquilinear form in ψ^*, ψ). If we rewrite that Hamiltonian in terms of the real and imaginary parts of ψ , then it would be a real quadratic form in terms of them (as seen in the theorem of normal modes). Because of this, we are insensitive to cubic or higher terms in the theory. Suppose we make some transformation of our field into a new field $\psi \rightarrow \psi'$ so that the Schrödinger Hamiltonian has the same form in terms of ψ' as it does in terms of ψ (possibly with a new Hamiltonian operator). We could express that transformation in terms of how the real and imaginary parts of ψ' depend on the real and imaginary parts of ψ . If the real and imaginary parts of ψ' depend linearly on the real and imaginary parts of ψ , then the new Hamiltonian will automatically be a quadratic form in the real and imaginary parts of ψ' just as we want. If the real and imaginary parts of ψ' depend nonlinearly on the real and imaginary parts of ψ then the new Hamiltonian will not automatically be a quadratic form in the real and imaginary parts of ψ' . Instead, all of the nonlinear terms (if we were express the real and imaginary parts of ψ' in terms of a Taylor series on the real and imaginary parts of ψ) would generate cubic and higher terms in the Hamiltonian. But, these are precisely terms we say we are insensitive to due to our truncation. And so, we are not interested in them. Because of this, we have no interest in nonlinear transformations of the real and imaginary parts of $|\psi\rangle$ as they generate terms that are irrelevant in our theory.

So, the only relevant transformations $\psi \rightarrow \psi'$ are those for which ψ' is a linear combination of the real and imaginary parts of our untransformed ψ , or equivalently a linear combination of ψ and ψ^* (because the real and imaginary parts of a complex number can be written as linear combinations of the complex number and its conjugate):

$$|\psi'\rangle = \hat{U}|\psi\rangle + \hat{V}|\psi^*\rangle \quad (8.3.1)$$

where $\hat{U}$ and $\hat{V}$ are as yet unspecified linear operators. It will be useful to note that any complex number is by definition equal to its own transpose and therefore for any operator $\hat{O}$ and vectors $|\psi\rangle$ and $|\phi\rangle$:

$$\langle\psi|\hat{O}|\phi\rangle = \langle\psi|\hat{O}|\phi\rangle^T = (|\phi\rangle)^T \hat{O}^T (\langle\psi|^T) = (|\phi\rangle^*)^\dagger \hat{O}^T (\langle\psi|^*)^\dagger = \langle\phi^*|\hat{O}^T|\psi^*\rangle. \quad (8.3.2)$$

By definition $\langle\psi|\psi\rangle = 1$ and so to preserve this:

$$\langle\psi'|\psi'\rangle = \left(\langle\psi|\hat{U}^\dagger + \langle\psi^*|\hat{V}^\dagger\right) \left(\hat{U}|\psi\rangle + \hat{V}|\psi^*\rangle\right) \quad (8.3.3)$$

$$= \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle + \langle\psi^*|\hat{V}^\dagger\hat{U}|\psi\rangle + \langle\psi|\hat{U}^\dagger\hat{V}|\psi^*\rangle + \langle\psi^*|\hat{V}^\dagger\hat{V}|\psi^*\rangle \quad (8.3.4)$$

$$= \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle + \langle\psi^*|\hat{V}^\dagger\hat{U}|\psi\rangle + \langle\psi|\hat{V}^T\hat{U}^*|\psi^*\rangle + \langle\psi|\hat{V}^T\hat{V}^*|\psi^*\rangle \quad (8.3.5)$$

$$= \langle\psi|\left(\hat{U}^\dagger\hat{U} + \hat{V}^T\hat{V}^*\right)|\psi\rangle + \langle\psi^*|\hat{V}^\dagger\hat{U}|\psi\rangle + \langle\psi|\hat{V}^T\hat{U}^*|\psi^*\rangle \quad (8.3.6)$$

$$\stackrel{!}{=} \langle\psi|\psi\rangle \quad \forall|\psi\rangle \quad (8.3.7)$$

$$\implies \langle\psi|\left(\hat{U}^\dagger\hat{U} + \hat{V}^T\hat{V}^* - \mathbb{1}\right)|\psi\rangle + \langle\psi^*|\hat{V}^\dagger\hat{U}|\psi\rangle + \langle\psi|\hat{V}^T\hat{U}^*|\psi^*\rangle = 0. \quad (8.3.8)$$

Let us put equation (8.3.8) in components by using a real orthonormal basis $|n\rangle$:

$$|\psi\rangle = \sum_n \psi_n |n\rangle, \quad \hat{A} = \hat{U}^\dagger\hat{U} + \hat{V}^T\hat{V}^* - \mathbb{1}, \quad \hat{B} = \hat{V}^\dagger\hat{U} \quad (8.3.9)$$

$$A_{nm} = \langle n|\hat{A}|m\rangle, \quad B_{nm} = \langle n|\hat{B}|m\rangle. \quad (8.3.10)$$

Then, define $F(\psi, \psi^*)$ by:

$$F(\psi, \psi^*) = \langle\psi|\hat{A}|\psi\rangle + \langle\psi^*|\hat{B}|\psi\rangle + \langle\psi|\hat{B}^*|\psi^*\rangle \quad (8.3.11)$$

$$= \sum_n \psi_n^* \langle n|\hat{A} \sum_m \psi_m |m\rangle + \sum_n \psi_n \langle n|\hat{B} \sum_m \psi_m |m\rangle + \sum_n \psi_n^* \langle n|\hat{B}^* \sum_m \psi_m^* |m\rangle \quad (8.3.12)$$

$$= \sum_{nm} \left(\langle n|\hat{A}|m\rangle \psi_n^* \psi_m + \langle n|\hat{B}|m\rangle \psi_n \psi_m + \langle n|\hat{B}^*|m\rangle \psi_n^* \psi_m^* \right) \quad (8.3.13)$$

$$= \sum_{nm} (A_{nm} \psi_n^* \psi_m + B_{nm} \psi_n \psi_m + B_{nm}^* \psi_n^* \psi_m^*). \quad (8.3.14)$$

This function is required to vanish for all ψ . Consequently, all of its derivatives must vanish for all ψ . Then:

$$\frac{\partial^2 F}{\partial \psi_n \partial \psi_m} = B_{nm} + B_{mn} = 0 \implies \hat{B}^T = -\hat{B}. \quad (8.3.15)$$

Thus, $\hat{B}$ must be antisymmetric. Then by equation (8.3.2):

$$\langle \psi^* | \hat{B} | \psi \rangle = \langle \psi^* | \hat{B}^T | \psi \rangle = -\langle \psi^* | \hat{B} | \psi \rangle \implies \langle \psi^* | \hat{B} | \psi \rangle = 0. \quad (8.3.16)$$

Consequently, F simplifies to:

$$F(\psi, \psi^*) = \langle \psi | \hat{A} | \psi \rangle = \sum_{nm} A_{nm} \psi_n^* \psi_m \quad (8.3.17)$$

Further requiring the derivatives of F to vanish:

$$\frac{\partial^2 F}{\partial \psi_n^* \partial \psi_m} = A_{nm} = 0 \implies \hat{A} = 0 \implies F = 0. \quad (8.3.18)$$

Thus, we must have:

$$\hat{U}^\dagger \hat{U} + \hat{V}^T \hat{V}^* = \mathbb{1}, \quad \hat{V}^\dagger \hat{U} = -\hat{U}^T \hat{V}^*. \quad (8.3.19)$$

Now let us transform our Lagrangian and for complete generality allow time to be transformed:

$$\mathcal{L}' = i\hbar \langle \psi' | \dot{\psi}' \rangle - \langle \psi' | \hat{H}' | \psi' \rangle \quad (8.3.20)$$

$$= i\hbar \left(\langle \psi | \hat{U}^\dagger + \langle \psi^* | \hat{V}^\dagger \right) \frac{d}{dt'} \left(\hat{U} | \psi \rangle + \hat{V} | \psi^* \rangle \right) - \left(\langle \psi | \hat{U}^\dagger + \langle \psi^* | \hat{V}^\dagger \right) \hat{H}' \left(\hat{U} | \psi \rangle + \hat{V} | \psi^* \rangle \right) \quad (8.3.21)$$

$$\begin{aligned} &= i\hbar \frac{dt}{dt'} \left(\langle \psi | \hat{U}^\dagger \hat{U} | \dot{\psi} \rangle + \langle \psi | \hat{U}^\dagger \dot{\hat{U}} | \psi \rangle + \langle \psi^* | \hat{V}^\dagger \hat{U} | \dot{\psi} \rangle + \langle \psi^* | \hat{V}^\dagger \dot{\hat{U}} | \psi \rangle \right) \\ &\quad + i\hbar \frac{dt}{dt'} \left(\langle \psi | \hat{U}^\dagger \hat{V} | \dot{\psi}^* \rangle + \langle \psi | \hat{U}^\dagger \dot{\hat{V}} | \psi^* \rangle + \langle \psi^* | \hat{V}^\dagger \hat{V} | \dot{\psi}^* \rangle + \langle \psi^* | \hat{V}^\dagger \dot{\hat{V}} | \psi^* \rangle \right) \\ &\quad - \langle \psi | \hat{U}^\dagger \hat{H}' \hat{U} | \psi \rangle - \langle \psi^* | \hat{V}^\dagger \hat{H}' \hat{U} | \psi \rangle - \langle \psi | \hat{U}^\dagger \hat{H}' \hat{V} | \psi^* \rangle - \langle \psi^* | \hat{V}^\dagger \hat{H}' \hat{V} | \psi^* \rangle \end{aligned} \quad (8.3.22)$$

$$\begin{aligned} &= i\hbar \frac{dt}{dt'} \left(\langle \psi | \hat{U}^\dagger \hat{U} | \dot{\psi} \rangle + \langle \psi | \hat{U}^\dagger \dot{\hat{U}} | \psi \rangle + \langle \psi^* | \hat{V}^\dagger \hat{U} | \dot{\psi} \rangle + \langle \psi^* | \hat{V}^\dagger \dot{\hat{U}} | \psi \rangle \right) \\ &\quad + i\hbar \frac{dt}{dt'} \left(\langle \psi | \hat{V}^T \hat{U}^* | \dot{\psi}^* \rangle + \langle \psi | \hat{U}^\dagger \dot{\hat{V}} | \psi^* \rangle + \langle \psi | \hat{V}^T \hat{V}^* | \dot{\psi} \rangle + \langle \psi | \dot{\hat{V}}^T \hat{V}^* | \psi \rangle \right) \\ &\quad - \langle \psi | \hat{U}^\dagger \hat{H}' \hat{U} | \psi \rangle - \langle \psi^* | \hat{V}^\dagger \hat{H}' \hat{U} | \psi \rangle - \langle \psi | \hat{U}^\dagger \hat{H}' \hat{V} | \psi^* \rangle - \langle \psi | \hat{V}^T \hat{H}'^T \hat{V}^* | \psi \rangle. \end{aligned} \quad (8.3.23)$$

Let σ be the sign of $\frac{dt'}{dt}$ so that $\frac{dt'}{dt} = \sigma \left| \frac{dt'}{dt} \right|$. Then by (1.9.107) in order for our transformed Lagrangian to be of the same form as our untransformed Lagrangian we must have for some function $f(t, |\psi\rangle, \langle\psi|)$:

$$\mathcal{L}' = \sigma \frac{dt}{dt'} \left(\mathcal{L} + \frac{df}{dt} \right). \quad (8.3.24)$$

Explicitly:

$$\mathcal{L}' = \sigma \frac{dt}{dt'} \left(i\hbar \langle \psi | \dot{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle + \frac{\partial f}{\partial t} + \sum_n \frac{\partial f}{\partial \psi_n} \dot{\psi}_n + \sum_n \frac{\partial f}{\partial \psi_n^*} \dot{\psi}_n^* \right). \quad (8.3.25)$$

For convenience of notation, define:

$$\frac{\partial f}{\partial |\psi\rangle} = \sum_n \frac{\partial f}{\partial \psi_n} \langle n |, \quad \frac{\partial f}{\partial \langle \psi |} = \sum_n \frac{\partial f}{\partial \psi_n^*} | n \rangle \quad (8.3.26)$$

$$\implies \mathcal{L}' = \sigma \frac{dt}{dt'} \left(i\hbar \langle \psi | \dot{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial |\psi\rangle} |\dot{\psi}\rangle + \langle \dot{\psi}| \frac{\partial f}{\partial \langle \psi |} \right). \quad (8.3.27)$$

We can then match terms from equation (8.3.23) to (8.3.27). If t' has any dependence on $|\psi\rangle$ or $\langle\psi|$ then there would be nonlinear terms $\dot{\psi}$ in (8.3.27). However, there are no such terms to match against in (8.3.23) and therefore t' must be a function of t only. Now matching the $\langle \dot{\psi} |$ terms in both equations:

$$i\hbar \frac{dt}{dt'} \hat{V}^T \hat{V}^* | \dot{\psi} \rangle + i\hbar \frac{dt}{dt'} \hat{V}^T \dot{\hat{U}}^* | \psi^* \rangle = \sigma \frac{dt}{dt'} \frac{\partial f}{\partial \langle \psi |} \quad (8.3.28)$$

$$\implies \frac{\partial f}{\partial \langle \psi |} = i\hbar \sigma \hat{V}^T \hat{V}^* | \dot{\psi} \rangle + i\hbar \sigma \hat{V}^T \dot{\hat{U}}^* | \psi^* \rangle. \quad (8.3.29)$$

In components and making use of (8.3.19):

$$\frac{\partial f}{\partial \psi_n^*} = i\hbar\sigma \sum_m \left(\langle n|\hat{V}^T \hat{V}^*|m\rangle \psi_m + \langle n|\hat{V}^T \hat{U}^*|m\rangle \psi_m^* \right) \quad (8.3.30)$$

$$\implies \frac{\partial^2 f}{\partial \psi_n^* \partial \psi_m^*} = \langle n|\hat{V}^T \hat{U}^*|m\rangle \implies \langle n|\hat{V}^T \hat{U}^*|m\rangle = \langle m|\hat{V}^T \hat{U}^*|n\rangle \quad (8.3.31)$$

$$\implies \hat{V}^T \hat{U}^* = (\hat{V}^T \hat{U}^*)^T = \hat{U}^\dagger \hat{V} \quad (8.3.32)$$

$$\implies \hat{V}^\dagger \hat{U} = -\hat{U}^T \hat{V}^* = -(\hat{V}^T \hat{U}^*)^\dagger = -(\hat{U}^\dagger \hat{V}) = -\hat{V}^\dagger \hat{U} \quad (8.3.33)$$

$$\implies \hat{V}^\dagger \hat{U} = 0. \quad (8.3.34)$$

With this (8.3.30) becomes:

$$\frac{\partial f}{\partial \langle \psi|} = i\hbar\sigma \hat{V}^T \hat{V}^* |\psi\rangle \implies f(t, \psi, \psi^*) = i\hbar\sigma \langle \psi|\hat{V}^T \hat{V}^*|\psi\rangle + g(t, \psi). \quad (8.3.35)$$

Next matching the $|\psi\rangle$ terms:

$$i\hbar \frac{dt}{dt'} \langle \psi|\hat{U}^\dagger \hat{U} = i\hbar\sigma \frac{dt}{dt'} \langle \psi| + \sigma \frac{dt}{dt'} \frac{\partial f}{\partial |\psi\rangle} \quad (8.3.36)$$

$$\implies \frac{\partial g}{\partial |\psi\rangle}(t, \psi) = i\hbar\sigma \langle \psi| \left(\hat{U}^\dagger \hat{U} - \hat{V}^T \hat{V}^* - \sigma \mathbb{1} \right). \quad (8.3.37)$$

The left hand side is a function of ψ only. Therefore, its ψ^* derivative must vanish. Taking the ψ^* derivative of both sides then gives:

$$\hat{U}^\dagger \hat{U} - \hat{V}^T \hat{V}^* - \sigma \mathbb{1} = 0. \quad (8.3.38)$$

Using equation (8.3.19) then gives:

$$\hat{U}^\dagger \hat{U} = \frac{1+\sigma}{2} \mathbb{1}, \quad \hat{V}^\dagger \hat{V} = \frac{1-\sigma}{2} \mathbb{1}. \quad (8.3.39)$$

Returning this result, it follows that:

$$\frac{\partial g}{\partial |\psi\rangle} = 0 \implies g(t, \psi) = g(t). \quad (8.3.40)$$

So, $g(t)$ appears only in the transformed Lagrangian through the $\frac{\partial f}{\partial t}$ term in (8.3.27). $\frac{\partial g}{\partial t}$ does not depend on ψ or ψ^* and so there is no other term to match it against. Thus, it must be 0. As such, $g(t)$ must just be some constant number. However, because the surface term only enters the Lagrangian through its derivatives, we can choose such a constant to be 0 so that $g(t) = 0$, giving:

$$f(t, \psi, \psi^*) = i\hbar\sigma \langle \psi|\hat{V}^T \hat{V}^*|\psi\rangle. \quad (8.3.41)$$

Now let us do some case analysis. First, assume time is not reversed so that $\sigma = 1$. Then by (8.3.39):

$$\hat{U}^\dagger \hat{U} = \mathbb{1}, \quad \hat{V}^\dagger \hat{V} = 0. \quad (8.3.42)$$

So, for all $|\psi\rangle$:

$$\langle \psi|\hat{V}^\dagger \hat{V}|\psi\rangle = 0 \implies \left\| \hat{V}|\psi\rangle \right\|^2 = 0 \implies \hat{V}|\psi\rangle = 0 \implies \hat{V} = 0. \quad (8.3.43)$$

The last step only following because this is true for all $|\psi\rangle$. Because $\hat{V}$ is 0, we then have:

$$|\psi'\rangle = \hat{U}|\psi\rangle. \quad (8.3.44)$$

As well, because a coordinate transformation is by definition invertible, $\hat{U}^{-1}$ must exist and from equation (8.3.42) we see that:

$$\hat{U}^{-1} = \hat{U}^\dagger. \quad (8.3.45)$$

So, $\hat{U}$ must be unitary. We immediately have $f = 0$ and the remaining terms in matching the transformed Lagrangians give:

$$i\hbar \frac{dt}{dt'} \langle \psi|\hat{U}^\dagger \dot{\hat{U}}|\psi\rangle - \langle \psi|\hat{U}^\dagger \hat{H}' \hat{U}|\psi\rangle = -\frac{dt}{dt'} \langle \psi|\hat{H}|\psi\rangle \quad \forall \psi \quad (8.3.46)$$

$$\implies \hat{U}^\dagger \hat{H}' \hat{U} = \frac{dt}{dt'} \left(\hat{H} + i\hbar \hat{U}^\dagger \dot{\hat{U}} \right) \quad (8.3.47)$$

Using the unitarity of $\hat{U}$ we can see that:

$$\hat{U}^\dagger \hat{U} = \mathbb{1} \implies \dot{\hat{U}}^\dagger \hat{U} + \hat{U}^\dagger \dot{\hat{U}} = 0 \implies \dot{\hat{U}} = -\hat{U} \dot{\hat{U}}^\dagger \hat{U}. \quad (8.3.48)$$

Then, we can solve for $\hat{H}'$ as:

$$\implies \hat{H}' = \frac{dt}{dt'} \left(\hat{U} \hat{H} \hat{U}^\dagger + i\hbar \dot{\hat{U}} \hat{U}^\dagger \right) \quad (8.3.49)$$

$$\implies \hat{H}' = \frac{dt}{dt'} \hat{U} \left(\hat{H} - i\hbar \frac{\partial}{\partial t} \right) \hat{U}^\dagger. \quad (8.3.50)$$

Now let us analyze the case in which time is reversed so that $\sigma = -1$. Then by (8.3.39):

$$\hat{U}^\dagger \hat{U} = 0, \quad \hat{V}^\dagger \hat{V} = \mathbb{1}. \quad (8.3.51)$$

So, for all $|\psi\rangle$:

$$\langle \psi | \hat{U}^\dagger \hat{U} | \psi \rangle = 0 \implies \left\| \hat{U} | \psi \rangle \right\|^2 = 0 \implies \hat{U} | \psi \rangle = 0 \implies \hat{U} = 0. \quad (8.3.52)$$

Again with the last step following because this was true for all $|\psi\rangle$. Because $\hat{U}$ is 0, we then have:

$$|\psi'\rangle = \hat{V} |\psi^*\rangle. \quad (8.3.53)$$

As well, because a coordinate transformation is by definition invertible $\hat{V}^{-1}$ must exist and from equation (8.3.51) we see that:

$$\hat{V}^{-1} = \hat{V}^\dagger \quad (8.3.54)$$

and so $\hat{V}$ is also unitary. We immediately have $f = -i\hbar \langle \psi | \psi \rangle$ and the remaining terms in matching the transformed Lagrangians give:

$$i\hbar \frac{dt}{dt'} \langle \psi | \dot{\hat{V}}^T \hat{V}^* | \psi \rangle - \langle \psi | \hat{V}^T \hat{H}'^T \hat{V}^* | \psi \rangle = \frac{dt}{dt'} \langle \psi | \hat{H} | \psi \rangle \quad \forall \psi \quad (8.3.55)$$

$$\implies \hat{V}^T \hat{H}'^T \hat{V}^* = \left| \frac{dt}{dt'} \right| \left(\hat{H} - i\hbar \dot{\hat{V}}^T \hat{V}^* \right) \quad (8.3.56)$$

$$\implies \hat{V}^\dagger \hat{H}' \hat{V} = \left| \frac{dt}{dt'} \right| \left(\hat{H}^T - i\hbar \hat{V}^\dagger \dot{\hat{V}} \right) \quad (8.3.57)$$

$$\implies \hat{H}' = \left| \frac{dt}{dt'} \right| \hat{V} \left(\hat{H}^T + i\hbar \frac{\partial}{\partial t} \right) \hat{V}^\dagger. \quad (8.3.58)$$

These two cases together give us:

Theorem 8.3: Wigner's Theorem

Any canonical transformation in quantum mechanics in which time is not reversed is given by some unitary operator $\hat{U}$ under which $|\psi\rangle$ and $\hat{H}$ transform as:

$$|\psi'\rangle = \hat{U} |\psi\rangle, \quad \hat{H}' = \frac{dt}{dt'} \hat{U} \left(\hat{H} - i\hbar \frac{\partial}{\partial t} \right) \hat{U}^\dagger. \quad (8.3.59)$$

As well, no surface term can be added to the action under such a transformation. Any canonical transformation in quantum mechanics in which time is reversed is given by some unitary operator $\hat{V}$ under which $|\psi\rangle$ and $\hat{H}$ transform as:

$$|\psi'\rangle = \hat{V} |\psi^*\rangle, \quad \hat{H}' = \left| \frac{dt}{dt'} \right| \hat{V} \left(\hat{H}^T + i\hbar \frac{\partial}{\partial t} \right) \hat{V}^\dagger. \quad (8.3.60)$$

As well, the surface term added to the action must be $f = -i\hbar \langle \psi | \psi \rangle$ under such a transformation.

Importantly, in the above the surface term $f = -i\hbar \langle \psi | \psi \rangle$ should not be set to $f = -i\hbar$ by using $\langle \psi | \psi \rangle = 1$ in the Lagrangian, because $\langle \psi | \psi \rangle = 1$ is actually a constraint on the initial condition. In order to use it in the Lagrangian, you are required first to add it as a Lagrange multiplier. If you do not use it in the Lagrangian and instead simply require it of the initial conditions used when actually solving the equations of motion, then dynamically it will be preserved.

When we very first studied time reversal as a subset of canonical transformations, we identified that all time reversing canonical transformations can be understood as a composition of a time nonreversing

(orthochronous) canonical transformation together with a simple time reversal. In a simple time reversal, $t' = -t$, $Q' = Q$. Consequently we found $P' = -P$ and $\mathcal{H}' = \mathcal{H}$. These considerations from chapter 1 were done assuming real valued canonical variables. In section 8.2 each component of $|\psi\rangle$ was defined so that a previous canonical coordinate was its real part (up to a constant multiplier) and the corresponding previous canonical momentum was its imaginary part. So, under a simple time reversal the real part should be unchanged but the imaginary part inverted (as Q is unchanged by P is inverted), which is precisely complex conjugation. Therefore, the quantum mechanical special case of a simple time reversal is the transformation:

$$|\psi'\rangle = |\psi^*\rangle. \quad (8.3.61)$$

Some readers may object to the notation $|\psi^*\rangle$ because it requires a meaningful notion of taking the complex conjugate of the coefficients of ψ without also taking the Hermitian adjoint of the basis elements. This is in general a basis dependent procedure, therefore ambiguous unless a natural basis is specified. This is okay, one just needs to understand that $|\psi^*\rangle$ is defined with respect to some basis. This is not surprising as the notion of a simple time reversal is coordinate dependent. (A simple time reversal in one set of coordinates is not a simple time reversal in another set of canonical coordinates.) In fact this property is essential because we need all time reversing transformations to be related to any designated simple time reversal by an orthochronous transformation, which is precisely a change of coordinates/basis.

While we considered only transformations so that ψ' depended linearly on ψ and ψ^* from the structure of the Hamiltonian, it is possible with significant extra effort to prove rigorously that this linearity is forced upon us. We can also prove the results of this section by instead requiring intensities $|\langle\psi_1|\psi_2\rangle|$ to be preserved instead of the form of the Hamiltonian. This is reasonable because such intensities are generally directly experimentally measurable. For a detailed proof of Wigner's theorem starting from this perspective, see [125].

Exercises

Problem 8.7: ★ The Time Evolution Operator. The Schrödinger equation for given initial conditions has a solution which exists and that solution is unique (for a finite dimensional Hilbert space this is easily proved because the Schrödinger equation is linear; for infinite dimensional Hilbert spaces it is more difficult to prove but still true). Because the Schrödinger equation is linear, the solution at time t is related to the solution at time t_0 linearly. That is, there exists an operator $\hat{U}(t, t_0)$ called the time evolution operator so that:

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle.$$

- (a) Show that the time evolution operator satisfies the identity condition:

$$\hat{U}(t_0, t_0) = \mathbb{1},$$

the composition condition:

$$\hat{U}(t, t_1)\hat{U}(t_1, t_0) = \hat{U}(t, t_0),$$

and the operator-Schrödinger equation:

$$i\hbar \frac{\partial \hat{U}(t, t_0)}{\partial t} = \hat{H}(t)\hat{U}(t, t_0).$$

- (b) Using the operator-Schrödinger equation, show that $\hat{U}(t, t_0)$ is unitary for all t . That is, show that:

$$\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{1}.$$

- (c) Using the composition condition, show that $\hat{U}(t, t_0)$ also satisfies:

$$i\hbar \frac{\partial \hat{U}(t, t_0)}{\partial t_0} = -\hat{U}(t, t_0)\hat{H}(t_0).$$

Because $\hat{U}$ is unitary and gives all quantum mechanical time evolution, by Wigner's theorem we see that once again time evolution is just a particular canonical transformation.

Problem 8.8: Hilbert's Hotel. For a finite dimensional vector space, if an operator has a left inverse then it has a right inverse and they are equal. This is not true for infinite dimensional vector spaces. Consequently, in order for any operator $\hat{U}$ to be unitary it is not enough to check $\hat{U}^\dagger \hat{U} = \mathbb{1}$. One must also show $\hat{U} \hat{U}^\dagger = \mathbb{1}$. We reserve the operator inverse notation only for operators which have both a left and right inverse and whose left and right inverses coincide. Consider an infinite dimensional Hilbert space with orthonormal basis

$|0\rangle, |1\rangle, |2\rangle, \dots$. Define the shift operator:

$$\hat{S}|n\rangle = |n+1\rangle.$$

(a) Show that:

$$\hat{S} = \sum_{n=0}^{\infty} |n+1\rangle\langle n|.$$

(b) Show that:

$$\hat{S}^\dagger \hat{S} = \mathbb{1}.$$

Thus, $S^\dagger$ is the left inverse of $\hat{S}$ and one may suspect that $\hat{S}$ is unitary.

(c) Show that:

$$\hat{S}\hat{S}^\dagger = \mathbb{1} - |0\rangle\langle 0|.$$

Thus, conclude that $S^\dagger$ is not the right inverse of $\hat{S}$ and $\hat{S}$ is not unitary.

8.4 Continuous Transformations in Quantum Mechanics

This section is based on [45]. As was true in classical physics, we are most often interested in continuous transformations. A continuous transformation is necessarily continuously connected to the identity transformation and of course the identity transformation does not reverse time. So, in quantum mechanics every continuous transformation is represented by a unitary transformation of the state vector due to Wigner's theorem:

$$|\psi'\rangle = \hat{U}|\psi\rangle, \quad \hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{1}. \quad (8.4.1)$$

From Noether's theorem, the generator G of a continuous transformation is given by:

$$G = \langle \pi | \mathcal{D} | \psi \rangle - \mathcal{H} \mathcal{D} t - \mathcal{D} f. \quad (8.4.2)$$

As we found in Wigner's theorem, $f = 0$ and so $\mathcal{D}f = 0$. If we consider transformations which leave time untransformed, $\mathcal{D}t = 0$ and so:

$$G = \langle \pi | \mathcal{D} | \psi \rangle = i\hbar \langle \psi | \mathcal{D} | \psi \rangle. \quad (8.4.3)$$

Now using equation (8.4.1):

$$\mathcal{D}|\psi\rangle = \left. \frac{d|\psi'\rangle}{d\varepsilon} \right|_{\varepsilon=0} = \left. \frac{d(\hat{U}|\psi\rangle)}{d\varepsilon} \right|_{\varepsilon=0} = \left. \frac{d\hat{U}}{d\varepsilon} \right|_{\varepsilon=0} |\psi\rangle = (\mathcal{D}\hat{U})|\psi\rangle. \quad (8.4.4)$$

Thus, G becomes:

$$G = i\hbar \langle \psi | (\mathcal{D}\hat{U}) | \psi \rangle \quad (8.4.5)$$

and so a generator in quantum mechanics is defined by some linear operator $\hat{G} = i\hbar(\mathcal{D}\hat{U})$. Studying what unitarity implies near the identity:

$$\left. \frac{d}{d\varepsilon} (\hat{U}^\dagger \hat{U}) \right|_{\varepsilon=0} = \left. \frac{d\mathbb{1}}{d\varepsilon} \right|_{\varepsilon=0} = 0 \quad (8.4.6)$$

$$\Rightarrow \left(\frac{d\hat{U}^\dagger}{d\varepsilon} \hat{U} + \hat{U}^\dagger \frac{d\hat{U}}{d\varepsilon} \right) \Big|_{\varepsilon=0} = 0 \quad (8.4.7)$$

$$\Rightarrow (\mathcal{D}\hat{U})^\dagger \mathbb{1} + \mathbb{1}(\mathcal{D}\hat{U}) = 0 \Rightarrow (\mathcal{D}\hat{U})^\dagger = -\mathcal{D}\hat{U} \quad (8.4.8)$$

$$\Rightarrow \hat{G}^\dagger = -i\hbar(\mathcal{D}\hat{U})^\dagger = i\hbar(\mathcal{D}\hat{U}) = \hat{G}. \quad (8.4.9)$$

Thus, every generator of continuous transformations of the wavefunction in quantum mechanics is of the form:

$$G = \langle \psi | \hat{G} | \psi \rangle \quad (8.4.10)$$

where $\hat{G}$ is a self-adjoint operator. One tends to also call $\hat{G}$ the generator of the transformation, because there is a one-to-one correspondence between G and $\hat{G}$, however this is a bit of abuse of language. It is common to call these G and $\hat{G}$ "observables" rather than generators. I will avoid this terminology as it is overly metaphysical and seems to suggest that all experimentally observable quantities are of this form and that all quantities of this form are experimentally observable, neither of which is true. (For examples, the parameters of the Hamiltonian, such as a particle mass, can be extracted from experimental observables and so are observable but not of this form and there are many quantities one could write down of this form which are not gauge-invariant and so not observable in that they aren't even experimentally well-defined.) From the self-adjointness of $\hat{G}$ it immediately follows that G is real valued:

$$G^* = (\langle \psi | \hat{G} | \psi \rangle)^* = (\langle \psi | \hat{G} | \psi \rangle)^\dagger = \langle \psi | \hat{G}^\dagger | \psi \rangle = \langle \psi | \hat{G} | \psi \rangle = G. \quad (8.4.11)$$

Now recall the Poisson bracket for classical field theory from equation (3.2.58). Written for our wavefunction it becomes:

$$\{A, B\} = \int_{\mathbb{S}} \left(\frac{\delta A}{\delta \psi^a(\vec{x})} \frac{\delta B}{\delta \pi_a(\vec{x})} - \frac{\delta A}{\delta \pi_a(\vec{x})} \frac{\delta B}{\delta \psi^a(\vec{x})} \right) d\mathbb{S} = \frac{1}{i\hbar} \int_{\mathbb{S}} \left(\frac{\delta A}{\delta \psi(\vec{x})} \frac{\delta B}{\delta \psi^\dagger(\vec{x})} - \frac{\delta B}{\delta \psi(\vec{x})} \frac{\delta A}{\delta \psi^\dagger(\vec{x})} \right) d\mathbb{S}. \quad (8.4.12)$$

Next consider how $|\psi\rangle$ evolves under the transformation generated by G using equation (1.4.1):

$$\frac{d|\psi\rangle}{d\varepsilon} = \{|\psi\rangle, G\}. \quad (8.4.13)$$

$$\frac{\delta|\psi\rangle}{\delta\psi(\vec{x})} = \frac{\delta}{\delta\psi(\vec{x})} \int_{\mathbb{S}} \psi(\vec{x}') |\vec{x}'\rangle d^d\vec{x}' = \int_{\mathbb{S}} \delta(\vec{x} - \vec{x}') |\vec{x}'\rangle d^d\vec{x}' = |\vec{x}\rangle \quad (8.4.14)$$

$$\frac{\delta|\psi\rangle}{\delta\psi^\dagger(\vec{x})} = \frac{\delta}{\delta\psi^\dagger(\vec{x})} \int_{\mathbb{S}} \psi(\vec{x}') |\vec{x}'\rangle d^d\vec{x}' = 0 \quad (8.4.15)$$

$$\frac{\delta G}{\delta\psi(\vec{x})} = \frac{\delta}{\delta\psi(\vec{x})} \langle\psi|\hat{G}|\psi\rangle = \frac{\delta\langle\psi|}{\delta\psi(\vec{x})} \hat{G}|\psi\rangle + \langle\psi|\hat{G} \frac{\delta|\psi\rangle}{\delta\psi(\vec{x})} = \left(\frac{\delta|\psi\rangle}{\delta\psi^\dagger(\vec{x})} \right)^\dagger \hat{G}|\psi\rangle + \langle\psi|\hat{G}|\vec{x}\rangle = \langle\psi|\hat{G}|\vec{x}\rangle \quad (8.4.16)$$

$$\frac{\delta G}{\delta\psi^\dagger(\vec{x})} = \left(\frac{\delta G}{\delta\psi(\vec{x})} \right)^\dagger = \left(\langle\psi|\hat{G}|\vec{x}\rangle \right)^\dagger = \langle\vec{x}|\hat{G}|\psi\rangle. \quad (8.4.17)$$

And so, computing the Poisson bracket:

$$\frac{d|\psi\rangle}{d\varepsilon} = \{|\psi\rangle, G\} = \frac{1}{i\hbar} \int_{\mathbb{S}} \left(\frac{\delta|\psi\rangle}{\delta\psi(\vec{x})} \frac{\delta G}{\delta\psi^\dagger(\vec{x})} - \frac{\delta G}{\delta\psi(\vec{x})} \frac{\delta|\psi\rangle}{\delta\psi^\dagger(\vec{x})} \right) d\mathbb{S} \quad (8.4.18)$$

$$= \frac{1}{i\hbar} \int_{\mathbb{S}} \left(|\vec{x}\rangle \langle\vec{x}|\hat{G}|\psi\rangle - \langle\psi|\hat{G}|\vec{x}\rangle 0 \right) d\mathbb{S} \quad (8.4.19)$$

$$= \frac{1}{i\hbar} \left(\int_{\mathbb{S}} |\vec{x}\rangle \langle\vec{x}| d\mathbb{S} \right) \hat{G}|\psi\rangle \quad (8.4.20)$$

$$= -\frac{i}{\hbar} \hat{G}|\psi\rangle. \quad (8.4.21)$$

This allows us to compute the n^{th} derivative of $|\psi\rangle$ with respect to ε :

$$\frac{d^n|\psi\rangle}{d\varepsilon^n} = \left(\frac{d}{d\varepsilon} \right)^{n-1} \left(-\frac{i}{\hbar} \hat{G}|\psi\rangle \right) = -\frac{i}{\hbar} \hat{G} \frac{d^{n-1}|\psi\rangle}{d\varepsilon^{n-1}} = \dots = \left(-\frac{i}{\hbar} \hat{G} \right)^n |\psi\rangle \quad (8.4.22)$$

and so applying the Taylor expansion for $|\psi\rangle$ in terms of ε :

$$|\psi'\rangle = |\psi(\varepsilon)\rangle = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \left(\frac{d^n|\psi\rangle}{d\varepsilon^n} \right) \Big|_{\varepsilon=0} = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \left(-\frac{i}{\hbar} \varepsilon \hat{G} \right)^n |\psi\rangle = e^{-\frac{i}{\hbar} \varepsilon \hat{G}} |\psi\rangle. \quad (8.4.23)$$

Comparing equation (8.4.23) with equation (8.4.1) we can see that the operator $\hat{U}$ is related to the transformation parameter ε and the generating operator $\hat{G}$ by:

$$\hat{U} = e^{-\frac{i}{\hbar} \varepsilon \hat{G}}. \quad (8.4.24)$$

Thus, we have:

Theorem 8.4: Continuous Transformations in Quantum Mechanics

Any continuous transformation which leaves time unchanged in quantum mechanics is generated by a function G so that there exists a self-adjoint operator $\hat{G}$ such that:

$$G = \langle\psi|\hat{G}|\psi\rangle \quad (8.4.25)$$

Under such a transformation with transformation parameter ε , $|\psi\rangle$ changes as:

$$|\psi'\rangle = e^{-\frac{i}{\hbar} \varepsilon \hat{G}} |\psi\rangle. \quad (8.4.26)$$

We see that $\hat{G}$ is self-adjoint and $\hat{U}$ must be unitary. Let us now establish an important fact: **for an operator $\hat{U}$, there exists a self-adjoint $\hat{F}$ so that $\hat{U} = e^{-i\hat{F}}$ if and only if $\hat{U}$ is unitary.** Suppose $\hat{U}$ can be written in the form $\hat{U} = e^{-i\hat{F}}$ for a self-adjoint $\hat{F}$. Then, because $\hat{F}$ is self-adjoint it is diagonalizable by the spectral theorem and we can identify an orthonormal eigenbasis $|n\rangle$ for $\hat{F}$. Automatically then by the definition of the operator exponential:

$$\hat{F} = \sum_n F_n |n\rangle \langle n|, \quad \hat{U} = e^{-i\hat{F}} \implies \hat{U} = \sum_n e^{-iF_n} |n\rangle \langle n| \quad (8.4.27)$$

and the F_n coefficients are real. With this, we immediately have that $\hat{U}$ is unitary:

$$\hat{U}\hat{U}^\dagger = \sum_{nn'} e^{-iF_n} e^{iF_{n'}} |n\rangle \langle n| n'\rangle \langle n'| = \sum_n |n\rangle \langle n| = \mathbb{1} \quad (8.4.28)$$

$$\hat{U}^\dagger \hat{U} = \sum_{nn'} e^{iF_n} e^{-iF_{n'}} |n\rangle \langle n| n'\rangle \langle n'| = \sum_n |n\rangle \langle n| = \mathbb{1}. \quad (8.4.29)$$

Now for the other direction. Suppose that $\hat{U}$ is unitary. Then, it is diagonalizable by the spectral theorem

with some orthonormal eigenbasis $|n\rangle$. Let u_n be the eigenvalues of $\hat{U}$:

$$\hat{U}|n\rangle = u_n|n\rangle. \quad (8.4.30)$$

Take the norm of both sides:

$$\|\hat{U}|n\rangle\|^2 = \|u_n|n\rangle\|^2 \quad (8.4.31)$$

$$\implies \langle n|\hat{U}^\dagger\hat{U}|n\rangle = u_n^*u_n\langle n|n\rangle \quad (8.4.32)$$

$$\implies |u_n|^2 = 1 \quad (8.4.33)$$

by using that $\hat{U}$ is unitary. So, for each n we can define real numbers F_n so that $u_n = e^{-iF_n}$. From these real numbers define $\hat{F}$ by:

$$\hat{F} = \sum F_n|n\rangle\langle n|. \quad (8.4.34)$$

Automatically it follows that:

$$\hat{U} = e^{-i\hat{F}} \quad (8.4.35)$$

as desired.

Because the form $\langle\psi|\hat{G}|\psi\rangle$ will continue to appear often, it is useful to give it a name. For an operator $\hat{O}$, the quantity $\langle\psi|\hat{O}|\psi\rangle$ is called the **operator summary** or “operator expectation” of $\hat{O}$. I will avoid the term operator expectation because the word expectation invokes concepts from probability and statistics which are not intended. There is an emergent connection between operator summaries and statistical expectations that is experimentally important, but the mechanism behind that is statistical mechanics and the detailed explanation for it isn’t appropriate until chapter 9. We can see from theorem 8.2 that even the Hamiltonian is the operator summary of a self-adjoint operator, the Hamiltonian operator. We also introduce a short hand notation for operator summaries:

$$G = \langle\hat{G}\rangle = \langle\psi|\hat{G}|\psi\rangle. \quad (8.4.36)$$

The Poisson bracket of two operator summaries leads to a very nice structure. Consider $A = \langle\hat{A}\rangle$ and $B = \langle\hat{B}\rangle$ for some operators $\hat{A}$ and $\hat{B}$. Then:

$$\{A, B\} = \{\langle\hat{A}\rangle, \langle\hat{B}\rangle\} = \frac{1}{i\hbar} \int_{\mathbb{S}} \left(\frac{\delta\langle\hat{A}\rangle}{\delta\psi(\vec{x})} \frac{\delta\langle\hat{B}\rangle}{\delta\psi^\dagger(\vec{x})} - \frac{\delta\langle\hat{B}\rangle}{\delta\psi(\vec{x})} \frac{\delta\langle\hat{A}\rangle}{\delta\psi^\dagger(\vec{x})} \right) d\mathbb{S} \quad (8.4.37)$$

$$= \frac{1}{i\hbar} \int_{\mathbb{S}} \left(\langle\psi|\hat{A}|\vec{x}\rangle\langle\vec{x}|\hat{B}|\psi\rangle - \langle\psi|\hat{B}|\vec{x}\rangle\langle\vec{x}|\hat{A}|\psi\rangle \right) d\mathbb{S} \quad (8.4.38)$$

$$= \frac{1}{i\hbar} \left(\langle\psi|\hat{A} \int_{\mathbb{S}} |\vec{x}\rangle\langle\vec{x}| d\mathbb{S} \hat{B} |\psi\rangle - \langle\psi|\hat{B} \int_{\mathbb{S}} |\vec{x}\rangle\langle\vec{x}| d\mathbb{S} \hat{A} |\psi\rangle \right) \quad (8.4.39)$$

$$= \frac{1}{i\hbar} \left(\langle\psi|\hat{A}\hat{B}|\psi\rangle - \langle\psi|\hat{B}\hat{A}|\psi\rangle \right) \quad (8.4.40)$$

$$= \langle\psi|\frac{1}{i\hbar}[\hat{A}, \hat{B}]|\psi\rangle. \quad (8.4.41)$$

This argument is due to [91]. Hence, the Poisson bracket of two operator summaries is itself an operator summary. Furthermore, suppose $\hat{A}$ and $\hat{B}$ are self-adjoint. Then by (8.2.105) the Poisson bracket of two operator summaries of two self-adjoint operators is itself an operator summary of a self-adjoint operator.

Now suppose we have some generators which together form a Lie algebra. That is, we have generators τ_a whose Poisson brackets, for some constant $f_{ab}{}^c$ satisfy:

$$\{\tau_a, \tau_b\} = f_{ab}{}^c \tau_c. \quad (8.4.42)$$

It follows from theorem 8.4 that we must have self-adjoint operators $\hat{\tau}_a$ so that $\tau_a = \langle\hat{\tau}_a\rangle$. Then, from equation (8.4.41):

$$\{\langle\tau_a\rangle, \langle\tau_b\rangle\} = f_{ab}{}^c \langle\tau_c\rangle \quad (8.4.43)$$

$$\implies \langle\frac{1}{i\hbar}[\hat{\tau}_a, \hat{\tau}_b]\rangle = f_{ab}{}^c \langle\tau_c\rangle \quad (8.4.44)$$

$$\implies \langle\psi|([\hat{\tau}_a, \hat{\tau}_b] - i\hbar f_{ab}{}^c \hat{\tau}_c)|\psi\rangle = 0, \quad \forall|\psi\rangle \quad (8.4.45)$$

$$\implies [\hat{\tau}_a, \hat{\tau}_b] = i\hbar f_{ab}{}^c \hat{\tau}_c. \quad (8.4.46)$$

Hence, the Lie bracket structure of the generators reproduces itself on the generating operators with $\frac{1}{i\hbar}[\cdot, \cdot]$

replacing the Poisson bracket.

Now suppose we have a wavefunction with internal degrees of freedom. Under many transformations of interest, the way that the transformation acts on $|\psi\rangle$ will be to transform the spatial dependence in a particular way and to transform the internal components of $|\psi\rangle$ in a completely independent way. That is, the continuous transformation $\hat{U}$ corresponding to the overall transformation factors into a piece $\hat{U}_S$ which acts on the spatial dependence of $|\psi\rangle$ and $\hat{U}_{\text{int}}$ which acts on the internal space for $|\psi\rangle$:

$$|\psi'\rangle = \hat{U}|\psi\rangle = \hat{U}_S \hat{U}_{\text{int}} |\psi\rangle. \quad (8.4.47)$$

Certainly it is not necessarily the case that all transformations must take this form but it so happens that a broad class of transformations we will be interested in do. In order for $\hat{U}$ to be unitary, it immediately follows that $\hat{U}_S$ and $\hat{U}_{\text{int}}$ must individually be unitary on their respective spaces. As well, they commute with each other because they are operators on different vector spaces:

$$\hat{U}^{-1} = \hat{U}^\dagger \implies \hat{U}_S^{-1} \hat{U}_{\text{int}}^{-1} = \hat{U}_S^\dagger \hat{U}_{\text{int}}^\dagger \implies \hat{U}_S^{-1} = \hat{U}_S^\dagger, \quad \hat{U}_{\text{int}}^{-1} = \hat{U}_{\text{int}}^\dagger. \quad (8.4.48)$$

Then, differentiating equation (8.4.47) with respect to the transformation parameter about the identity:

$$\frac{d|\psi\rangle}{d\varepsilon} = \left(\left(\mathcal{D}\hat{U}_S \right) \mathbb{1} + \mathbb{1} \left(\mathcal{D}\hat{U}_{\text{int}} \right) \right) |\psi\rangle. \quad (8.4.49)$$

Thus, if we define:

$$\hat{G} = i\hbar(\mathcal{D}\hat{U}), \quad \hat{G}_S = i\hbar(\mathcal{D}\hat{U}_S), \quad \hat{G}_{\text{int}} = i\hbar(\mathcal{D}\hat{U}_{\text{int}}) \quad (8.4.50)$$

we can see that the overall generating operator $\hat{G}$ can be written as a sum of a generator on the spatial dependence of the wavefunction and a generator on the internal space of the wavefunction:

$$\hat{G}|\psi\rangle = \left(\hat{G}_S + \hat{G}_{\text{int}} \right) |\psi\rangle, \quad \forall |\psi\rangle \quad (8.4.51)$$

$$\implies \hat{G} = \hat{G}_S + \hat{G}_{\text{int}}. \quad (8.4.52)$$

If we have a group of transformations which all factorize in the above way, then let $\hat{\tau}_a$ be the generating operators for those transformations as identified in equation (8.4.46). Then, we must have:

$$\hat{\tau}_a = \hat{\tau}_a^S + \hat{\tau}_a^{\text{int}}, \quad [\hat{\tau}_a, \hat{\tau}_b] = i\hbar f_{ab}^c \hat{\tau}_c \quad (8.4.53)$$

$$\implies [\hat{\tau}_a^S, \hat{\tau}_b^S] + [\hat{\tau}_a^{\text{int}}, \hat{\tau}_b^{\text{int}}] = i\hbar f_{ab}^c \hat{\tau}_c^S + i\hbar f_{ab}^c \hat{\tau}_c^{\text{int}} \quad (8.4.54)$$

where this last line follows because the internal and spatial generators necessarily commute with each other. Because the internal and spatial generators act on different spaces, these pieces must cancel independently and so we have:

$$[\hat{\tau}_a^S, \hat{\tau}_b^S] = i\hbar f_{ab}^c \hat{\tau}_c^S, \quad [\hat{\tau}_a^{\text{int}}, \hat{\tau}_b^{\text{int}}] = i\hbar f_{ab}^c \hat{\tau}_c^{\text{int}} \quad (8.4.55)$$

and so the Lie algebra structure reproduces itself independently on the spatial and internal spaces⁴. Together this gives us:

Theorem 8.5: Quantum Poisson Brackets Theorem

The Poisson bracket of two operator summaries is itself an operator summary given by:

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\} = \left\langle \frac{1}{i\hbar} [\hat{A}, \hat{B}] \right\rangle. \quad (8.4.56)$$

If $\hat{A}$ and $\hat{B}$ are self-adjoint then the Poisson bracket of their summaries is itself the operator summary of a self-adjoint operator.

In quantum mechanics, any Lie algebra of generators τ_a with structure constants f_{ab}^c can be written in the form $\tau_a = \langle \hat{\tau}_a \rangle$ for some operators $\hat{\tau}_a$ which satisfy:

$$[\hat{\tau}_a, \hat{\tau}_b] = i\hbar f_{ab}^c \hat{\tau}_c. \quad (8.4.57)$$

If those generators correspond to transformations which factorize in how they act on the spatial and internal degrees of freedom of the wavefunction then the generating operators can be written

⁴There is a subtlety that one could add a term proportional to the identity to one of these if one subtracts the same term from the other. However, this effect would cancel in the combined transformation and so can essentially be reabsorbed into the definition of $\hat{U}_S$ and $\hat{U}_{\text{int}}$ so that no such term appears.

as $\hat{\tau}_a = \hat{\tau}_a^{\text{S}} + \hat{\tau}_a^{\text{int}}$ where the $\hat{\tau}_a^{\text{S}}$ act only on the spatial dependence of the wavefunction and the $\hat{\tau}_a^{\text{int}}$ act only on the internal degrees of freedom. As well, the spatial and internal generating operators independently reproduce the Lie algebra as:

$$[\hat{\tau}_a^{\text{S}}, \hat{\tau}_b^{\text{S}}] = i\hbar f_{ab}^c \hat{\tau}_c^{\text{S}}, \quad [\hat{\tau}_a^{\text{int}}, \hat{\tau}_b^{\text{int}}] = i\hbar f_{ab}^c \hat{\tau}_c^{\text{int}} \quad (8.4.58)$$

From the Schrödinger equation, if we consider two wavefunctions which are related by multiplying by a constant phase $|\psi'\rangle = e^{i\varphi}|\psi\rangle$, we can see that they both satisfy the same equation of motion:

$$i\hbar \frac{d|\psi'\rangle}{dt} - \hat{H}|\psi'\rangle = e^{i\varphi} \left(i\hbar \frac{d|\psi\rangle}{dt} - \hat{H}|\psi\rangle \right) = 0 \quad (8.4.59)$$

Thus, this fixed phase difference is preserved for all time. As well, any operator summary is completely unaffected by this phase:

$$\langle \psi' | \hat{G} | \psi' \rangle = \langle \psi | e^{-i\varphi} \hat{G} e^{i\varphi} | \psi \rangle = \langle \psi | \hat{G} | \psi \rangle. \quad (8.4.60)$$

So, because all generators in quantum mechanics and terms appearing in the Lagrangian are of this form, this overall phase drops out of the results of anything which couples the wavefunction to other variables (such as electromagnetism) or any of its mechanical quantities such as energy, momentum, or angular momentum. Because it is through such quantities that we make measurements, this overall phase φ has no experimental consequences. This is to say, **the wavefunction can be modified by an arbitrary overall constant phase with no physical effects**. This is unsurprising as such a phase could have been absorbed into our original definition of the components of the wavefunction in equation (8.2.3) without changing any of the arguments which followed. Because the wavefunction's normalization is set to 1 and the phase is arbitrary, any vector $|\phi\rangle \in \mathbb{H}$ which is proportional to $|\psi\rangle$ by a complex number: $|\phi\rangle = z|\psi\rangle$ produces all of the same physical predictions as $|\psi\rangle$, independent of the value of z . A family of vectors which are all mutually proportional to each other by a complex number is called a ray. Because of this you will often hear people who are being careful say “the state of a quantum system is represented by a ray in Hilbert space” as the ray corresponding to $|\psi\rangle$ is unique, not $|\psi\rangle$ itself. Later on we will generalize our approach to quantum mechanics in terms of a quantity known as the density matrix, in which meaningless junk like this overall phase doesn't appear. It is essential to understand that only the overall phase of $|\psi\rangle$ is meaningless, the relative phases of the ψ_n when $|\psi\rangle$ is written in a basis are extremely important.

It turns out further that $|\psi\rangle$ can be determined up to an overall phase (so the physical state, the ray to which $|\psi\rangle$ corresponds, can be determined) from the operator summaries of self-adjoint operators. To see how, consider a set of orthonormal basis vectors $|n\rangle$ and the operators $\hat{S}_{mn}$ and $\hat{A}_{mn}$ defined by:

$$\hat{S}_{mn} = \frac{|m\rangle\langle n| + |n\rangle\langle m|}{2} \implies \hat{S}_{mn}^\dagger = \frac{|n\rangle\langle m| + |m\rangle\langle n|}{2} = \hat{S}_{mn} \quad (8.4.61)$$

$$\hat{A}_{mn} = \frac{|m\rangle\langle n| - |n\rangle\langle m|}{2i} \implies \hat{A}_{mn}^\dagger = \frac{|n\rangle\langle m| - |m\rangle\langle n|}{-2i} = \hat{A}_{mn}. \quad (8.4.62)$$

Then, consider the expansion of the wavefunction in this basis:

$$|\psi\rangle = \sum_n \psi_n |n\rangle \quad (8.4.63)$$

$$\langle \hat{S}_{mn} \rangle = \frac{\psi_m^* \psi_n + \psi_n^* \psi_m}{2}, \quad \langle \hat{A}_{mn} \rangle = \frac{\psi_m^* \psi_n - \psi_n^* \psi_m}{2i} \quad (8.4.64)$$

$$\implies \langle \hat{S}_{mn} \rangle + i \langle \hat{A}_{mn} \rangle = \psi_m^* \psi_n. \quad (8.4.65)$$

Take a particular value of n , n_0 , such that $\langle \hat{S}_{n_0 n_0} \rangle \neq 0$. Such an n_0 must exist because the diagonal elements of $\langle \hat{S}_{mn} \rangle$ are automatically real, nonnegative, and sum to 1 by definition:

$$\langle \hat{S}_{nn} \rangle = \psi_n^* \psi_n \implies \sum_n \langle \hat{S}_{nn} \rangle = \sum_n \psi_n^* \psi_n = \sum_n \langle \psi | n \rangle \langle n | \psi \rangle = \langle \psi | \psi \rangle = 1. \quad (8.4.66)$$

Choose the phase of ψ so that ψ_{n_0} is real and positive. Then,

$$\langle \hat{S}_{n_0 n_0} \rangle = |\psi_{n_0}|^2 \implies \psi_{n_0} = \sqrt{\langle \hat{S}_{n_0 n_0} \rangle} \quad (8.4.67)$$

$$\langle \hat{S}_{n_0 n} \rangle + i \langle \hat{A}_{n_0 n} \rangle = \psi_{n_0}^* \psi_n = \sqrt{\langle \hat{S}_{n_0 n_0} \rangle} \psi_n \quad (8.4.68)$$

$$\Rightarrow \psi_n = \frac{\langle \hat{S}_{n_0 n} \rangle + i \langle \hat{A}_{n_0 n} \rangle}{\sqrt{\langle \hat{S}_{n_0 n_0} \rangle}}. \quad (8.4.69)$$

So the wavefunction can be fully reconstructed from these summaries by:

$$|\psi\rangle = \sum_n \psi_n |n\rangle = \sum_n \left(\frac{\langle \hat{S}_{n_0 n} \rangle + i \langle \hat{A}_{n_0 n} \rangle}{\sqrt{\langle \hat{S}_{n_0 n_0} \rangle}} \right) |n\rangle. \quad (8.4.70)$$

So we see that a complete set of these generators is enough to reconstruct ψ and thus determine the physical state. If a complete set of generators can be measured experimentally (which is typically true, in the sense that it is possible to measure an arbitrarily large number and approximate the full series), it follows that **the wavefunction (viewed as a ray in Hilbert space) is observable**. Reconstructing the quantum state of a system systematically through operator summaries is known as **quantum tomography**. A very careful reader will notice that only a subset of the operator summaries $\langle \hat{S}_{mn} \rangle$ and $\langle \hat{A}_{mn} \rangle$ were sufficient to determine $|\psi\rangle$ and may worry about the possibility that if a different subset had been chosen a different $|\psi\rangle$ would have been found. Later we will realize that interacting quantum systems necessitate representing the state of the system by a more general object known as the density matrix. It is possible that a given set of operator summaries may be incompatible with the existence of a $|\psi\rangle$, and in that case a density matrix is necessary. However, for describing a single matter particle at a time with a definite known state as we are committing to in this chapter, a wavefunction description is sufficient.

Exercises

Problem 8.9: ★ Ehrenfest's Theorem and the Quantum Noether Theorem. Let $G = \langle \psi | \hat{G}(t) | \psi \rangle$ for some self-adjoint operator $\hat{G}$ be a generator of interest. Derive Ehrenfest's theorem and derive quantum version of Noether's Theorem.

(a) Using the Schrödinger equation, show that:

$$\frac{d\langle \hat{G} \rangle}{dt} = \left\langle \frac{\partial \hat{G}}{\partial t} \right\rangle + \left\langle \frac{1}{i\hbar} [\hat{G}, \hat{H}] \right\rangle.$$

This result is known as Ehrenfest's Theorem. You should be able to see that it is a special case of (1.4.24). Because of this result, it is sometimes a useful shorthand to introduce the convective derivative $\frac{D}{Dt}$ defined so that:

$$\frac{D\hat{G}}{Dt} = \frac{\partial \hat{G}}{\partial t} + \frac{1}{i\hbar} [\hat{G}, \hat{H}].$$

(b) Consider the continuous transformation generated by G with parameter ε . Show using Noether's theorem that regardless of whether this transformation is a symmetry:

$$\left. \frac{\partial \hat{H}'(\varepsilon, t')}{\partial \varepsilon} \right|_{\varepsilon=0} = \frac{D\hat{G}}{Dt}.$$

Show that the transformation is a symmetry if and only if:

$$\frac{D\hat{G}}{Dt} = 0.$$

This is the quantum mechanical special case of Noether's theorem.

Problem 8.10: ★ Active vs. Passive Picture. Just like with statistical mechanics and continuum mechanics, it is possible and sometimes useful to introduce a notion of an active picture and a passive picture. The passive picture (also known as the Schrödinger picture) is the one we have been using in which the operators are specified in how they act on Hilbert space and the wavefunction evolves in time according to the Schrödinger equation. Using the time evolution operator, one can see:

$$\langle \psi(t) | \hat{G}(t) | \psi(t) \rangle = \langle \psi(t_0) | \hat{U}^\dagger(t, t_0) \hat{G}(t) \hat{U}(t, t_0) | \psi(t_0) \rangle.$$

The active picture operator $\hat{G}_A(t, t_0)$ defined relative to the time t_0 is then defined so that:

$$\hat{G}_A(t, t_0) = \hat{U}^\dagger(t, t_0) \hat{G}(t) \hat{U}(t, t_0).$$

Because operator summaries are the quantities of interest in quantum mechanics and these active picture operators can be used to compute all operator summaries using the constant state vector $|\psi(t_0)\rangle$ (for a fixed

t_0), the evolution of these operators contains all of the time evolution of quantum mechanics.

(a) Show that the active picture operators satisfy:

$$\frac{d\hat{G}_A}{dt} = \hat{U}^\dagger \frac{D\hat{G}}{Dt} \hat{U}.$$

(b) Suppose that $\hat{G}$ does not explicitly depend on time. Show that:

$$\frac{d\hat{G}_A}{dt} = \frac{1}{i\hbar} [\hat{G}_A, \hat{H}_A]$$

Readers familiar with quantum mechanics are likely to have been taught to refer to the active picture as the Heisenberg picture, named after Werner Heisenberg. One of Heisenberg's roles in life was as scientific head of the Nazi nuclear program. While the program failed and was inadequately staffed or resourced to succeed, his willing participation in the program and persistent nationalism during the Nazi era make him, in the author's view, ineligible for veneration, rehabilitation, or apologism.

8.5 Summary and Spread Coordinates

The argument of this section is based on [90], [91]. Now that we have the form of the Lagrangian and Hamiltonian for our new theory, we would like to understand how it relates to our previous theories. Previously when we modeled matter by point particles, a point was specified by its position $\vec{x}(t)$ and its conjugate linear momentum $\vec{p}(t)$. Now that we are considering a wave theory, we ought to expect that point-like behavior would be approximately valid whenever the wave is contained in a region of space small enough to treat as point-like for our experimental purposes and when that whole wave packet is all moving together with itself at about the same overall velocity so that it remains essentially localized relative to our experimental resolution over time. In such an approximation, the point around which the wavefunction is essentially localized defines the classical position $\vec{x}_{cl}$. To translate that position defined by the center of the whole wave, one must then translate the whole wave. Thus, its conjugate linear momentum is the generator of translations of the entire wave which is by definition its total linear momentum. So, the conjugate momentum $\vec{p}_{cl}$ to the classical position should be the total momentum carried by the wave packet.

We can directly compute $\vec{p}_{cl}$ using Noether's theorem. By definition, under a translation by $\vec{\varepsilon}$, a Dirac delta with peak at $\vec{x}$ becomes a Dirac delta with peak at $\vec{x} + \vec{\varepsilon}$. Let $\hat{T}(\vec{\varepsilon})$ to be the unitary operator corresponding to a translation by $\vec{\varepsilon}$:

$$\hat{T}|\vec{x}\rangle \stackrel{\text{def}}{=} |\vec{x} + \vec{\varepsilon}\rangle \quad (8.5.1)$$

$$\implies \hat{T} \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} = \int_{\mathbb{S}} |\vec{x} + \vec{\varepsilon}\rangle \langle \vec{x}| d^d \vec{x} \quad (8.5.2)$$

$$\implies \hat{T} = \int_{\mathbb{S}} |\vec{x} + \vec{\varepsilon}\rangle \langle \vec{x}| d^d \vec{x}. \quad (8.5.3)$$

A short calculation confirms that $\hat{T}$ is unitary. Under a translation the translated wavefunction $\psi_{\varepsilon}(t, \vec{x})$ becomes:

$$\psi_{\varepsilon}(t, \vec{x}) = \langle \vec{x} | \psi_{\varepsilon} \rangle = \langle \vec{x} | \hat{T} | \psi \rangle = \langle \vec{x} | \hat{T} \int_{\mathbb{S}} |\vec{x}'\rangle \langle \vec{x}' | d^d \vec{x}' | \psi \rangle = \int_{\mathbb{S}} \langle \vec{x} | \vec{x}' + \vec{\varepsilon} \rangle \langle \vec{x}' | \psi \rangle d^d \vec{x}' \quad (8.5.4)$$

$$= \int_{\mathbb{S}} \delta(\vec{x}' + \vec{\varepsilon} - \vec{x}) \psi(t, \vec{x}') d^d \vec{x}' = \psi(t, \vec{x} - \vec{\varepsilon}). \quad (8.5.5)$$

So, a translation simply shifts the argument of the wavefunction. Then, by theorem 8.4 and equation (8.4.5), the total linear momentum of the wave ($\vec{p}_{cl}$) is given by the generator of translations of that wave as:

$$\vec{p}_{cl} = i\hbar \langle \psi | \left(\vec{\mathcal{D}} \hat{T} \right) | \psi \rangle = i\hbar \int_{\mathbb{S}} \langle \psi | \vec{x} \rangle \langle \vec{x} | \left(\vec{\mathcal{D}} \hat{T} \right) | \psi \rangle d^d \vec{x} \quad (8.5.6)$$

$$= i\hbar \int_{\mathbb{S}} \psi^{\dagger}(t, \vec{x}) \left. \frac{d\psi_{\varepsilon}(\vec{x})}{d\vec{\varepsilon}} \right|_{\vec{\varepsilon}=0} d^d \vec{x} = i\hbar \int_{\mathbb{S}} \psi^{\dagger} \left. \frac{d\psi(t, \vec{x} - \vec{\varepsilon})}{d\vec{\varepsilon}} \right|_{\vec{\varepsilon}=0} d^d \vec{x} \quad (8.5.7)$$

$$= i\hbar \int_{\mathbb{S}} \psi^{\dagger} (-\nabla \psi) d^d \vec{x} = \langle \psi | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \right) | \psi \rangle. \quad (8.5.8)$$

So, the total linear momentum of the wavefunction can be written as the operator summary of “the momentum operator” $\hat{\vec{p}}$ defined by:

$$\hat{\vec{p}} \stackrel{\text{def}}{=} -i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \quad (8.5.9)$$

$$\implies \vec{p}_{cl} = \langle \psi | \hat{\vec{p}} | \psi \rangle. \quad (8.5.10)$$

We can see that this momentum operator is self-adjoint, as we know it should be from theorem 8.4, by considering its inner product between two functions ϕ and ψ :

$$\langle \phi | \hat{\vec{p}}^{\dagger} | \psi \rangle = \langle \phi | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \right)^{\dagger} | \psi \rangle = \langle \phi | i\hbar \int_{\mathbb{S}} (\nabla |\vec{x}\rangle) \langle \vec{x}| d^d \vec{x} | \psi \rangle \quad (8.5.11)$$

$$= i\hbar \int_{\mathbb{S}} (\nabla \phi(\vec{x})^*) \psi(\vec{x}) d^d \vec{x} = i\hbar \int_{\mathbb{S}} (\nabla(\phi^* \psi) - \phi^* \nabla \psi) d^d \vec{x}. \quad (8.5.12)$$

Functions ϕ and ψ which are square-integrable (meaning $\langle \psi | \psi \rangle$ and $\langle \phi | \phi \rangle$ are finite, precisely the class of wavefunctions for which our theory is defined) must decay sufficiently quickly for $|\vec{x}| \rightarrow \infty$ for their normalization integrals to converge. As such, the total derivative term in the above integral becomes a

vanishing surface term for large $|\vec{x}|$. So:

$$\langle \phi | \hat{p}^\dagger | \psi \rangle = 0 - i\hbar \int_{\mathbb{S}} \phi^* \nabla \psi d^d \vec{x} = \langle \phi | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \right) | \psi \rangle = \langle \phi | \hat{p} | \psi \rangle. \quad (8.5.13)$$

Because this holds for all such ϕ and ψ , we have:

$$\hat{p}^\dagger = \hat{p}. \quad (8.5.14)$$

With this momentum operator by equation theorem 8.4 we can express the translation operator as:

$$\hat{T} = e^{-\frac{i}{\hbar} \vec{\varepsilon} \cdot \hat{p}}. \quad (8.5.15)$$

In this form we can see quite explicitly how the translation operator actually just reproduces Taylor's theorem for analytic functions in the position basis. Using the exponential form:

$$\psi_\varepsilon(t, \vec{x}) = \langle \vec{x} | \psi_\varepsilon \rangle = \langle \vec{x} | \hat{T} | \psi \rangle = \langle \vec{x} | e^{-\frac{i}{\hbar} \vec{\varepsilon} \cdot \hat{p}} | \psi \rangle \quad (8.5.16)$$

$$= \langle \vec{x} | \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n (\vec{\varepsilon} \cdot \hat{p})^n | \psi \rangle = \sum_{n=0}^{\infty} \frac{(-i)^n}{n! \hbar^n} \langle \vec{x} | (\vec{\varepsilon} \cdot \hat{p})^n | \psi \rangle \quad (8.5.17)$$

Using:

$$\langle \vec{x} | \hat{p} | \psi \rangle = \langle \vec{x} | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}'\rangle \nabla' \langle \vec{x}' | d^d \vec{x}' \right) | \psi \rangle = -i\hbar \int_{\mathbb{S}} \langle \vec{x} | \vec{x}' \rangle \nabla' \langle \vec{x}' | \psi \rangle d^d \vec{x}' \quad (8.5.18)$$

$$= -i\hbar \int_{\mathbb{S}} \delta(\vec{x} - \vec{x}') \nabla' \psi(t, \vec{x}') d^d \vec{x}' = -i\hbar \nabla \psi(t, \vec{x}) \quad (8.5.19)$$

we can evaluate⁵ the inner product above by applying this formula n times:

$$\langle \vec{x} | (\vec{\varepsilon} \cdot \hat{p})^n | \psi \rangle = \langle \vec{x} | (\vec{\varepsilon} \cdot \hat{p}) \left((\vec{\varepsilon} \cdot \hat{p})^{n-1} | \psi \rangle \right) = i\hbar (\vec{\varepsilon} \cdot \nabla) (\langle \vec{x} | (\vec{\varepsilon} \cdot \hat{p})^{n-1} | \psi \rangle) = \dots = (-i\hbar)^n (\vec{\varepsilon} \cdot \nabla)^n \psi(t, \vec{x}). \quad (8.5.20)$$

Then, equation (8.5.17) becomes:

$$\psi_\varepsilon(t, \vec{x}) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n! \hbar^n} (-i\hbar)^n (\vec{\varepsilon} \cdot \nabla)^n \psi(t, \vec{x}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (\vec{\varepsilon} \cdot \nabla)^n \psi(t, \vec{x}). \quad (8.5.21)$$

This last expression is the formula for the Taylor expansion of $\psi(t, \vec{x} - \vec{\varepsilon})$ in powers of $\vec{\varepsilon}$ around $\vec{\varepsilon} = 0$ and so from this we recover:

$$\psi_\varepsilon(t, \vec{x}) = \psi(t, \vec{x} - \vec{\varepsilon}) \quad (8.5.22)$$

exactly as expected.

There is another way we can arrive at the expression for the momentum operator. From our study of the Legendre transformation, we know that the conjugate momentum P to a coordinate Q can be computed from the Lagrangian by:

$$P = \frac{\partial \mathcal{L}}{\partial \dot{Q}}. \quad (8.5.23)$$

Therefore, if we compute the right hand side of equation (8.5.23) with Q as the amount we had translated ψ , then the conjugate momentum to that Q will be the generator of translations of ψ . From our Lagrangian:

$$\mathcal{L} = i\hbar \langle \psi | \dot{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle \quad (8.5.24)$$

$$= i\hbar \langle \psi | \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} | \dot{\psi} \rangle - \langle \psi | \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} \hat{H} \int_{\mathbb{S}} |\vec{x}'\rangle \langle \vec{x}'| d^d \vec{x}' | \psi \rangle \quad (8.5.25)$$

$$= \int_{\mathbb{S}} i\hbar \langle \psi | \vec{x} \rangle \langle \vec{x} | \dot{\psi} \rangle d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \langle \psi | \vec{x} \rangle \langle \vec{x} | \hat{H} | \vec{x}' \rangle \langle \vec{x}' | \psi \rangle d^d \vec{x} d^d \vec{x}' \quad (8.5.26)$$

$$= i\hbar \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \dot{\psi}(t, \vec{x}) d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}'. \quad (8.5.27)$$

We can see actually that this field theory may be non-local depending on the coefficients $\langle \vec{x} | \hat{H} | \vec{x}' \rangle$. We don't know at this point what to choose for $\hat{H}$ but we will return to that issue soon. For now the choice does not

⁵In many beginning quantum books one is likely to see the equation " $\hat{p} = -i\hbar \nabla$ ", which is horrible notation. The left hand side is supposed to be an operator in the Dirac notation while the right hand side represents how that operator acts as a differential operator in the position basis. The correct version of this statement is $\langle \vec{x} | \hat{p} | \psi \rangle = -i\hbar \nabla \psi$.

matter. If we make a time dependent translation of an untranslated wavefunction ψ_0 :

$$\psi(t, \vec{x}) = \psi_0(t, \vec{x} - \vec{\varepsilon}(t)) \quad (8.5.28)$$

$$\implies \dot{\psi}(t, \vec{x}) = \frac{\partial \psi_0}{\partial t}(t, \vec{x} - \vec{\varepsilon}(t)) - \dot{\vec{\varepsilon}} \cdot \nabla \psi_0(t, \vec{x} - \vec{\varepsilon}(t)) = \frac{\partial \psi}{\partial t} - \dot{\vec{\varepsilon}} \cdot \nabla \psi. \quad (8.5.29)$$

Here the partial time derivative of ψ indicates differentiating the explicit time dependence but not $\vec{\varepsilon}$. Then, applying a time dependent translation to the Lagrangian gives:

$$\mathcal{L} = i\hbar \int_{\mathbb{S}} \psi^\dagger \dot{\psi} d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}' \quad (8.5.30)$$

$$= i\hbar \int_{\mathbb{S}} \psi^\dagger \left(\frac{\partial \psi}{\partial t} - \dot{\vec{\varepsilon}} \cdot \nabla \psi \right) d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}' \quad (8.5.31)$$

$$= -i\hbar \dot{\vec{\varepsilon}} \cdot \int_{\mathbb{S}} \psi^\dagger \nabla \psi d^d \vec{x} + i\hbar \int_{\mathbb{S}} \psi^\dagger \frac{\partial \psi}{\partial t} d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}'. \quad (8.5.32)$$

And so, the conjugate momentum to a translation is given by the derivative of the Lagrangian with respect to the velocity of translation in accordance with equation (8.5.23):

$$\vec{p}_{\text{cl}} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{\varepsilon}}} = -i\hbar \int_{\mathbb{S}} \psi^\dagger \nabla \psi d^d \vec{x} = \langle \psi | \hat{\vec{p}} | \psi \rangle \quad (8.5.33)$$

exactly as we had before.

Let us study the properties of the momentum operator. Because it is self-adjoint it is normal and so we begin by searching for its eigenvectors. That is, consider an eigenvector $|\vec{p}\rangle$ of the momentum operator which is labeled by a vector $\vec{p}$ intended to indicate its eigenvalue:

$$\hat{\vec{p}} |\vec{p}\rangle = \vec{p} |\vec{p}\rangle. \quad (8.5.34)$$

This notation is always a little hard to parse the first time you see it. Taking the inner product with $\langle \vec{x} |$ we have:

$$\langle \vec{x} | \hat{\vec{p}} |\vec{p}\rangle = \vec{p} \langle \vec{x} | \vec{p} \rangle \quad (8.5.35)$$

$$\implies \langle \vec{x} | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}'\rangle \nabla' \langle \vec{x}' | d^d \vec{x}' \right) |\vec{p}\rangle = \vec{p} \langle \vec{x} | \vec{p} \rangle \quad (8.5.36)$$

$$\implies -i\hbar \int_{\mathbb{S}} \langle \vec{x} | \vec{x}' \rangle \nabla' \langle \vec{x}' | \vec{p} \rangle d^d \vec{x}' = \vec{p} \langle \vec{x} | \vec{p} \rangle \quad (8.5.37)$$

$$\implies -i\hbar \int_{\mathbb{S}} \delta(\vec{x} - \vec{x}') \nabla' \langle \vec{x}' | \vec{p} \rangle d^d \vec{x}' = \vec{p} \langle \vec{x} | \vec{p} \rangle \quad (8.5.38)$$

$$\implies -i\hbar \nabla \langle \vec{x} | \vec{p} \rangle = \vec{p} \langle \vec{x} | \vec{p} \rangle \quad (8.5.39)$$

$$\implies \frac{1}{\langle \vec{x} | \vec{p} \rangle} \nabla \langle \vec{x} | \vec{p} \rangle = \frac{i}{\hbar} \vec{p} \quad (8.5.40)$$

$$\implies \nabla \ln(\langle \vec{x} | \vec{p} \rangle) = \frac{i}{\hbar} \vec{p} \quad (8.5.41)$$

$$\implies \ln(\langle \vec{x} | \vec{p} \rangle) = \frac{i}{\hbar} \vec{p} \cdot \vec{x} + C \quad (8.5.42)$$

$$\implies \langle \vec{x} | \vec{p} \rangle = N e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}} \quad (8.5.43)$$

where here N is an arbitrary constant. Thus, we can see that the eigenvectors of the momentum operator are just complex exponentials. We can choose the normalization factor N so that the $|\vec{p}\rangle$ vectors satisfy the same orthonormality condition as the $|\vec{x}\rangle$ vectors:

$$\langle \vec{p} | \vec{p}' \rangle = \langle \vec{p} | \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x} | d^d \vec{x} |\vec{p}' \rangle = \int_{\mathbb{S}} \langle \vec{p} | \vec{x} \rangle \langle \vec{x} | \vec{p}' \rangle d^d \vec{x} \quad (8.5.44)$$

$$= \int_{\mathbb{S}} \left(N e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}} \right)^* N e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}'} d^d \vec{x} = |N|^2 \int_{\mathbb{S}} e^{\frac{i}{\hbar} \vec{x} \cdot (\vec{p}' - \vec{p})} d^d \vec{x} \quad (8.5.45)$$

$$= |N|^2 (2\pi)^d \delta\left(\frac{\vec{p} - \vec{p}'}{\hbar}\right) = (2\pi\hbar)^d |N|^2 \delta(\vec{p} - \vec{p}'). \quad (8.5.46)$$

So, by convention we choose the normalization N as:

$$N = \frac{1}{(2\pi\hbar)^{\frac{d}{2}}} \quad (8.5.47)$$

$$\implies \boxed{\langle \vec{x} | \vec{p} \rangle = \frac{e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}}}{(2\pi\hbar)^{\frac{d}{2}}}, \quad \langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}')} \quad (8.5.48)$$

Consequently, the momentum eigenstates also satisfy the same completeness relation as the position eigenstates and the momentum operator admits a nice expression in terms of its eigenstates (letting $\mathbb{K}$ be the $\mathbb{R}^d$ vector space of all values of $\vec{p}$):

$$\int_{\mathbb{K}} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} = \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} \int_{\mathbb{K}} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} \int_{\mathbb{S}} |\vec{x}'\rangle \langle \vec{x}'| d^d \vec{x}' \quad (8.5.49)$$

$$= \int_{\mathbb{S}} \int_{\mathbb{K}} \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| \vec{p}\rangle \langle \vec{p}| \vec{x}'\rangle \langle \vec{x}'| d^d \vec{x} d^d \vec{p} d^d \vec{x}' \quad (8.5.50)$$

$$= \int_{\mathbb{S}} \int_{\mathbb{K}} \int_{\mathbb{S}} |\vec{x}\rangle \frac{e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}}}{(2\pi\hbar)^{\frac{d}{2}}} \frac{e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{x}'}}{(2\pi\hbar)^{\frac{d}{2}}} \langle \vec{x}'| d^d \vec{x} d^d \vec{p} d^d \vec{x}' \quad (8.5.51)$$

$$= \int_{\mathbb{S}} \int_{\mathbb{K}} \int_{\mathbb{S}} |\vec{x}\rangle \frac{e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{x} - \vec{x}')}}{(2\pi\hbar)^d} \langle \vec{x}'| d^d \vec{x} d^d \vec{p} d^d \vec{x}' \quad (8.5.52)$$

$$= \int_{\mathbb{S}} \int_{\mathbb{S}} |\vec{x}\rangle \delta(\vec{x} - \vec{x}') \langle \vec{x}'| d^d \vec{x} d^d \vec{x}' \quad (8.5.53)$$

$$= \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} = \mathbb{1}. \quad (8.5.54)$$

$$\hat{p} = -i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} = -i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \int_{\mathbb{K}} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} \quad (8.5.55)$$

$$= -i\hbar \int_{\mathbb{K}} \int_{\mathbb{S}} |\vec{x}\rangle \frac{\partial \langle \vec{x} | \vec{p} \rangle}{\partial \vec{x}} \langle \vec{p}| d^d \vec{x} d^d \vec{p} = -i\hbar \int_{\mathbb{K}} \int_{\mathbb{S}} |\vec{x}\rangle \frac{i}{\hbar} \vec{p} \langle \vec{x} | \vec{p} \rangle \langle \vec{p}| d^d \vec{x} d^d \vec{p} \quad (8.5.56)$$

$$= \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} \int_{\mathbb{K}} \vec{p} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} = \int_{\mathbb{K}} \vec{p} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p}. \quad (8.5.57)$$

Thus, there is a momentum eigenvector for each real vector $\vec{p}$ and these vectors are orthonormal and complete. This allows us to make a few nice identifications. For example, we can define the “momentum space wavefunction” $\tilde{\psi}(t, \vec{p})$ analogously to our “position space wavefunction” $\psi(t, \vec{x})$ by:

$$\tilde{\psi}(t, \vec{p}) = \langle \vec{p} | \psi(t) \rangle. \quad (8.5.58)$$

Using the completeness relation, this function just gives the expansion coefficients for $|\psi\rangle$ when written as a linear combination of the elements of the momentum basis:

$$|\psi\rangle = \int_{\mathbb{K}} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} |\psi\rangle = \int_{\mathbb{K}} \tilde{\psi}(t, \vec{p}) |\vec{p}\rangle d^d \vec{p}. \quad (8.5.59)$$

Let us see how the position and momentum space wavefunctions relate:

$$\tilde{\psi}(t, \vec{p}) = \langle \vec{p} | \psi(t) \rangle = \langle \vec{p} | \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} |\psi\rangle = \int_{\mathbb{S}} \langle \vec{p} | \vec{x} \rangle \langle \vec{x} | \psi \rangle d^d \vec{x} = \int_{\mathbb{S}} \frac{e^{-\frac{i}{\hbar} \vec{x} \cdot \vec{p}}}{(2\pi\hbar)^{\frac{d}{2}}} \psi(t, \vec{x}) d^d \vec{x}. \quad (8.5.60)$$

The momentum space wavefunction is simply the Fourier transform of the position space wavefunction with the wavenumber $\vec{k} = \frac{\vec{p}}{\hbar}$. This is actually quite straightforward to understand. We found that the momentum operator in the position basis is (proportional to) the spatial derivative and so its eigenvectors will be eigenvectors of the derivative which as we already know are exponential functions. The inverse Fourier transform exactly expresses a spatial function as a linear combination of complex exponentials and the Fourier transform gives the coefficients of linear combination. That is all that has happened by identifying the momentum basis; we have simply put the Fourier transform into Dirac notation.

Now that we understand the momentum basis a bit better, we can naturally define “translations” of the momentum space in exactly the same way as we did for position. That is, define the operator $\hat{S}(\vec{\varepsilon})$ as the unitary operator which acts as:

$$\hat{S}(\vec{\varepsilon}) |\vec{p}\rangle \stackrel{\text{def}}{=} |\vec{p} + \vec{\varepsilon}\rangle \quad (8.5.61)$$

$$\implies \hat{S}|\vec{p}\rangle\langle\vec{p}| = |\vec{p} + \vec{\varepsilon}\rangle\langle\vec{p}| \quad (8.5.62)$$

$$\implies \hat{S} \int_{\mathbb{K}} |\vec{p}\rangle\langle\vec{p}| d^d \vec{p} = \int_{\mathbb{K}} |\vec{p} + \vec{\varepsilon}\rangle\langle\vec{p}| d^d \vec{p} \quad (8.5.63)$$

$$\implies \hat{S} = \int_{\mathbb{K}} |\vec{p} + \vec{\varepsilon}\rangle\langle\vec{p}| d^d \vec{p}. \quad (8.5.64)$$

Then, under a momentum translation the wavefunction $\psi_\varepsilon(t, \vec{x})$ becomes:

$$\psi_\varepsilon(t, \vec{x}) = \langle \vec{x} | \psi_\varepsilon(t) \rangle = \langle \vec{x} | \hat{S} | \psi(t) \rangle = \langle \vec{x} | \int_{\mathbb{K}} |\vec{p} + \vec{\varepsilon}\rangle\langle\vec{p}| d^d \vec{p} | \psi(t) \rangle \quad (8.5.65)$$

$$= \langle \vec{x} | \int_{\mathbb{K}} |\vec{p} + \vec{\varepsilon}\rangle\langle\vec{p}| d^d \vec{p} | \int_{\mathbb{S}} |\vec{x}'\rangle\langle\vec{x}'| d^d \vec{x}' \psi(t) \rangle = \int_{\mathbb{K}} \int_{\mathbb{S}} \langle \vec{x} | \vec{p} + \vec{\varepsilon} \rangle \langle \vec{p} | \vec{x}' \rangle \langle \vec{x}' | \psi(t) \rangle d^d \vec{x}' d^d \vec{p} \quad (8.5.66)$$

$$= \int_{\mathbb{S}} \int_{\mathbb{K}} \frac{e^{\frac{i}{\hbar} \vec{x} \cdot (\vec{p} + \vec{\varepsilon})}}}{(2\pi\hbar)^{\frac{d}{2}}} \frac{e^{-\frac{i}{\hbar} \vec{x}' \cdot \vec{p}}}{(2\pi\hbar)^{\frac{d}{2}}} \psi(t, \vec{x}') d^d \vec{p} d^d \vec{x}' = e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \int_{\mathbb{S}} \int_{\mathbb{K}} \frac{e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{x} - \vec{x}')}}{(2\pi\hbar)^d} \psi(t, \vec{x}') d^d \vec{p} d^d \vec{x}' \quad (8.5.67)$$

$$= e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \int_{\mathbb{S}} \delta(\vec{x} - \vec{x}') \psi(t, \vec{x}') d^d \vec{x}' = e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \psi(t, \vec{x}). \quad (8.5.68)$$

Hence, a translation in momentum simply multiplies the wavefunction by a phase factor which is linear in position. We can see by direct calculation that this does in fact add momentum $\vec{\varepsilon}$:

$$\vec{p}'_{\text{cl}} = \langle \psi_\varepsilon | \hat{p} | \psi_\varepsilon \rangle = \langle \psi_\varepsilon | \left(-i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x} \right) | \psi_\varepsilon \rangle = -i\hbar \int_{\mathbb{S}} \langle \psi_\varepsilon | \vec{x} \rangle \nabla \langle \vec{x} | \psi_\varepsilon \rangle d^d \vec{x} \quad (8.5.69)$$

$$= -i\hbar \int_{\mathbb{S}} \psi_\varepsilon^\dagger \nabla \psi_\varepsilon d^d \vec{x} = -i\hbar \int_{\mathbb{S}} \psi^\dagger e^{-\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \nabla \left(e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \psi \right) d^d \vec{x} \quad (8.5.70)$$

$$= -i\hbar \int_{\mathbb{S}} \psi^\dagger e^{-\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \left(\frac{i}{\hbar} \vec{\varepsilon} e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \psi + e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \nabla \psi \right) d^d \vec{x} \quad (8.5.71)$$

$$= -i\hbar \int_{\mathbb{S}} \psi^\dagger \nabla \psi d^d \vec{x} + \vec{\varepsilon} \int_{\mathbb{S}} \psi^\dagger \psi d^d \vec{x} \quad (8.5.72)$$

$$= \langle \psi | \hat{p} | \psi \rangle + \vec{\varepsilon} \langle \psi | \psi \rangle \quad (8.5.73)$$

$$= \vec{p}_{\text{cl}} + \vec{\varepsilon}. \quad (8.5.74)$$

Now that we have a bit of understanding of the momentum of the wavefunction, how should we extract the classical position? In classical mechanics, a particle's position and momentum satisfy the canonical Poisson brackets and so now that we have identified $\vec{p}_{\text{cl}}$ we can find the associated classical position $\vec{x}_{\text{cl}}$ by finding the quantity which satisfies the canonical Poisson brackets with $\vec{p}_{\text{cl}}$. Notice that $Q' = P$, $P' = -Q$, $t' = t$, $\mathcal{H}' = \mathcal{H}$ is in fact a canonical transformation. That is to say the conjugate momentum to P is actually $-Q$. Applying this, one could consider the Lagrangian $\mathcal{L}'(t, Q', \dot{Q}')$ gotten by Legendre transforming in these primed coordinates:

$$\mathcal{L}'(t, Q', \dot{Q}') = \dot{Q}' P' - \mathcal{H} \quad (8.5.75)$$

$$\implies P' = \frac{\partial \mathcal{L}}{\partial \dot{Q}'}. \quad (8.5.76)$$

In the unprimed coordinates, this reads:

$$\mathcal{L}'(t, P, \dot{P}) = -\dot{P} Q - \mathcal{H} \quad (8.5.77)$$

$$\implies -Q = \frac{\partial \mathcal{L}'}{\partial \dot{P}}. \quad (8.5.78)$$

Thus if we write the Lagrangian in terms of P and $\dot{P}$, we can actually recover Q from equation (8.5.78) in the same way we would usually get P from a Lagrangian written in terms of Q and $\dot{Q}$ ⁶. Before we derived the expression for $\vec{p}_{\text{cl}}$ by differentiating the Lagrangian with respect to a time dependent translation of position because $\vec{p}_{\text{cl}}$ is conjugate to that position. This line of reasoning allows us to derive $\vec{x}_{\text{cl}}$ by differentiating the Lagrangian with respect to a time dependent translation of momentum because $-\vec{x}_{\text{cl}}$ is conjugate to that

⁶One may be concerned about calling both of these quantities the Lagrangian. Notice that this new “Lagrangian” in terms of P and $\dot{P}$ is actually related to the typical expression for $\mathcal{L}$ by adding a total time derivative and so there is nothing to worry about.

momentum. Applying a time dependent translation of momentum to our untranslated wavefunction ψ_0 gives:

$$\psi(t, \vec{x}) = e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \psi_0(t, \vec{x}) \quad (8.5.79)$$

$$\implies \dot{\psi} = \frac{i}{\hbar} \dot{\vec{\varepsilon}} \cdot \vec{x} e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \psi_0(t, \vec{x}) + e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \vec{x}} \frac{\partial \psi_0}{\partial t}(t, \vec{x}) \quad (8.5.80)$$

$$\implies \dot{\psi} = \frac{i}{\hbar} \dot{\vec{\varepsilon}} \cdot \vec{x} \psi + \frac{\partial \psi}{\partial t}. \quad (8.5.81)$$

Then, applying this to the Lagrangian:

$$\mathcal{L} = i\hbar \int_{\mathbb{S}} \psi^\dagger \dot{\psi} d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}' \quad (8.5.82)$$

$$= i\hbar \int_{\mathbb{S}} \psi^\dagger \left(\frac{i}{\hbar} \dot{\vec{\varepsilon}} \cdot \vec{x} \psi + \frac{\partial \psi}{\partial t} \right) d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}' \quad (8.5.83)$$

$$= -\dot{\vec{\varepsilon}} \cdot \int_{\mathbb{S}} \psi^\dagger \vec{x} \psi d^d \vec{x} + i\hbar \int_{\mathbb{S}} \psi^\dagger \frac{\partial \psi}{\partial t} d^d \vec{x} - \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H} | \vec{x}' \rangle \psi(t, \vec{x}') d^d \vec{x} d^d \vec{x}'. \quad (8.5.84)$$

And so, the classical position is given from equation (8.5.78) as:

$$\vec{x}_{\text{cl}} = -\frac{\partial \mathcal{L}}{\partial \dot{\vec{\varepsilon}}} = \int_{\mathbb{S}} \psi^\dagger \vec{x} \psi d^d \vec{x} \quad (8.5.85)$$

$$= \int_{\mathbb{S}} \langle \psi | \vec{x} | \psi \rangle d^d \vec{x} = \langle \psi | \int_{\mathbb{S}} \vec{x} | \vec{x} \rangle \langle \vec{x} | d^d \vec{x} | \psi \rangle. \quad (8.5.86)$$

Defining then the position operator $\hat{\vec{x}}$:

$$\hat{\vec{x}} = \int_{\mathbb{S}} \vec{x} | \vec{x} \rangle \langle \vec{x} | d^d \vec{x} \quad (8.5.87)$$

$$\implies \vec{x}_{\text{cl}} = \langle \psi | \hat{\vec{x}} | \psi \rangle. \quad (8.5.88)$$

The position operator is immediately self-adjoint:

$$\hat{\vec{x}}^\dagger = \int_{\mathbb{S}} \vec{x} | \vec{x} \rangle \langle \vec{x} | d^d \vec{x} = \hat{\vec{x}}. \quad (8.5.89)$$

As well, we can see that the form in equation (8.5.87) is analogous to equation (8.5.57) for the momentum operator. Equation (8.5.87) is quite a reasonable expression for what we mean by the position operator as from equation (8.5.85):

$$\vec{x}_{\text{cl}} = \langle \psi | \hat{\vec{x}} | \psi \rangle = \int_{\mathbb{S}} \vec{x} |\psi|^2 d^d \vec{x} \quad (8.5.90)$$

and so the result is a weighted average position where the weight is $|\psi|^2$. Thus, when the wavefunction is essentially all located around a particular position, $|\psi|^2$ will only make significant contributions to this integral near that position and so $\vec{x}_{\text{cl}}$ will coincide with that position, exactly as we intended with the meaning of classical position. Because $-\vec{x}_{\text{cl}}$ is the generator of momentum translations, by theorem 8.4 we can express the momentum translation operator as:

$$\hat{S}(\vec{\varepsilon}) = e^{\frac{i}{\hbar} \vec{\varepsilon} \cdot \hat{\vec{x}}}. \quad (8.5.91)$$

Now that we have identified the classical position and momentum within the wavefunction, we ought to check that they are in fact canonically conjugate in the way we intended. By the canonical brackets in equation (1.4.7) then we would like to check:

$$\{\vec{x}_{\text{cl}}, \vec{x}_{\text{cl}}\} \stackrel{?}{=} 0, \quad \{\vec{x}_{\text{cl}}, \vec{p}_{\text{cl}}\} \stackrel{?}{=} \mathbb{1}, \quad \{\vec{p}_{\text{cl}}, \vec{p}_{\text{cl}}\} \stackrel{?}{=} 0. \quad (8.5.92)$$

From theorem 8.5, these are equivalent to:

$$[\hat{\vec{x}}, \hat{\vec{x}}] \stackrel{?}{=} 0, \quad [\hat{\vec{x}}, \hat{\vec{p}}] \stackrel{?}{=} i\hbar \mathbb{1}, \quad [\hat{\vec{p}}, \hat{\vec{p}}] \stackrel{?}{=} 0. \quad (8.5.93)$$

So, let us compute these commutators. To do so, it is easiest to work in components and to consider these operators acting on an arbitrary vector $|\psi\rangle$:

$$[\hat{x}^a, \hat{x}^b] |\psi\rangle = (\hat{x}^a \hat{x}^b - \hat{x}^b \hat{x}^a) |\psi\rangle = \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x} | d^d \vec{x} (\hat{x}^a \hat{x}^b - \hat{x}^b \hat{x}^a) |\psi\rangle \quad (8.5.94)$$

$$= \int_{\mathbb{S}} |\vec{x}\rangle (x^a x^b - x^b x^a) \langle \vec{x} | \psi \rangle d^d \vec{x} = \int_{\mathbb{S}} |\vec{x}\rangle 0 \langle \vec{x} | \psi \rangle d^d \vec{x} = 0. \quad \checkmark \quad (8.5.95)$$

$$[\hat{x}^a, \hat{p}_b]|\psi\rangle = (\hat{x}^a \hat{p}_b - \hat{p}_b \hat{x}^a)|\psi\rangle = \int |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} (\hat{x}^a \hat{p}_b - \hat{p}_b \hat{x}^a)|\psi\rangle \quad (8.5.96)$$

$$= \int_{\mathbb{S}} |\vec{x}\rangle (x^a \langle \vec{x}|\hat{p}_b|\psi\rangle - \langle \vec{x}|\hat{p}_b \hat{x}^a|\psi\rangle) d^d \vec{x} = \int_{\mathbb{S}} |\vec{x}\rangle \left(-i\hbar x^a \frac{\partial \psi}{\partial x^b} + i\hbar \frac{\partial}{\partial x^b} (\langle \vec{x}|\hat{x}^a|\psi\rangle) \right) d^d \vec{x} \quad (8.5.97)$$

$$= \int_{\mathbb{S}} |\vec{x}\rangle \left(-i\hbar x^a \frac{\partial \psi}{\partial x^b} + i\hbar \frac{\partial}{\partial x^b} (x^a \psi) \right) d^d \vec{x} = \int_{\mathbb{S}} |\vec{x}\rangle \left(-i\hbar x^a \frac{\partial \psi}{\partial x^b} + i\hbar \delta_b^a \psi + i\hbar x^a \frac{\partial \psi}{\partial x^b} \right) d^d \vec{x} \quad (8.5.98)$$

$$= i\hbar \delta_b^a \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}|\psi\rangle d^d \vec{x} = i\hbar \delta_b^a |\psi\rangle. \quad \checkmark \quad (8.5.99)$$

$$[\hat{p}_a, \hat{p}_b]|\psi\rangle = (\hat{p}_a \hat{p}_b - \hat{p}_b \hat{p}_a)|\psi\rangle = \int_{\mathbb{K}} |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} (\hat{p}_a \hat{p}_b - \hat{p}_b \hat{p}_a)|\psi\rangle \quad (8.5.100)$$

$$= \int_{\mathbb{K}} |\vec{p}\rangle (p_a p_b - p_b p_a) \langle \vec{p}|\psi\rangle d^d \vec{p} = \int_{\mathbb{K}} |\vec{p}\rangle 0 \langle \vec{p}|\psi\rangle d^d \vec{p} = 0. \quad \checkmark. \quad (8.5.101)$$

These computations should remind you of section 1.3. The commutation relations are exactly as suspected in equation (8.5.93) and thus the Poisson brackets are exactly as suspected in equation (8.5.92). Thus we have:

Theorem 8.6: Classical Variables in Quantum Mechanics

The position and momentum operators are self-adjoint operators defined by:

$$\hat{x} = \int_{\mathbb{S}} \vec{x} |\vec{x}\rangle \langle \vec{x}| d^d \vec{x}, \quad \hat{p} = -i\hbar \int_{\mathbb{S}} |\vec{x}\rangle \nabla \langle \vec{x}| d^d \vec{x}. \quad (8.5.102)$$

They satisfy the canonical commutation relations:

$$[\hat{x}, \hat{x}] = 0, \quad [\hat{x}, \hat{p}] = i\hbar \mathbb{1}, \quad [\hat{p}, \hat{p}] = 0. \quad (8.5.103)$$

The quantities $\vec{x}_{\text{cl}} = \langle \hat{x} \rangle$ and $\vec{p}_{\text{cl}} = \langle \hat{p} \rangle$ correspond to the spatial-average position and total linear momentum of the wavefunction and correspond to the position and momentum present in the classical theory of point matter when the wavefunction is approximately localized. They always satisfy the canonical brackets:

$$\{\vec{x}_{\text{cl}}, \vec{x}_{\text{cl}}\} = 0, \quad \{\vec{x}_{\text{cl}}, \vec{p}_{\text{cl}}\} = \mathbb{1}, \quad \{\vec{p}_{\text{cl}}, \vec{p}_{\text{cl}}\} = 0. \quad (8.5.104)$$

8.5.1 Operator Spreads

We say that $\vec{x}_{\text{cl}}$ and $\vec{p}_{\text{cl}}$ correspond to classical particle-like position and momentum, but under what circumstances should we recover classical mechanics from our wave theory of matter? As we said, this wave should produce essentially classical dynamics for $\vec{x}_{\text{cl}}$ and $\vec{p}_{\text{cl}}$ whenever that wave is essentially localized in its position and the whole wave moves with an essentially well-defined velocity. Because the Legendre transformation acts as a way to trade in position and velocity dependence for position and momentum dependence, having an essentially well-defined position and velocity implies having an essentially well-defined position and momentum. Thus, we expect classical mechanics to be recovered for $\vec{x}_{\text{cl}}$ and $\vec{p}_{\text{cl}}$ whenever the wavefunction is not very spread out over space and simultaneously also not very spread out in momentum space. This should remind you of problem 4.50 (in fact its exactly the same thing). Let us study how to quantify such conditions.

Consider an operator $\hat{\mathcal{O}}$ and a normalized eigenstate $|\psi\rangle$ of that operator with eigenvalue λ . Then:

$$\hat{\mathcal{O}}|\psi\rangle = \lambda|\psi\rangle \implies \langle \psi|\hat{\mathcal{O}}|\psi\rangle = \lambda\langle \psi|\psi\rangle \implies \lambda = \langle \hat{\mathcal{O}} \rangle. \quad (8.5.105)$$

Further consider the nonlinear operator $\delta\hat{\mathcal{O}}$ defined by:

$$\delta\hat{\mathcal{O}} = \hat{\mathcal{O}} - \langle \psi|\hat{\mathcal{O}}|\psi\rangle \mathbb{1} \quad (8.5.106)$$

$$\implies \delta\hat{\mathcal{O}}|\psi\rangle = \hat{\mathcal{O}}|\psi\rangle - \langle \hat{\mathcal{O}} \rangle|\psi\rangle = \lambda|\psi\rangle - \lambda|\psi\rangle = 0. \quad (8.5.107)$$

And so, $\delta\hat{\mathcal{O}}$ annihilates any normalized eigenstate of $\hat{\mathcal{O}}$. In fact, the converse is true as suppose instead that for a vector $|\phi\rangle$ the operator $\delta\hat{\mathcal{O}}$ annihilates that vector:

$$\delta\hat{\mathcal{O}}|\phi\rangle = 0 \implies \hat{\mathcal{O}}|\phi\rangle - \langle \phi|\hat{\mathcal{O}}|\phi\rangle|\phi\rangle = 0 \implies \hat{\mathcal{O}}|\phi\rangle = \langle \phi|\hat{\mathcal{O}}|\phi\rangle|\phi\rangle. \quad (8.5.108)$$

Hence, $|\phi\rangle$ must be an eigenvector of $\hat{\mathcal{O}}$ with eigenvalue $\langle \phi|\hat{\mathcal{O}}|\phi\rangle$. It further follows by taking the inner

product of both sides with $\langle\phi|$ that $\langle\phi|\phi\rangle = 1$ ⁷. And so, $\delta\hat{\mathcal{O}}$ annihilates a vector if and only if that vector is a normalized eigenstate of $\hat{\mathcal{O}}$. A vector in a normed vector space has norm 0 if and only if it is the 0 vector:

$$\|u\|^2 = \langle u|u\rangle = 0 \iff |u\rangle = 0 \quad (8.5.109)$$

and so the fact that $\delta\hat{\mathcal{O}}$ annihilates a vector if and only if that vector $|\psi\rangle$ is a normalized eigenstate of $\hat{\mathcal{O}}$ is equivalent in both directions to the condition that $\delta\hat{\mathcal{O}}|\psi\rangle$ has norm 0:

$$|\psi\rangle \text{ is a normalized eigenstate of } \hat{\mathcal{O}} \iff \delta\hat{\mathcal{O}}|\psi\rangle = 0 \iff \|\delta\hat{\mathcal{O}}|\psi\rangle\|^2 = \langle\psi|\delta\hat{\mathcal{O}}^\dagger\delta\hat{\mathcal{O}}|\psi\rangle = 0. \quad (8.5.110)$$

Thus, the quantity $\delta\mathcal{O}^2$ defined by:

$$\delta\mathcal{O}^2 = \langle\psi|\delta\hat{\mathcal{O}}^\dagger\delta\hat{\mathcal{O}}|\psi\rangle \quad (8.5.111)$$

for a general state $|\psi\rangle$ is 0 if and only if $|\psi\rangle$ is a normalized eigenstate of $\hat{\mathcal{O}}$. This expression is called the operator spread of $\hat{\mathcal{O}}$ in the state $|\psi\rangle$ and is generally written as:

$$\text{Spr}(\hat{\mathcal{O}}) = \delta\mathcal{O}^2 = \langle\psi|(\hat{\mathcal{O}}^\dagger - \langle\hat{\mathcal{O}}\rangle^*\mathbb{1})(\hat{\mathcal{O}} - \langle\hat{\mathcal{O}}\rangle\mathbb{1})|\psi\rangle. \quad (8.5.112)$$

Because the operator spread is expressible as the norm of a vector, it is non-negative. Further, if $\hat{\mathcal{O}}$ is normal then using the spectral expansion of the operator $\hat{\mathcal{O}}$:

$$\text{Spr}(\hat{\mathcal{O}}) = \langle\psi|(\hat{\mathcal{O}}^\dagger - \langle\hat{\mathcal{O}}\rangle^*\mathbb{1})\left(\sum_n \lambda_n |n\rangle\langle n| - \langle\hat{\mathcal{O}}\rangle \sum_n |n\rangle\langle n|\right)|\psi\rangle \quad (8.5.113)$$

$$= \sum_n \langle\psi|(\hat{\mathcal{O}}^\dagger - \langle\hat{\mathcal{O}}\rangle^*\mathbb{1})|n\rangle (\lambda_n - \langle\hat{\mathcal{O}}\rangle) \langle n|\psi\rangle \quad (8.5.114)$$

$$= \sum_n (\lambda_n^* - \langle\hat{\mathcal{O}}\rangle^*)(\lambda_n - \langle\hat{\mathcal{O}}\rangle) \langle\psi|n\rangle \langle n|\psi\rangle \quad (8.5.115)$$

$$= \sum_n |\lambda_n - \langle\hat{\mathcal{O}}\rangle|^2 |\psi_n|^2 \quad (8.5.116)$$

So when all of the non-zero ψ_n correspond to eigenvalues λ_n which are near each other, $\langle\hat{\mathcal{O}}\rangle$ will be near those λ_n and all of the $|\lambda_n - \langle\hat{\mathcal{O}}\rangle|^2$ will be small, leading to a small spread. Thus, when $|\psi\rangle$ is nearly an eigenstate of $\hat{\mathcal{O}}$ the operator spread of $\hat{\mathcal{O}}$ will be nearly 0. The operator spread of $\hat{\mathcal{O}}$ essentially measures the extent to which $|\psi\rangle$ fails to be an eigenstate of $\hat{\mathcal{O}}$. When we want to consider a wavefunction which is localized in position, we will concretely mean a wavefunction for which the operator spread of the position for that wavefunction is negligible (for the purposes at hand; how large of a spread will count as negligible will of course depend on experimental resolution). As well, a wavefunction which is localized in momentum will mean that it has operator spread of the momentum which is negligible.

An occasionally useful way of interpreting the operator spread comes from what it tells us about how far the operator summary is from the nearest eigenvalue of $\hat{\mathcal{O}}$. For a normal operator $\hat{\mathcal{O}}$ and fixed normalized $|\psi\rangle$ which is not necessarily an eigenvector of $\hat{\mathcal{O}}$, define the operator $\hat{V}_\psi$ by:

$$\hat{V}_\psi = (\hat{\mathcal{O}}^\dagger - \langle\psi|\hat{\mathcal{O}}|\psi\rangle^*\mathbb{1})(\hat{\mathcal{O}} - \langle\psi|\hat{\mathcal{O}}|\psi\rangle\mathbb{1}) - \text{Spr}_\psi(\hat{\mathcal{O}})\mathbb{1} \quad (8.5.117)$$

where the operator spread given above is intended as being taken with respect to the vector $|\psi\rangle$. It immediately follows by computation of $[\hat{V}_\psi, \hat{V}_\psi^\dagger]$ that $\hat{V}_\psi$ is normal as well. Further, any eigenvector $|n\rangle$ of $\hat{\mathcal{O}}$ with eigenvalue λ_n is also an eigenvector of $\hat{V}_\psi$ with eigenvalue v_n given as:

$$\hat{V}_\psi|n\rangle = (\hat{\mathcal{O}}^\dagger - \langle\hat{\mathcal{O}}\rangle^*\mathbb{1})(\hat{\mathcal{O}} - \langle\hat{\mathcal{O}}\rangle\mathbb{1})|n\rangle - \text{Spr}_\psi(\hat{\mathcal{O}})|n\rangle \quad (8.5.118)$$

$$= (\hat{\mathcal{O}}^\dagger - \langle\hat{\mathcal{O}}\rangle^*\mathbb{1})(\lambda_n - \langle\hat{\mathcal{O}}\rangle)|n\rangle - \text{Spr}_\psi(\hat{\mathcal{O}})|n\rangle \quad (8.5.119)$$

$$= ((\lambda_n^* - \langle\hat{\mathcal{O}}\rangle^*)(\lambda_n - \langle\hat{\mathcal{O}}\rangle) - \text{Spr}_\psi(\hat{\mathcal{O}}))|n\rangle \quad (8.5.120)$$

$$= (|\lambda_n - \langle\hat{\mathcal{O}}\rangle|^2 - \text{Spr}_\psi(\hat{\mathcal{O}}))|n\rangle \quad (8.5.121)$$

$$\implies v_n = |\lambda_n - \langle\hat{\mathcal{O}}\rangle|^2 - \text{Spr}_\psi(\hat{\mathcal{O}}). \quad (8.5.122)$$

So, all of the eigenvalues of $\hat{V}_\psi$ are real. Let v_* be the least eigenvalue of $\hat{V}_\psi$ (or, more rigorously, the greatest

⁷There is a slight exception in the case that $\langle\phi|\hat{\mathcal{O}}|\phi\rangle = 0$ in which case no condition on normalization can be derived. The rest of the steps of reasoning presented here still follow, just with the word normalized removed. Ultimately, this case will not affect our final conclusion.

real number less than or equal to v_n for all n , also known as the infimum of the spectrum of $\hat{V}_\psi$). Let λ_* be the associated eigenvalue of $\hat{O}$ corresponding to v_* :

$$v_* = |\lambda_* - \langle \hat{O} \rangle|^2 - \text{Spr}_\psi(\hat{O}) \quad (8.5.123)$$

Then, we have:

$$\langle \psi | \hat{V}_\psi | \psi \rangle = \langle \psi | (\hat{V}_\psi - v_* \mathbb{1} + v_* \mathbb{1}) | \psi \rangle = v_* \langle \psi | \psi \rangle + \langle \psi | (\hat{V}_\psi - v_* \mathbb{1}) \sum_n |n\rangle \langle n| \psi \rangle \quad (8.5.124)$$

$$= v_* + \sum_n (v_n - v_*) \langle \psi | n \rangle \langle n | \psi \rangle = v_* + \sum_n (v_n - v_*) |\psi_n|^2. \quad (8.5.125)$$

The last term in the final equality is a sum of $(v_n - v_*) |\psi_n|^2$. $v_n - v_*$ is non-negative by the definition of v_* and $|\psi_n|^2$ is always non-negative and so we have:

$$\langle \psi | \hat{V}_\psi | \psi \rangle \geq v_*. \quad (8.5.126)$$

Using the definitions of $\hat{V}_\psi$ and λ_* :

$$\langle \psi | \left((\hat{O}^\dagger - \langle \psi | \hat{O} | \psi \rangle^* \mathbb{1}) (\hat{O} - \langle \psi | \hat{O} | \psi \rangle \mathbb{1}) - \text{Spr}_\psi(\hat{O}) \mathbb{1} \right) | \psi \rangle \geq v_* \quad (8.5.127)$$

$$\implies \text{Spr}(\hat{O}) - \text{Spr}(\hat{O}) \geq v_* \quad (8.5.128)$$

$$\implies 0 \geq |\lambda_* - \langle \hat{O} \rangle|^2 - \text{Spr}(\hat{O}) \quad (8.5.129)$$

$$\implies |\lambda_* - \langle \hat{O} \rangle| \leq \sqrt{\text{Spr}(\hat{O})}. \quad (8.5.130)$$

Hence, for any state $|\psi\rangle$ and normal operator $\hat{O}$, there always exists an eigenvalue of $\hat{O}$ within one square-root of the spread of $\hat{O}$ from the summary of $\hat{O}$. Thus the operator spread tells you how far the operator spread is at most from an eigenvalue of the operator.

Another quantity which is very closely related to the operator spread but generalized to two operators is the operator correlation. For two operators $\hat{A}$ and $\hat{B}$, their correlation is defined by:

$$\text{Cor}(\hat{A}, \hat{B}) = \langle \psi | \frac{(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) + (\hat{B} - \langle \hat{B} \rangle \mathbb{1})(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})}{2} | \psi \rangle. \quad (8.5.131)$$

One can see immediately that the correlation satisfies: $\text{Cor}(\hat{A}, \hat{B}) = \text{Cor}(\hat{B}, \hat{A})^*$. In the case of a normal operator, we can see that the operator spread is a special case:

$$\text{Cor}(\hat{O}, \hat{O}) = \langle \psi | \frac{(\hat{O}^\dagger - \langle \hat{O} \rangle^* \mathbb{1})(\hat{O} - \langle \hat{O} \rangle \mathbb{1}) + (\hat{O} - \langle \hat{O} \rangle \mathbb{1})(\hat{O}^\dagger - \langle \hat{O} \rangle^* \mathbb{1})}{2} | \psi \rangle \quad (8.5.132)$$

$$= \langle \psi | (\hat{O}^\dagger - \langle \hat{O} \rangle^* \mathbb{1})(\hat{O} - \langle \hat{O} \rangle \mathbb{1}) | \psi \rangle = \text{Spr}(\hat{O}). \quad (8.5.133)$$

All of this gives us:

Theorem 8.7: Spectral Spread Theorem

The operator correlation in a state $|\psi\rangle$ between two operators $\hat{A}$ and $\hat{B}$ is defined by:

$$\text{Cor}(\hat{A}, \hat{B}) = \langle \psi | \frac{(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) + (\hat{B} - \langle \hat{B} \rangle \mathbb{1})(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})}{2} | \psi \rangle \quad (8.5.134)$$

and satisfies:

$$\text{Cor}(\hat{B}, \hat{A}) = \text{Cor}(\hat{A}, \hat{B})^*. \quad (8.5.135)$$

The operator spread in a state $|\psi\rangle$ of an operator $\hat{O}$ is defined by:

$$\text{Spr}(\hat{O}) = \text{Cor}(\hat{O}, \hat{O}) = \langle (\hat{O}^\dagger - \langle \hat{O} \rangle^* \mathbb{1})(\hat{O} - \langle \hat{O} \rangle \mathbb{1}) \rangle. \quad (8.5.136)$$

The operator spread is 0 if and only if $|\psi\rangle$ is a normalized eigenstate of $\hat{O}$. The spread is non-negative and acts as a measure of the extent to which $|\psi\rangle$ fails to be an eigenstate of $\hat{O}$. For any $|\psi\rangle$ and normal operator $\hat{O}$, there is always an eigenvalue of $\hat{O}$ within a distance of $\sqrt{\text{Spr}(\hat{O})}$ from $\langle \hat{O} \rangle$.

The summary position can be written in a way which makes it look quite like our original definition of

the center of mass:

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle = \int_{\mathbb{S}} \vec{x} |\psi|^2 d^d \vec{x}. \quad (8.5.137)$$

This precisely corresponds to equation (2.9.29) if we interpret $dm = m|\psi|^2 d^d \vec{x}$ and thus interpret the wavefunction as having mass density $\rho_m = m|\psi|^2$ where m is its total mass. As well, the correlations of the components of the position are quite closely related to the moment of inertia tensor:

$$\text{Cor}(\hat{x}^a, \hat{x}^b) = \int_{\mathbb{S}} (x^a - \langle \hat{x}^a \rangle)(x^b - \langle \hat{x}^b \rangle) |\psi|^2 d^d \vec{x}. \quad (8.5.138)$$

Making that same identification for the mass density, we have:

$$\frac{1}{m} I^{ab} = \left(\sum_c \text{Spr}(\hat{x}^c) \right) \delta^{ab} - \text{Cor}(\hat{x}^a, \hat{x}^b) \quad (8.5.139)$$

where I^{ab} are the components of the moment of inertia. We will find that this identification for the mass density is more than just an analogy in the coming sections. The fact that we are not dealing with a rigid body is expressed in I^{ab} having generic time dependence.

Because we have a wave instead of a point, its position spread and momentum spread will be non-zero. The position spread naturally corresponds to the fact that the wave will have non-zero size in space and the momentum spread corresponds to the fact that the different parts of the wave will not all move together; it all sloshes around in a non-trivial way. This tells us precisely the conditions under which we should expect the wave theory to act like our point theory. A wave approximates a point when its position spread is small enough that its spatial size is negligible (on the scale of the experiment) and its momentum spread is small enough that the whole wave moves approximately together (again, on the scale of the experiment). Therefore, the point limit (also called the classical limit) is the limit that both the position and momentum spreads are sufficiently small for our experimental precision. It turns out though that there are basic restrictions on the extent to which the wavefunction can have both small position spread and small momentum spread.

Consider two vectors $|u\rangle$ and $|v\rangle$ and assume $|v\rangle \neq 0$. Define a third vector $|w\rangle$ by:

$$|w\rangle = |u\rangle + \alpha |v\rangle \quad (8.5.140)$$

for some constant α . Let us choose α so that $|w\rangle$ and $|v\rangle$ are orthogonal:

$$\langle v | w \rangle = \langle v | u \rangle + \alpha \langle v | v \rangle \stackrel{!}{=} 0 \implies \alpha = -\frac{\langle v | u \rangle}{\langle v | v \rangle}. \implies |w\rangle = |u\rangle - \frac{\langle v | u \rangle}{\langle v | v \rangle} |v\rangle. \quad (8.5.141)$$

By definition of the norm, $\langle w | w \rangle \geq 0$ with equality if and only if $|w\rangle = 0$. Therefore:

$$\langle w | w \rangle = \left(\langle u | - \frac{\langle u | v \rangle}{\langle v | v \rangle} \langle v | \right) \left(|u\rangle - \frac{\langle v | u \rangle}{\langle v | v \rangle} |v\rangle \right) \quad (8.5.142)$$

$$= \langle u | u \rangle - \frac{\langle u | v \rangle \langle v | u \rangle}{\langle v | v \rangle} - \frac{\langle u | v \rangle \langle v | u \rangle}{\langle v | v \rangle} + \frac{\langle u | v \rangle \langle v | u \rangle}{\langle v | v \rangle^2} \langle v | v \rangle \quad (8.5.143)$$

$$= \langle u | u \rangle - \frac{|\langle u | v \rangle|^2}{\langle v | v \rangle} \geq 0 \quad (8.5.144)$$

$$\implies \boxed{\langle u | u \rangle \langle v | v \rangle \geq |\langle u | v \rangle|^2}. \quad (8.5.145)$$

Precise equality can only hold in the event $|w\rangle$ is 0. When $|w\rangle = 0$, $|u\rangle$ and $|v\rangle$ are then colinear and in fact one can see immediately that the converse holds: if $|u\rangle$ and $|v\rangle$ are colinear then by equation (8.5.141) $|w\rangle = 0$. As well, to derive this inequality we had to assume $|v\rangle \neq 0$. However, if $|v\rangle = 0$ the inequality holds automatically as an equality and so it is true in general. That is, for all vectors $|u\rangle$ and $|v\rangle$:

$$\langle u | u \rangle \langle v | v \rangle \geq |\langle u | v \rangle|^2 \quad (8.5.146)$$

with equality holding if and only if the two vectors are colinear. This result is known as the **Cauchy-Schwarz inequality**. Now let us consider two operators $\hat{A}$ and $\hat{B}$ and a state $|\psi\rangle$ and define:

$$|u\rangle = (\hat{A} - \langle \hat{A} \rangle \mathbb{1}) |\psi\rangle, \quad |v\rangle = (\hat{B} - \langle \hat{B} \rangle \mathbb{1}) |\psi\rangle. \quad (8.5.147)$$

Then:

$$\langle u | u \rangle = \langle \psi | (\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1}) (\hat{A} - \langle \hat{A} \rangle \mathbb{1}) | \psi \rangle = \text{Spr}(\hat{A}) \quad (8.5.148)$$

$$\langle v | v \rangle = \langle \psi | (\hat{B}^\dagger - \langle \hat{B} \rangle^* \mathbb{1}) (\hat{B} - \langle \hat{B} \rangle \mathbb{1}) | \psi \rangle = \text{Spr}(\hat{B}) \quad (8.5.149)$$

$$\langle u|v\rangle = \langle \psi | (\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) | \psi \rangle \quad (8.5.150)$$

$$\begin{aligned} &= \langle \psi | \left(\frac{(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) - (\hat{B} - \langle \hat{B} \rangle \mathbb{1})(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})}{2} \right. \\ &\quad \left. + \frac{(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) + (\hat{B} - \langle \hat{B} \rangle \mathbb{1})(\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1})}{2} \right) | \psi \rangle \end{aligned} \quad (8.5.151)$$

$$= \langle \psi | \frac{1}{2} [\hat{A}^\dagger - \langle \hat{A} \rangle^* \mathbb{1}, \hat{B} - \langle \hat{B} \rangle \mathbb{1}] | \psi \rangle + \text{Cor}(\hat{A}, \hat{B}) \quad (8.5.152)$$

$$= \frac{1}{2} \langle [\hat{A}^\dagger, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}). \quad (8.5.153)$$

Thus, by the Cauchy-Schwarz inequality:

$$\text{Spr}(\hat{A})\text{Spr}(\hat{B}) \geq \left| \frac{1}{2} \langle [\hat{A}^\dagger, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \right|^2. \quad (8.5.154)$$

For the special case of $\hat{A}$ and $\hat{B}$ being self-adjoint, we have:

$$\langle v|u\rangle = \frac{1}{2} \langle [\hat{A}, \hat{B}] \rangle^* + \text{Cor}(\hat{A}, \hat{B})^* \quad (8.5.155)$$

$$= -\frac{1}{2} \langle [\hat{A}, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \quad (8.5.156)$$

$$|\langle u|v\rangle|^2 = \langle u|v\rangle \langle v|u\rangle \quad (8.5.157)$$

$$= \left(\frac{1}{2} \langle [\hat{A}, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \right) \left(-\frac{1}{2} \langle [\hat{A}, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \right) \quad (8.5.158)$$

$$= \text{Cor}(\hat{A}, \hat{B})^2 - \frac{1}{4} \langle [\hat{A}, \hat{B}] \rangle^2 = \text{Cor}(\hat{A}, \hat{B})^2 + \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2. \quad (8.5.159)$$

And so, equation (8.5.154) becomes:

$$\text{Spr}(\hat{A})\text{Spr}(\hat{B}) \geq \text{Cor}(\hat{A}, \hat{B})^2 + \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2. \quad (8.5.160)$$

Together this gives us:

Theorem 8.8: Uncertainty Theorem

For any two operators $\hat{A}$ and $\hat{B}$:

$$\text{Spr}(\hat{A})\text{Spr}(\hat{B}) \geq \left| \frac{1}{2} \langle [\hat{A}^\dagger, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \right|^2. \quad (8.5.161)$$

For the special case of two self-adjoint operators:

$$\text{Spr}(\hat{A})\text{Spr}(\hat{B}) \geq \text{Cor}(\hat{A}, \hat{B})^2 + \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2. \quad (8.5.162)$$

8.5.2 The Classical Limit

The correlation and commutator of $\hat{A}$ and $\hat{B}$ place limits on how small the spreads of $\hat{A}$ and $\hat{B}$ can be made. A particular special case of interest is when the operators are the position and momentum operators in the same direction $\vec{n}$. That is, define $\hat{x} = \vec{n} \cdot \hat{\vec{x}}$ and $\hat{p} = \vec{n} \cdot \hat{\vec{p}}$ where $\vec{n}$ is a constant unit vector. Then:

$$[\hat{x}, \hat{p}] = [\vec{n} \cdot \hat{\vec{x}}, \vec{n} \cdot \hat{\vec{p}}] = \vec{n} \cdot [\hat{\vec{x}}, \hat{\vec{p}}] \cdot \vec{n} = \vec{n} \cdot i\hbar \mathbb{1} \cdot \vec{n} = i\hbar \mathbb{1}. \quad (8.5.163)$$

Consequently:

$$\text{Spr}(\hat{x})\text{Spr}(\hat{p}) \geq \text{Cor}(\hat{x}, \hat{p})^2 + \left(\frac{1}{2i} \langle [\hat{x}, \hat{p}] \rangle \right)^2 \geq \left(\frac{1}{2i} \langle i\hbar \mathbb{1} \rangle \right)^2 = \frac{\hbar^2}{4}. \quad (8.5.164)$$

Thus, there is a limit to how small the spreads of position and momentum can be made simultaneously. This is not surprising. As a state's position spread gets smaller, it comes closer to being an eigenstate of the position

operator and thus gets closer to being a Dirac delta. As a state's momentum spread gets smaller, it comes closer to being an eigenstate of the momentum operator and thus gets closer to being a complex exponential. A Dirac delta is entirely localized to a point whereas a complex exponential does not decay in magnitude at all with distance. So, there is a limit to how well a function can simultaneously approximate these two very different behaviors. **This is a general fact about the Fourier transform, is purely mathematical, and is not derived from any physics.** There is a limited sense in which equation (8.5.164) can be applied to physics. Suppose we have the experimental sensitivity to physics only on length scales of at least w_x and momenta up to a resolution w_p . The classical regime is whenever the wavefunction spreads are essentially negligible compared to these resolutions:

$$\text{Spr}(\hat{x}) \ll w_x^2, \quad \text{Spr}(\hat{p}) \ll w_p^2. \quad (8.5.165)$$

Using equation (8.5.164):

$$w_p^2 \gg \text{Spr}(\hat{p}) \geq \frac{\hbar^2}{4\text{Spr}(\hat{x})} \implies \text{Spr}(\hat{x}) \gg \frac{\hbar^2}{4w_p^2} \quad (8.5.166)$$

$$w_x^2 \gg \text{Spr}(\hat{x}) \geq \frac{\hbar^2}{4\text{Spr}(\hat{p})} \implies \text{Spr}(\hat{p}) \gg \frac{\hbar^2}{4w_x^2} \quad (8.5.167)$$

So, we have that in order for a wavefunction to be in the “classical regime” for given experimental resolutions we must have the position and momentum spreads sit in the ranges:

$$\frac{\hbar^2}{4w_p^2} \ll \text{Spr}(\hat{x}) \ll w_x^2 \quad (8.5.168)$$

$$\frac{\hbar^2}{4w_x^2} \ll \text{Spr}(\hat{p}) \ll w_p^2. \quad (8.5.169)$$

As well, simply multiplying the two pieces of equation (8.5.165) gives:

$$\frac{\hbar^2}{4} \leq \text{Spr}(\hat{x})\text{Spr}(\hat{p}) \ll w_x^2 w_p^2 \quad (8.5.170)$$

$$\implies w_x w_p \gg \frac{\hbar}{2}. \quad (8.5.171)$$

That is, the classical limit is only achievable in an experiment with position and momentum resolutions satisfying equation (8.5.171) and for wavefunctions satisfying equations (8.5.168) and (8.5.169). If your experimental resolution is too good, so that $w_x w_p$ is too small, then you will intrinsically have to deal with the full wavefunction and cannot expect any sort of simplification to classical mechanics. Because much of the world is well described by classical mechanics, the constant $\hbar$ in equation (8.5.171) must have a very small value in the SI unit system (as in the SI unit system we classically can measure to several decimal points in the base units of meters, seconds, kilograms that comprise the units of $\hbar$). We will find that in SI units the value of $\hbar$ is in fact very small.

The requirement that under classical conditions the Schrödinger equation should reproduce classical mechanics places some restrictions on what $\hat{H}$ can be. The quantum Hamiltonian is exactly $\langle \psi | \hat{H} | \psi \rangle$ and the exact dynamics of the operator summaries of the position and momenta are given by:

$$\frac{d\vec{x}_{\text{cl}}}{dt} = \{\vec{x}_{\text{cl}}, \mathcal{H}\} = \left\langle \frac{1}{i\hbar} [\hat{x}, \hat{H}] \right\rangle \quad (8.5.172)$$

$$\frac{d\vec{p}_{\text{cl}}}{dt} = \{\vec{p}_{\text{cl}}, \mathcal{H}\} = \left\langle \frac{1}{i\hbar} [\hat{p}, \hat{H}] \right\rangle. \quad (8.5.173)$$

These are reflections of a more general result that if we consider a generator $G(t, \psi, \psi^*)$ which we know from theorem 8.4 must be given by $\langle \psi | \hat{G} | \psi \rangle$ for a self-adjoint operator $\hat{G}$ then its time evolution is given by:

$$\frac{dG}{dt} = \frac{\partial G}{\partial t} + \{G, \mathcal{H}\} = \left\langle \frac{\partial \hat{G}}{\partial t} \right\rangle + \left\langle \frac{1}{i\hbar} [\hat{G}, \hat{H}] \right\rangle \quad (8.5.174)$$

$$\implies \frac{d}{dt} \langle \hat{G} \rangle = \left\langle \left(\frac{\partial \hat{G}}{\partial t} + \frac{1}{i\hbar} [\hat{G}, \hat{H}] \right) \right\rangle. \quad (8.5.175)$$

This is known as Ehrenfest's theorem; it's the quantum mechanical special case of equation (1.4.24). Under approximately classical conditions, this should reproduce Hamilton's equations for the corresponding classical

system. Therefore, for approximately classical wavefunctions, we must have:

$$\langle \frac{1}{i\hbar} [\hat{x}, \hat{H}] \rangle \approx \frac{\partial \mathcal{H}_{\text{cl}}}{\partial \vec{p}_{\text{cl}}}, \quad \langle \frac{1}{i\hbar} [\hat{p}, \hat{H}] \rangle \approx -\frac{\partial \mathcal{H}_{\text{cl}}}{\partial \vec{x}_{\text{cl}}} \quad (8.5.176)$$

where $\mathcal{H}_{\text{cl}}(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}})$ is the Hamiltonian of the corresponding classical system that our quantum system is supposed to reproduce. Generally, these conditions will **NOT** be enough to determine the Hamiltonian operator $\hat{H}$. However, requiring that the quantum system should have some symmetries of interest and reproduce the classical equations of motion in the classical limit is often (but still not always) enough to determine what the Hamiltonian operator $\hat{H}$ should be for the system.

We can see a little more about what classical physics tells us about the Hamiltonian operator by using our results from problem 4.50 for wave packet solutions to a generic quadratic field theory. The Schrödinger Hamiltonian can be written explicitly in the position basis:

$$\mathcal{H} = \langle \psi | \hat{H} | \psi \rangle = \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H}(t) | \vec{x}' \rangle \psi(t, \vec{x}') d^3 \vec{x}' d^3 \vec{x}. \quad (8.5.177)$$

Using the Taylor expansion of $\psi(t, \vec{x})$:

$$\mathcal{H} = \int_{\mathbb{S}} \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) \langle \vec{x} | \hat{H}(t) | \vec{x}' \rangle \sum_{n=0}^{\infty} \frac{1}{n!} (x'^{a_1} - x^{a_1}) \dots (x'^{a_n} - x^{a_n}) \partial_{a_1 \dots a_n}^n \psi(t, \vec{x}) d^3 \vec{x}' d^3 \vec{x}. \quad (8.5.178)$$

Then, we can define the differential operator $H(t, \vec{x}, -i\hbar \nabla)$ by:

$$H(t, \vec{x}, -i\hbar \nabla) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int_{\mathbb{S}} \langle \vec{x} | \hat{H}(t) | \vec{x}' \rangle (x'^{a_1} - x^{a_1}) \dots (x'^{a_n} - x^{a_n}) d^3 \vec{x}' \right) \partial_{a_1 \dots a_n}^n. \quad (8.5.179)$$

With this, the Schrödinger Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{S}} \psi^\dagger(t, \vec{x}) H(t, \vec{x}, -i\hbar \nabla) \psi(t, \vec{x}) d^3 \vec{x} \quad (8.5.180)$$

precisely in the form found in problem 4.50.

If we consider a wavefunction which is approximately localized in position space, $|\psi(t, \vec{x})|^2$ will be small outside of a small neighborhood surrounding the classical position $\vec{x}_{\text{cl}}(t)$. If our wavefunction is also approximately localized in momentum space then $|\tilde{\psi}(t, \vec{p})|^2$ (where $\tilde{\psi}(t, \vec{p}) = \langle \vec{p} | \psi(t) \rangle$) will be small outside of a small neighborhood surrounding the classical momentum $\vec{p}_{\text{cl}}(t)$. The momentum space wavefunction $\tilde{\psi}$ is just the Fourier transform of $\psi(t, \vec{x})$ up to multiplying by $\frac{1}{h^{3/2}}$ and replacing the wavenumber $\vec{k}$ with $\frac{\vec{p}}{\hbar}$. Therefore, if the wavefunction is approximately localized in momentum space then it is also approximately localized in Fourier wavenumber space around a wavenumber $\vec{K}(t)$ which is related to $\vec{p}_{\text{cl}}(t)$ by:

$$\vec{p}_{\text{cl}} = \hbar \vec{K}(t). \quad (8.5.181)$$

This is known as the **de Broglie relation**. If the wavefunction is approximately localized in momentum space then the $H(t, \vec{x}, -i\hbar \nabla)$ operator immediately acts on ψ by:

$$H(t, \vec{x}, -i\hbar \nabla) \psi(t, \vec{x}) \approx H(t, \vec{x}, \vec{p}_{\text{cl}}) \psi(t, \vec{x}) \quad (8.5.182)$$

Then, if the wavefunction is approximately localized in position space we can complete the position integral in (8.5.180) to find:

$$\mathcal{H} \approx H(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}}). \quad (8.5.183)$$

In order for this to produce classical physics then, H must approximately be the classical Hamiltonian $\mathcal{H}_{\text{cl}}(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}})$. This does not fully fix H (one can't simply just say $H = \mathcal{H}_{\text{cl}}$ as functions) because no wavefunction is exactly localized in both position and momentum space and so there is no exactly classical wavefunction. Instead, we can only require that $H = \mathcal{H}_{\text{cl}} +$ corrections which are small when the wavefunction is approximately classical. We can be more formal and exact about how what extra terms can be in H that are missing from $\mathcal{H}_{\text{cl}}$, but we will save this for chapter 9.

Under the classical limit, we can also use (8.5.182) in the Schrödinger equation to see:

$$i\hbar \dot{\psi}(t, \vec{x}) \approx H(t, \vec{x}, \vec{p}_{\text{cl}}) \psi(t, \vec{x}). \quad (8.5.184)$$

If $\vec{x}$ is near $\vec{x}_{\text{cl}}$ then we can approximately replace $H(t, \vec{x}, \vec{p}_{\text{cl}})$ with $H(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}})$. If $\vec{x}$ is far from $\vec{x}_{\text{cl}}$ and ψ is approximately classical then $\psi(t, \vec{x}) \approx 0$. In either case:

$$H(t, \vec{x}, \vec{p}_{\text{cl}}) \psi(t, \vec{x}) \approx H(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}}) \psi(t, \vec{x}) \quad (8.5.185)$$

and so we can see that an approximately classical wavefunction has approximately well defined angular frequency Ω given by:

$$i\hbar\dot{\psi}(t, \vec{x}) \approx H(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}})\psi(t, \vec{x}) \implies H(t, \vec{x}_{\text{cl}}, \vec{p}_{\text{cl}}) = \hbar\Omega. \quad (8.5.186)$$

This last condition is known as the **Planck relation**. The equations of motion derived for $\vec{x}_{\text{cl}}$ and $\vec{K}$ in problem 4.50 were:

$$\frac{d\vec{x}_{\text{cl}}}{dt} = \frac{\partial\Omega}{\partial\vec{K}}, \quad \frac{d\vec{K}}{dt} = -\frac{\partial\Omega}{\partial\vec{x}_{\text{cl}}}. \quad (8.5.187)$$

Using the Planck and de Broglie relations we have:

$$\frac{d\vec{x}_{\text{cl}}}{dt} = \frac{\partial H}{\partial\vec{p}_{\text{cl}}}, \quad \frac{d\vec{p}_{\text{cl}}}{dt} = -\frac{\partial H}{\partial\vec{x}_{\text{cl}}} \quad (8.5.188)$$

which are just Hamilton's equations (when we use that $H \approx \mathcal{H}_{\text{cl}}$). Therefore, **classical physics emerges as the wave packet approximation of quantum mechanics**.

8.5.3 The meaning of $\hbar$

The constant $\hbar$ that appears in the Schrödinger Lagrangian now also appears in our classicality conditions and so is evidently something important to understand. Let us first find the units of $\hbar$. From the normalization condition we can identify the units of the wavefunction:

$$\langle\psi|\psi\rangle = \int_{\mathbb{S}} |\psi|^2 d^d\vec{x} = 1 \implies [\psi]^2 L^d = 1 \implies [\psi] = \frac{1}{L^{\frac{d}{2}}} \quad (8.5.189)$$

where L is the unit of length. Then, from the Schrödinger Lagrangian we can identify the units of $\hbar$:

$$\mathcal{L} = i\hbar\langle\psi|\dot{\psi}\rangle - \langle\psi|\hat{H}|\psi\rangle \implies [\mathcal{L}] = [\hbar] \left[\int_{\mathbb{S}} \psi^\dagger \dot{\psi} d^d\vec{x} \right] \quad (8.5.190)$$

$$\implies \frac{[S]}{T} = [\hbar] \frac{1}{L^{\frac{d}{2}}} \frac{1}{T} \frac{1}{L^{\frac{d}{2}}} L^d \implies [\hbar] = [S] \quad (8.5.191)$$

where T is the unit of time. So, $\hbar$ has the same units as the action. We introduced the symbol $\hbar$ previously in problem 4.50, in equation (5.2.4), and in (5.12.114); this is not an accident. The use of $\hbar$ in equation (5.2.4) was allowed to be any positive constant with the units of the action, and we take from now on by definition that $\hbar$ to be chosen to be the same $\hbar$ appearing in the Schrödinger Lagrangian, which is known as Planck's constant (sometimes $\hbar$ is called the reduced Planck's constant and $2\pi\hbar$ is called Planck's constant; we will not do this). Electromagnetism is a field theory with a quadratic Hamiltonian and so by the argument of section 8.2 can be put into the form of the Schrödinger equation (in fact the homework questions in section 4.6 basically do this) and so the $\hbar$ appearing in problem 4.50 enters the same way it does in the Schrödinger Lagrangian. It isn't obvious right now that the $\hbar$ introduced in problem 4.50 has the same value as the $\hbar$ introduced in the Schrödinger Lagrangian in general; it does, but we won't be able to derive that fact until the end of this chapter.

In equations (5.2.68) and (5.2.70) we found that the whole of analytical mechanics is agnostic to the choice of the units of the action and that rescaling our choice of units of action is equivalent to rescaling our choice of units of mass. Therefore, when we chose the kilogram as a reference unit of mass it implicitly (when combined with our choices of units for length and time) determined a numerical value of $\hbar$ in that unit system. This is just like how when one chooses the meter as a reference unit of length and the second as a reference unit of time it implicitly determines a numerical value of c . However, we know that c can be eliminated from all equations and set to a numerical value of 1 by choosing our unit of length to be the distance traveled by light in our unit of time. This choice is uniquely special because c is the only invariant speed (due to Lorentz symmetry). A very similar choice can be made for $\hbar$. Due to the Planck and de Broglie relations, the momentum 4-vector $(E, \vec{p})$ of a normalized wave with well defined angular frequency and wave number is related to the wavenumber 4-vector $(\omega, \vec{k})$ by:

$$p^\mu = \hbar k^\mu. \quad (8.5.192)$$

But, the units of energy and momentum depend on our choice of the units of action and so can be rescaled one time only by an arbitrary factor. So, **if we define our units of the action so that the energy of a normalized Schrödinger wave of well-defined angular frequency is equal to that angular frequency then $\hbar = 1$ identically**. Thus, just like c , $\hbar$ is not a fundamental constant.

In units in which $c \neq 1$, one needs to perform an experiment in order to measure c as it appears in the equations of the theory. This can be accomplished through any experiment which can measure how far light travels in a measurable time. Alternatively, in units in which $c = 1$, one needs to perform the same experiment in order to calibrate what numerical value to assign to the distance traveled by the light. That is, if one lets light travel for 1 nanosecond and measures how far it goes, marking the start and end points of its travel, the distance between those two points defines the distance of a light-nanosecond. Then, light travels one light-nanosecond per nanosecond and so the speed of light is simply 1. Similarly, in units in which $\hbar \neq 1$, one needs to perform an experiment in order to measure $\hbar$ as it appears in the equations of the theory. We will discuss how to do this in the homework of later sections (for example when we study the Hydrogen atom). Alternatively, in units in which $\hbar = 1$, one needs to perform the same experiment in order to calibrate what numerical value to assign to the mass used in that experiment. That is, no more or less experimental information is necessary regardless of which unit system one uses (as it should be).

There is further analogy between c and $\hbar$. How velocities compare to c controls the nonrelativistic limit. So, formally taking $c \rightarrow \infty$ (as it is the equivalent of $v/c \rightarrow 0$) turns relativistic equations into their nonrelativistic counterparts. Similarly, due to the classicality conditions in (8.5.168), (8.5.169), (8.5.171), how the experimental resolutions w_x and w_p compare to the wavefunction spreads and $\hbar$ controls the classical limit. Due to the uncertainty theorem, it isn't possible to have a wavefunction which is simultaneously completely localized in position space and momentum space and the extent to which this is impossible is proportional to $\hbar$. If we formally take the $\hbar \rightarrow 0$ limit then it would be possible to have $\text{Spr}(\hat{x})$ and $\text{Spr}(\hat{p})$ both go to 0 so that our wavepacket would be completely like a classical particle. Therefore, just as $c \rightarrow \infty$ formally gives the nonrelativistic limit, $\hbar \rightarrow 0$ formally gives the classical limit. The reason I am saying these are *formal* limits is that c and $\hbar$ in reality always have fixed numerical values (and are 1 in my favorite units). In every experiment they are always fixed; there is no experiment in which $c \rightarrow \infty$ or $\hbar \rightarrow 0$. Properly, the nonrelativistic or classical limit is approximately achieved whenever the genuinely dynamical relevant experimental parameters (velocities or wavepacket spreads) are small.

For the rest of this chapter we will keep around factors of $\hbar$ and not choose its value to be 1. However, beginning next chapter we will set it to 1 just as we have with c and ϵ_0 and we will keep it that way unless stated otherwise. While we keep it around, let us look at its units. The units of the action are $\frac{ML^2}{T}$, which we can derive by using any known Lagrangian, for example the free nonrelativistic particle:

$$\mathcal{L} = \frac{1}{2}m|\dot{x}|^2 \implies [\mathcal{L}] = \left[\frac{dS}{dt} \right] = \frac{[S]}{T} = M \frac{L^2}{T^2} \implies [S] = \frac{ML^2}{T}. \quad (8.5.193)$$

Therefore, in SI units, $\hbar$ has the units of $\frac{\text{kg m}^2}{\text{s}}$. In particular, in modern SI units the kilogram is defined so that $\hbar$ takes the exact value:

$$\hbar = \frac{6.62607015}{2\pi} \times 10^{-34} \frac{\text{kg m}^2}{\text{s}}. \quad (8.5.194)$$

In order to establish this value experimentally (meaning to take an object and measure its mass in kilograms as defined by $\hbar$ having this value) requires an experiment that can compare macroscopically measurable quantities to $\hbar$. We describe a few ways to do this in the homework throughout this chapter such as in problems 8.45, 8.46, 8.47. Once we have defined our unit of mass so that $\hbar = 1$, we will have an induced unit of mass so that the action is unitless. In particular, the units of mass in $\hbar = 1$ units are:

$$[S] = \frac{ML^2}{T} = 1 \implies M = \frac{T}{L^2}. \quad (8.5.195)$$

The unit system in which $\epsilon_0 = 1$ and $\hbar = 1$ we call **Schrödinger Natural Units (SNU)**. This leaves time and length as the only independent units. We have not set $c = 1$ because for the bulk of this chapter we will consider Galilean symmetry and so the speed of light will not directly appear and so time and length are considered independent units. If we use meters and seconds as our units of length and time, then in SNU the unit of mass would be $\frac{\text{s}}{\text{m}^2}$.

Quantum mechanics also makes it possible to define the second at a level of precision that was previously impossible. In SI units, the second is defined exactly as the duration of 9192631770 periods of the electromagnetic radiation emitted by the transition between the hyperfine levels of the unperturbed ground state of the ^{133}Cs atom. To unpack this phrase, when modeled as a quantum system, the Cesium-133 atom has a lowest energy state (the ground state) and due to the interactions of the electromagnetic fields generated by the atomic nucleus with the electrons in the atom, there is a characteristic resonant angular frequency ω of electromagnetic waves emitted in the transition of this atom between its lowest energy configurations

(the ground state and its nearest neighbor eigenstate of the interacting Hamiltonian operator). That angular frequency of electromagnetic radiation then defines a period $\tau = \frac{2\pi}{\omega}$ and the second is defined to be exactly 9192631770τ . This gives the second a universally reproducible definition and it for all but the most precise of purposes coincides with the more colloquial understanding of a second as $1/86400^{\text{th}}$ of a solar day on Earth.

Looking ahead to when we do incorporate relativity and so use $c = 1$ units, using $\hbar = c = \epsilon_0 = k_B = 1$ units leaves only one single remaining independent unit. A unit of time can be converted to length using c , or to a mass using $\hbar$ and c , or to a charge using $\hbar$, c , and ϵ_0 , or to a temperature (in separate temperature units rather than energy units, gross) using $\hbar$, c , and k_B . This is our final unit system, and it is called either **Natural Units (NU)** or **High Energy Units (HEU)**, which are the units used in particle physics. For the last remaining unit, if one wants to correspond as closely to SI as possible, one should take the free unit to be the unit of time as the second (with the second defined as above in terms of Cesium). Alternatively, to correspond to particle physics practice as closely as possible, one should take the free unit to be the unit of energy as the electronvolt eV. The electronvolt is defined exactly as the energy gained by an electron when it is accelerated through an electrostatic potential difference of 1 Volt ($1 \text{ Volt} = 1 \frac{\text{kg m}^2}{\text{s}^2 \text{C}}$ in SI units where C is the SI unit of charge the Coulomb defined so that the electron charge is precisely $1.602176634 \times 10^{-19} \text{C}$). Using the SI definition of the second gives that in HEU the electronvolt and the second are exactly related by:

$$1\text{eV} = 2\pi \frac{1.602176634}{6.62607015} 10^{15} \frac{1}{\text{s}} \approx 1.51926744787862620125 \times 10^{15} \frac{1}{\text{s}}. \quad (8.5.196)$$

So, for HEU we take either the eV or the second as our one defining unit and use the number presented here as a conversion factor between those two choices. Alternatively, using the Cesium definition, the electronvolt is defined so that the energy difference due to hyperfine splitting of the unperturbed ground state of Cesium-133 is exactly:

$$\Delta E = \frac{6.62607015 \times 0.919263177}{1.602176634} \times 10^{-5} \text{ eV} \approx 38.0176702609049942617 \mu\text{eV} \quad (8.5.197)$$

in terms of microelectronvolts (10^{-6}eV). The electronvolt is an extremely convenient unit for atomic, nuclear, and particle physics. Unfortunately, it is a bit gross for every day quantities. Using $\hbar = c = \epsilon_0 = k_B = 1$ (and for the case of the Coulomb, the experimental value of the fine-structure constant α , see problem 8.48), all of the more familiar SI units of the meter, second, kilogram, Coulomb, and Kelvin can be expressed in terms of electronvolts. In particular:

SI Unit	eV Equivalent
1s	$\approx 1.5192674479 \times 10^{15} \text{ eV}^{-1}$
1m	$\approx 5.0677307162 \times 10^6 \text{ eV}^{-1}$
1kg	$\approx 5.6095886038 \times 10^{35} \text{ eV}$
1C	$\approx 1.8900670154 \times 10^{18}$
1K	$\approx 8.6173332621 \times 10^{-5} \text{ eV}.$

The huge range of exponents and unobvious way to verbally pronounce eV^{-1} makes it clear why for social purposes high energy units are pretty inconvenient. However, for scientific purposes applied to particle physics they are highly optimized. Conveniently, the range of human reasonable temperatures is pretty nice in electronvolts with the range -50°C to 50°C corresponding to 19.2meV to 27.8meV and a comfortable room temperature of 20°C corresponding to 25.2meV .

8.5.4 Rigged Hilbert Space

The position and momentum operators are surprisingly complicated objects mathematically even though in the position basis they simply multiply by a real number or take a derivative. We found that their eigenstates satisfy:

$$\langle \vec{x} | \vec{x}' \rangle = \delta(\vec{x} - \vec{x}'), \quad \langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}'). \quad (8.5.199)$$

Automatically it follows that if we set $|\phi\rangle = |\vec{x}\rangle$ for a particular value of $\vec{x}$, then $|\phi\rangle$ does not have finite norm:

$$\langle \phi | \phi \rangle = \delta(\vec{x} - \vec{x}) = \delta(0). \quad (8.5.200)$$

The $\delta(0)$ is effectively infinity. To understand it any meaningful sense one can consider a sequence of functions $|\phi_n\rangle$ which limit to $|\vec{x}\rangle$ and see that the norm of $|\phi_n\rangle$ limits to ∞ as $n \rightarrow \infty$. For example, if one takes $|\phi_n\rangle$ to be a Gaussian in position space centered at $\vec{x}$ and with width proportional to $\frac{1}{n}$ then one can find explicitly what the normalization of that Gaussian has to be in order for $|\phi_n\rangle$ to behave (when inner producted with

other functions) as $|\vec{x}\rangle$ in the $n \rightarrow \infty$ limit. One can then see explicitly that that normalization blows up for large n . The Gaussian is a particular choice where the calculation can be done completely explicitly but the result is independent of how $|\vec{x}\rangle$ is approached as a limit. Because $|\vec{x}\rangle$ has infinite norm, it isn't mathematically a proper element in the Hilbert space $\mathbb{H}$. The identical argument holds for $|\vec{p}\rangle$.

So, neither $|\vec{x}\rangle$ for any $\vec{x}$ nor $|\vec{p}\rangle$ for any $\vec{p}$ are in $\mathbb{H}$. This isn't actually a crazy thought. The Hilbert space is supposed to be the space of physically reasonable states of our system (finite momentum, finite energy, finite generators in general, and so finite norm) and both $|\vec{x}\rangle$ and $|\vec{p}\rangle$ are quite pathological states if taken too seriously. $|\vec{x}\rangle$ is entirely localized in position space, and so effectively represents a point particle, which we know from Part I is fundamentally an unphysical idea. $|\vec{p}\rangle$ is not localized at all in position space as it is a plane wave with infinite spatial extent. So, even though it carries a finite energy density, it carries that energy density throughout all space and so carries infinite total energy. The fact that neither $|\vec{x}\rangle$ nor $|\vec{p}\rangle$ is in our space of exactly allowed physical states is thus a good thing; they are quite unphysical!

However, mathematically $|\vec{x}\rangle$ and $|\vec{p}\rangle$ are useful tools for doing calculations. So, it is important to in some way formalize what they are and to what space they belong. After all, it doesn't make sense in a purely rigorous sense to say that the $|\vec{x}\rangle$ form a "basis" of the Hilbert space if they aren't even in the Hilbert space to begin with. The appropriate mathematical fix is called a Rigged Hilbert Space. A rigged Hilbert space is a set of three vector spaces, the first and smallest we call Φ , the second is our usual Hilbert space $\mathbb{H}$, and the third and largest we call $\tilde{\Phi}$. Φ is called the space of test functions and it is a subset of $\mathbb{H}$. Specifically, Φ is the space of smooth functions of compact support. Smooth here means that the functions in Φ are required to be infinitely many times differentiable and of compact support means that the functions in Φ are only nonzero in a closed finite region of space. The Hilbert space $\mathbb{H}$ of functions of finite norm is a subset of $\tilde{\Phi}$. $\tilde{\Phi}$ is the space of distributions. A distribution (like the Dirac delta) is an object that is not generally a well defined mathematical function but has well defined behavior when integrated against a test function. In other words, the inner product of a test function with a test function, Hilbert space element, or distribution is well defined and finite; the inner product of a Hilbert space element with a test function or Hilbert space element is well defined and finite but not generally so with a distribution; and, the inner product of a distribution is generally only well defined and finite when with a test function. Both $|\vec{x}\rangle$ and $|\vec{p}\rangle$ are distributions in $\tilde{\Phi}$, but not vectors in $\mathbb{H}$.

The spectral theorem guarantees that a normal operator has an orthogonal spanning set of generalized eigenvectors. Generalized eigenvector here means that a "vector" which is only guaranteed to be an element of $\tilde{\Phi}$, not necessarily of $\mathbb{H}$. These generalized eigenvectors are orthogonal in the sense that different ones have vanishing inner products with each other. They cannot generally be normalized to a finite value but a normalization condition can still be imposed (such as fixing $\langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}')$ with no prefactor on the Dirac delta). They are a spanning set in the sense that each element of $\mathbb{H}$ can be written as a (potentially infinite) linear combination of them. So, we informally say that the operator has an orthonormal basis of eigenvectors, in analogy with the finite dimensional linear algebra. Physicists tend to be pretty relaxed with this language as opposed to mathematicians that study functional analysis who are very careful. The takeaway from this subsection is that we will maintain only about the typical physics level of rigor in our discussions of Hilbert spaces but it should be known that an entirely rigorous treatment can be done and that while our proofs given here could be improved in term of rigor, our essential results are durable when treated with the higher level analysis (and phrased in appropriately rigorized language).

8.5.5 The Phenomenological Born Rule

An individual quantum particle, such as an electron, is extremely small and not directly detectable by human senses. In order to make meaningful measurements of quantum systems, we have to couple the microscopic system to a macroscopic measuring apparatus (we call it a detector). Beyond our control, that microscopic system will also inevitably be coupled (however weakly) to an enormous environment of variables (think of all the degrees of freedom in the all the air around you) which we for the purposes of the description include as part of the detector. The distinctions microscopic and macroscopic used here are precisely those from statistical mechanics, meaning that a microscopic quantum system is one whose state we do not have direct access to while a macroscopic meter is macroscopic in the sense that we can directly read the value reported by the meter. A macroscopic apparatus necessarily consists of an extremely large number of microscopic degrees of freedom, as physical objects are comprised of many many microscopic constituents. The part of the detector we can read is called the meter (some particular macroscopic variable of the detector) and all of the many microscopic parts of the detector we cannot read are called the environment. We might

wish that it would be possible to build a detector so that the reading of the meter was completely determined by the system we wish to measure, however the fact that the environment is necessarily large makes this overly optimistic. In order to make the meter sensitive to the microscopic system we want to measure, we have to make it able to be perturbed macroscopically by small microscopic fluctuations. This sensitivity inevitably also makes it at least partly sensitive to the environment, which has unaccounted for microscopic dynamics. Because we have to treat the environment as having many averaged out degrees of freedom, **a proper treatment of the measurement of quantum systems requires using statistical mechanics.**

A proper treatment of quantum measurement by statistical mechanics will have to wait for chapter 9, once we have built up more technical machinery. The main results of that analysis are two approximate effective principles known as the Born rule and the collapse rule. While we won't derive them yet, for making connection to experimental results it is useful to describe them now. An **ideal measurement** is the optimal measurement scheme possible consistent with quantum mechanics and statistical mechanics, in the sense of introducing the least error. Suppose we have a microscopic quantum system with state $|\psi\rangle$ for which we are going to measure a single property by an ideal detector. In an ideal measurement, it is possible to divide the Hilbert space $\mathbb{H}$ of our microscopic system into orthogonal subspaces $\mathbb{H}_1, \mathbb{H}_2, \dots$ which span the full Hilbert space and so that if $|\psi\rangle \in \mathbb{H}_n$ then the meter is guaranteed to read off a particular value M_n which is distinct for each different value of n . We can define the projector operator $\hat{\pi}_n$ as the operator that projects a vector in $\mathbb{H}$ into the subspace $\mathbb{H}_n$. Such a projector is automatically self-adjoint:

$$\hat{\pi}_n = \hat{\pi}_n^\dagger. \quad (8.5.201)$$

The requirement that the subspaces are orthogonal is given by:

$$\hat{\pi}_m \hat{\pi}_n = \delta_{mn} \hat{\pi}_n \quad (8.5.202)$$

where no implicit index summation is intended. The requirement that the subspaces span the full Hilbert space is given by:

$$\sum_n \hat{\pi}_n = \mathbb{1}. \quad (8.5.203)$$

One may wish that for each $|\psi\rangle \in \mathbb{H}$ there would be a guaranteed corresponding meter reading, however due to the statistical mechanics of the system-meter-environment interaction, this is too much to ask. The large number of interacting degrees of freedom makes the full system-meter-environment system chaotic, and consequently a probabilistic description of the effective results becomes necessary due to our imperfect knowledge of the exact microscopic initial state of the meter-environment system (the detector) and our inability to exactly calculate the dynamics of the interaction system. These subspaces $\mathbb{H}_n$ are stable, in the sense that under the full system interactions $|\psi\rangle$ will stay in one if it is already in one. But, if $|\psi\rangle$ is composed of a linear combination of subspaces, it will dynamically and chaotically (and so effectively randomly from a macroscopic perspective) decay into one of the subspaces and thus select a meter value. Which subspace is selected depends sensitively on the initial conditions of the full system, but by calibrating the detector to be unbiased on average, one can derive the probability of selection for each subspace. Doing so gives **the Born rule**: the probability that the meter M will read the value M_n is given by:

$$\text{Prob}(M = M_n) = \langle \psi | \hat{\pi}_n | \psi \rangle. \quad (8.5.204)$$

This use of projectors to generate probabilities is called a **projection valued measure (PVM)**.

After the interaction has occurred, the wavefunction will have been driven into the corresponding subspace $\mathbb{H}_n$ so that we also have **the collapse rule**: if the meter takes the value M_n , the system wavefunction $|\psi_n\rangle$ after the interaction is given by:

$$|\psi_n\rangle = \frac{\hat{\pi}_n |\psi\rangle}{\|\hat{\pi}_n |\psi\rangle\|}. \quad (8.5.205)$$

Sometimes it is useful to express the $\hat{\pi}_n$ explicitly in terms of an eigenbasis. Let $|n, a\rangle$ (with a a label) be a set of orthonormal vectors which span $\mathbb{H}_n$. The range of the label a is the dimension of $\mathbb{H}_n$. Then:

$$\hat{\pi}_n |n, a\rangle = \delta_{mn} |n, a\rangle. \quad (8.5.206)$$

Because the $\mathbb{H}_n$ span $\mathbb{H}$, varying over n and a in $|n, a\rangle$ gives an orthonormal basis of $\mathbb{H}$. Therefore:

$$\hat{\pi}_n = \hat{\pi}_n \sum_m \sum_a |m, a\rangle \langle m, a| = \sum_a |n, a\rangle \langle n, a|. \quad (8.5.207)$$

The resulting probability for $M = M_n$ in terms of this basis is then:

$$\text{Prob}(M = M_n) = \langle \psi | \hat{\pi}_n | \psi \rangle = \sum_a |\langle n, a | \psi \rangle|^2. \quad (8.5.208)$$

In the special case that the for a particular $n = n_*$ the corresponding subspace $\mathbb{H}_*$ is 1 dimensional, a only takes the value 1 and we can let $|\phi\rangle = |n_*, 1\rangle$. Under that circumstance, these formulas simply to:

$$\hat{\pi}_* = |\phi\rangle\langle\phi| \quad (8.5.209)$$

$$\text{Prob}(M = M_*) = |\langle\phi|\psi\rangle|^2. \quad (8.5.210)$$

Because of this expression, most sources will call the quantity $|\langle\phi|\psi\rangle|^2$ the probability that when $|\psi\rangle$ is measured, it will be found to become $|\phi\rangle$. Importantly, this is only valid for the special case of a 1 dimensional subspace and under the circumstances that a real measurement may be approximated by an ideal one. Further, it is only valid in the physical context of an actual measurement in which $|\phi\rangle\langle\phi|$ is one of the stable states produced by that particular measurement apparatus because measurement is a dynamical interactive process. Conceptualizing $|\langle\phi|\psi\rangle|^2$ as a probability is not a fundamental or exact principle, which is why I call $|\langle\phi|\psi\rangle|^2$ an intensity or projective intensity and avoid overuse/misuse of the term probability.

If the meter is going to tell us anything about our system of interest, we want the subspaces $\mathbb{H}_n$ on which it takes predictable values to be physically meaningful subspaces for that system. Consequently, in an ideal measurement we further require that these subspaces correspond to the eigenspaces of some operator of interest $\hat{G}$ in the quantum system. That way, there is a correspondence between the eigenvalues G_n of $\hat{G}$ and the meter readings M_n so that if $|\psi\rangle$ is an eigenstate of $\hat{G}$ with eigenvalue G_n , the meter predictably reads the value M_n . This structure lets us (in an ideal measurement) correlate as much as possible the reading of the meter with the value of some operator summary of interest in the system we are measuring. Using the properties of the $\hat{\pi}_n$, this condition gives a simple formula for any function f of $\hat{G}$:

$$f(\hat{G})|\psi\rangle = f(\hat{G}) \sum_n \hat{\pi}_n |\psi\rangle = \sum_n \|\hat{\pi}_n |\psi\rangle\| f(\hat{G}) |\psi_n\rangle = \sum_n \|\hat{\pi}_n |\psi\rangle\| f(G_n) |\psi_n\rangle = \sum_n f(G_n) \hat{\pi}_n |\psi\rangle, \quad \forall |\psi\rangle \quad (8.5.211)$$

$$\implies f(\hat{G}) = \sum_n f(G_n) \hat{\pi}_n. \quad (8.5.212)$$

To understand why in an ideal measurement a correspondence between the stable subspaces $\mathbb{H}_n$ and the eigenspaces of an operator of interest $\hat{G}$ is natural, let us consider an example. Suppose we have a detector screen with pixels sensitive to incoming charges. The width of a pixel is w . If the incoming wave-packet is entirely localized to a single pixel, then an ideal screen would only have that corresponding pixel light up. We can define the subspace $\mathbb{H}_n$ as the subspace of the Hilbert space which has wavefunctions that are only nonzero on the n^{th} pixel. Then, we could define the coarse-grained position of that pixel by the position value x_n at that pixel's center and then define the coarse-grained position operator by:

$$\hat{x}_w = \sum_n x_n \hat{\pi}_n. \quad (8.5.213)$$

Each eigenvalue x_n of $\hat{x}_w$ corresponds to the meter value, in this case n , of which pixel lights up when the charge is incident.

Most sources will typically say that an ideal measurement acts as an uncertain measurement of $\hat{G}$, which I think is very misleading (not maliciously, just a poor choice of words). Most pedantically, the meter is what is observed, not anything related to $\hat{G}$. Of course, we do want to interpret that meter result in terms of something about the system, so that element of the leap is forgivable. However, $\hat{G}$ isn't a variable, it is just an operator; the state of the system is $|\psi\rangle$ and any measurement reveals information about $|\psi\rangle$, not $\hat{G}$, which doesn't even depend on the system's state. Saying that a measurement measures an operator and gives some probability distribution makes $\hat{G}$ sound like a random variable. While it is possible in a limited sense to talk about operators as random variables, doing so out of context is incorrect, easily leads to contradictions, and generally muddles your thinking. Avoid it.

Instead, it is much more accurate to say that the repeated ideal measurement described above acts as an uncertain measurement of $\langle\hat{G}\rangle$ (which actually does depend on the state $|\psi\rangle$). Because an ideal measurement of a microscopic quantum system by a macroscopic detector gives probabilistic results, in order to learn specific facts about the state $|\psi\rangle$ one needs to prepare the system many times and perform many measurements. Suppose we prepare and measure the same state $|\psi\rangle$ a total of N times and that in observation k we observe the meter reading $M_{\sigma(k)}$ where $\sigma(k)$ is the function that maps which observation is considered to the specific

relevant value of n . Let K_n be the number of times we observe the value M_n , or in other words the number of values of k for which $\sigma(k) = n$. Then, because we have made N observations:

$$\sum_n K_n = N. \quad (8.5.214)$$

We can define the empirical frequency q_n of outcome M_n as:

$$q_n = \frac{K_n}{N}. \quad (8.5.215)$$

In the large N limit, $q_n \rightarrow \text{Prob}(M = M_n)$ due to the definition of probability. In an ideal measurement, if we read a value M_n on the meter, we infer that $|\psi\rangle$ has collapsed to $|\psi_n\rangle \in \mathbb{H}_n$ which is then an eigenstate of $\hat{G}$ with eigenvalue G_n . Correspondingly, in that state:

$$\langle \psi_n | \hat{G} | \psi_n \rangle = G_n. \quad (8.5.216)$$

Thus, we identify that our uncertain measurement of $\langle \hat{G} \rangle$ has given the value G_n a fraction q_n of the time. Consequently, our sample mean $\bar{G}$ of the empirical values is:

$$\bar{G} = \sum_n q_n \langle \psi_n | \hat{G} | \psi_n \rangle = \sum_n q_n G_n. \quad (8.5.217)$$

In the large N limit then we have:

$$\lim_{N \rightarrow \infty} \bar{G} = \sum_n G_n \text{Prob}(M = M_n) = \sum_n G_n \langle \psi | \hat{\pi}_n | \psi \rangle = \langle \psi | \sum_n G_n \hat{\pi}_n | \psi \rangle = \langle \psi | \hat{G} | \psi \rangle = \langle \hat{G} \rangle. \quad (8.5.218)$$

Therefore, $\bar{G}$ (which is fully determined by the meter readings) in the limit of large data converges to the value $\langle \hat{G} \rangle$. This is how repeated ideal measurement acts as a measurement of $\langle \hat{G} \rangle$. This correspondence between the statistical quantity $\bar{G}$ and the operator summary $\langle \hat{G} \rangle$ in the large data limit is why most sources call $\langle \hat{G} \rangle$ an expectation value or operator expectation. However, I view this as a derived correspondence emergent in the ideal measurement model, not a fundamental physical fact, and so avoid this language.

In life we always have a finite amount of data so let us determine the behavior of $\bar{G}$ at finite N . Let $p_n = \text{Prob}(M = M_n)$. We can alternatively write $\bar{G}$ as:

$$\bar{G} = \frac{1}{N} \sum_{k=1}^N G_{\sigma(k)}. \quad (8.5.219)$$

Because $\sigma(k)$ takes the value n with probability p_n , $G_{\sigma(k)}$ takes the value G_n with probability p_n . As well, the $\sigma(k)$ and hence $G_{\sigma(k)}$ are identically independently distributed. Thus:

$$\mathbb{E}\bar{G} = \frac{1}{N} \sum_{k=1}^N \mathbb{E}(G_{\sigma(k)}) = \frac{1}{N} \sum_{k=1}^N \sum_n p_n G_n = \frac{1}{N} N \langle \hat{G} \rangle = \langle \hat{G} \rangle. \quad (8.5.220)$$

As well:

$$\text{Var}(\bar{G}) = \mathbb{E}(\bar{G})^2 - (\mathbb{E}\bar{G})^2 = \frac{1}{N^2} \sum_{k=1}^N \sum_{k'=1}^N \mathbb{E}(G_{\sigma(k)} G_{\sigma(k')}) - \langle \hat{G} \rangle^2 \quad (8.5.221)$$

$$= \frac{1}{N^2} \sum_{k=1}^N \mathbb{E}(G_{\sigma(k)}^2) + \frac{1}{N^2} \sum_{k=1}^N \sum_{\substack{k'=1 \\ k' \neq k}}^N \mathbb{E}(G_{\sigma(k)} G_{\sigma(k')}) - \langle \hat{G} \rangle^2 \quad (8.5.222)$$

$$= \frac{1}{N^2} N \sum_n p_n G_n^2 + \frac{1}{N^2} \sum_{k=1}^N \sum_{\substack{k'=1 \\ k' \neq k}}^N \langle \hat{G} \rangle^2 - \langle \hat{G} \rangle^2 \quad (8.5.223)$$

$$= \frac{1}{N} \langle \psi | \sum_n G_n^2 \hat{\pi}_n | \psi \rangle + \frac{1}{N^2} N(N-1) \langle \hat{G} \rangle^2 - \langle \hat{G} \rangle^2 \quad (8.5.224)$$

$$= \frac{\langle \hat{G}^2 \rangle - \langle \hat{G} \rangle^2}{N} = \frac{\text{Spr}(\hat{G})}{N}. \quad (8.5.225)$$

Therefore, we can view $\bar{G}$ as giving a statistical measurement of $\langle \hat{G} \rangle$ with a quantifiable variance that decays with the number of trials. We can also identify the operator spread $\text{Spr}(\hat{G})$ as the variance of a single ideal measurement of $\langle \hat{G} \rangle$. Recalling the idea of quantum tomography, we now see that by preparing a system

many times with the same state $|\psi\rangle$ and measuring many different generators many different times each, we can develop increasingly precise knowledge of the value of each generator, and approximately reconstruct $|\psi\rangle$ from these values. Thus again, the state $|\psi\rangle$ as a ray in Hilbert space is entirely observable in the limit of large data. While for individual measurements we have statistical results due to the Born rule, for large numbers of measurements we have predictable statistical behavior. Consequently, beams of many particles produce reliable intensities.

The similarity between the Born rule and the adiabatic invariants of the Schrödinger Lagrangian is not accidental. In an ideal measurement, the interaction between the system-meter-environment will cause a distinct response of the meter on each subspace $\mathbb{H}_n$. Consequently, the term added to the Hamiltonian to account for the interaction between the system and the detector will be of the form:

$$\mathcal{H}_{\text{int}} = \sum_n \langle \psi | \hat{\pi}_n | \psi \rangle h_n \quad (8.5.226)$$

where h_n is a function of the meter-environment variables distinct for each n . By each h_n being distinct, the meter will have a distinct response on each subspace. During the interaction, $\mathcal{H}_{\text{int}}$ must completely dominate over the free Hamiltonians in order for the system and the detector to become properly correlated and so for the short time that the interaction happens, $\mathcal{H}_{\text{int}}$ is effectively the total Hamiltonian. Eigenstates of the Hamiltonian operator $\sum_n \hat{\pi}_n h_n$ are precisely the eigenstates $|n, a\rangle$ of the $\hat{\pi}_n$ and the adiabatic invariants of this Hamiltonian $|\langle n, a | \psi \rangle|^2$ are precisely the ingredients of the Born rule. In fact, it is because these Born rule intensities are stable enough on experimental time scales due to adiabatic invariance that allows them to have the experimental stability necessary for the Born rule to emerge as an effective macroscopic description of measurement.

One may wonder to what extent it is possible to simultaneously measure two properties of a single instance of a quantum system. Because the projectors $\hat{\pi}_n$ have to be selected based on the associated predictable response of the meter and the property $G = \langle \hat{G} \rangle$ of the quantum system which is measured is built after this selection in terms of those projectors, it is only self-consistent to infer values of another property $G' = \langle \hat{G}' \rangle$ as well if it can also be built out of those projectors in the same measurement process. Therefore, $\hat{G}$ and $\hat{G}'$ must commute (which is automatically true if they are both built out of the same $\hat{\pi}_n$). Conversely, if $\hat{G}$ and $\hat{G}'$ commute, it is possible to simultaneously diagonalize them and thus build a simultaneous set of eigenspace projectors around which an appropriate detector could be designed. Thus, in an ideal measurement two properties are simultaneously measurable in a single experimental instance if and only if the corresponding generating operators to those properties commute.

The inability in an ideal measurement to simultaneously measure properties corresponding to noncommuting operators emphasizes an important point: **probabilities in quantum mechanics are contextual**. What does this mean? Suppose that the probabilities of quantum measurement actually existed at all times, regardless of measurement or experimental context. Then, it would be possible to define a single probability space in which all of the probabilities of quantum mechanics live. So, it would be possible to answer the question of what is the probability of simultaneously reading off any two particular meter values corresponding to different properties. However, if the two properties do not commute there is no shared eigenspace, in contradiction with the conditions under which a meter value is read. Noncommuting operators indicate properties that cannot coexist in a single probability space. Consequently, the probabilities in quantum mechanics are only defined with respect to a specific measurement context. This makes perfect sense as it is the chaotic dynamical measurement process from which probabilities emerge. Measurements of different properties require physically different detector setups and so there is no physical reason to suspect that there should be a shared probability space of all possible different measurement processes. We will see rigorously when we study Bell inequalities that generically for a quantum system it is mathematically impossible to define a probability space that can describe all of the results of different possible measurements of that system.

Exercises

Problem 8.11: ★ Commutators becoming derivatives.

- Show by repeating and generalizing the arguments between equations (8.5.177) and (8.5.180) that a generic operator $\hat{F}$ on $\mathbb{H}_S$ may be written as a function $f(t, \hat{x}, \hat{p})$ (replace $\hat{H}$ in those equations by $\hat{F}$ and define f the way H is defined, then complete the argument).
- Show that if $\hat{F}$ commutes with $\hat{x}$ then it is not a function of $\hat{p}$.
- Show that if $\hat{F}$ commutes with $\hat{p}$ then it is not a function of $\hat{x}$.

(d) Show that if $\hat{F}$ is not a function of $\hat{x}$ then:

$$[\hat{x}, \hat{F}] = i\hbar \frac{\partial \hat{F}}{\partial \hat{p}}.$$

(e) Show that if $\hat{F}$ is not a function of $\hat{p}$ then:

$$[\hat{p}, \hat{F}] = -i\hbar \frac{\partial \hat{F}}{\partial \hat{x}}.$$

If treated appropriately, the results of this and the previous part actually hold for $\hat{F}$ which depend on both $\hat{x}$ and $\hat{p}$ (the partial derivative must be treated carefully in this case because the different terms within the function do not commute).

Problem 8.12: ★ Restoring factors of $\hbar$. Occasionally, one needs to compare equations with someone who prefers to use unit systems in which $\hbar$ is not set to 1 by definition. Suppose one has a quantity of interest F whose units are known in Schrödinger Natural Units (units in which $\hbar = \epsilon_0 = 1$) to be $[F]_{\text{SNU}} = T^\alpha L^\beta$ where L indicates units of length and T indicates units of time and known in your friend's unit system (for example SI units) to be $[F]_{\text{Friend}} = M^\gamma T^\lambda L^\mu Q^\nu$ where L indicates units of length and Q indicates units of charge. Show that:

$$\gamma + \lambda - \frac{\nu}{2} = \alpha, \quad -2\gamma + \mu + \frac{\nu}{2} = \beta$$

and that F in your two unit systems are related by:

$$F_{\text{Friend}} = \hbar^{\gamma + \frac{\nu}{2}} \epsilon_0^{\frac{\nu}{2}} F_{\text{SNU}}$$

with $\hbar$ and ϵ_0 being their respective values in your friend's unit system. Explain then that applying this to every quantity of interest in an equation allows one to restore powers of $\hbar$ and ϵ_0 in equations whenever one would like to and thus nothing is lost by choosing units which eliminate them.

Problem 8.13: Understanding Natural Units. From the defined values of $\hbar = c = \epsilon_0 = k_B = 1$ in natural units and the defined numerical values of $\hbar, c, k_B, q_e$ in SI units, together with the measured value of the fine-structure constant α (defined in problem 8.48), reproduce the values in the table (8.5.198).

Problem 8.14: The Dilation Operator. Consider a system with 1 spatial dimension so that $\mathbb{H}$ is the space of square-integrable complex functions of a single real variable. Define the Dilation Generator:

$$\hat{G} = \frac{(\hat{x} - \mathbb{1}\bar{x})(\hat{p} - \mathbb{1}\bar{p}) + (\hat{p} - \mathbb{1}\bar{p})(\hat{x} - \mathbb{1}\bar{x})}{2}$$

for constants $\bar{x}$ and $\bar{p}$. Further, define the Dilation Operator:

$$\hat{D}(\varepsilon) = e^{-\frac{i}{\hbar}\varepsilon\hat{G}}.$$

(a) Define $|\psi(\varepsilon)\rangle = \hat{D}(\varepsilon)|\psi_0\rangle$ for a fixed normalized wavefunction $|\psi_0\rangle$. Show that:

$$i\hbar \frac{d|\psi(\varepsilon)\rangle}{d\varepsilon} = \hat{G}|\psi\rangle.$$

(b) Show that the above in position space becomes:

$$\frac{\partial \psi}{\partial \varepsilon} + (x - \bar{x}) \frac{\partial \psi}{\partial x} - \frac{i}{\hbar} \bar{p}(x - \bar{x})\psi + \frac{\psi}{2} = 0$$

and show that this can be rewritten as:

$$\frac{\partial}{\partial \varepsilon} \left(e^{\frac{\varepsilon}{2} - \frac{i}{\hbar} \bar{p}x} \psi \right) + (x - \bar{x}) \frac{\partial}{\partial x} \left(e^{\frac{\varepsilon}{2} - \frac{i}{\hbar} \bar{p}x} \psi \right) = 0.$$

Show that this is solved by:

$$\psi(\varepsilon, x) = e^{-\frac{\varepsilon}{2} + \frac{i}{\hbar}(1 - e^{-\varepsilon})\bar{p}(x - \bar{x})} \psi(0, \bar{x} + e^{-\varepsilon}(x - \bar{x})).$$

(c) Suppose we choose the constants $\bar{x}$ and $\bar{p}$ so that they equal $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$ when $|\psi_0\rangle$ is used to compute these operator summaries. show that for all ε :

$$\langle \psi(\varepsilon) | \hat{x} | \psi(\varepsilon) \rangle = \bar{x}, \quad \langle \psi(\varepsilon) | \hat{p} | \psi(\varepsilon) \rangle = \bar{p}.$$

(d) Show that:

$$\frac{d}{d\varepsilon}(\hat{D}^\dagger(\hat{x} - \mathbb{1}\bar{x})\hat{D}) = \hat{D}^\dagger(\hat{x} - \mathbb{1}\bar{x})\hat{D}, \quad \frac{d}{d\varepsilon}(\hat{D}^\dagger(\hat{p} - \mathbb{1}\bar{p})\hat{D}) = -\hat{D}^\dagger(\hat{p} - \mathbb{1}\bar{p})\hat{D}$$

and that these are solved by:

$$\hat{D}^\dagger(\hat{x} - \mathbb{1}\bar{x})\hat{D} = e^\varepsilon(\hat{x} - \mathbb{1}\bar{x}), \quad \hat{D}^\dagger(\hat{p} - \mathbb{1}\bar{p})\hat{D} = e^{-\varepsilon}(\hat{p} - \mathbb{1}\bar{p}).$$

(e) Now define the central moments M_{mn} by:

$$M_{mn}(\varepsilon) = \langle \psi(\varepsilon) | \text{Sym}((\hat{x} - \mathbb{1}\bar{x}); m, (\hat{p} - \mathbb{1}\bar{p}); n) | \psi(\varepsilon) \rangle.$$

Here in the symmetrized product the ; m indicates that they are m factors of $\hat{x} - \bar{x}\mathbb{1}$ and ; n indicates there are n factors of $\hat{p} - \bar{p}\mathbb{1}$. Show that:

$$M_{mn}(\varepsilon) = e^{\varepsilon(m-n)} M_{mn}(0).$$

Use this result to explain how the dilation operator stretches the wavefunction out uniformly in position space and squeezes it in uniformly in momentum space. Explain further why if a transformation does one of these then it must do the other as well.

Problem 8.15: Nondegenerate Time Independent Perturbation Theory. As usual, in most systems are too hard to solve exactly. Suppose have a time independent Hamiltonian operator $\hat{H}_0$ whose eigenvector problem we can solve exactly with orthonormal eigenvectors $|n_0\rangle$ and eigenvalues $E_n^{(0)}$. Assume for this question that none of the eigenvalues of $\hat{H}_0$ are repeated. Suppose that the actual Hamiltonian operator $\hat{H}$ for our system is time independent and related to $\hat{H}_0$ by:

$$\hat{H} = \hat{H}_0 + \varepsilon \hat{H}_1$$

for a small parameter ε and $\hat{H}_1$ some operator. The goal of this question is to find the first few terms in powers of ε for the solution of the eigenvectors $|n\rangle$ and eigenvalues E_n of $\hat{H}$. These series will take the form:

$$E_n = E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)} + \mathcal{O}(\varepsilon^3)$$

$$|n\rangle = |n_0\rangle + \varepsilon |n_1\rangle + \varepsilon^2 |n_2\rangle + \mathcal{O}(\varepsilon^3).$$

(a) Expand the eigenvector equation for $\hat{H}$ to order ε^2 to show that:

$$\hat{H}_0 |n_1\rangle + \hat{H}_1 |n_0\rangle = E_n^{(0)} |n_1\rangle + E_n^{(1)} |n_0\rangle$$

$$\hat{H}_0 |n_2\rangle + \hat{H}_1 |n_1\rangle = E_n^{(0)} |n_2\rangle + E_n^{(1)} |n_1\rangle + E_n^{(2)} |n_0\rangle.$$

(b) The phase of eigenvectors can in general be chosen arbitrarily. Show that we can choose the phase of $|n\rangle$ so that:

$$\langle n_0 | n_1 \rangle = 0.$$

(c) Assume we have made the above phase choice. Show that the first two energy corrections and first state correction are given by:

$$E_n^{(1)} = \langle n_0 | \hat{H}_1 | n_0 \rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle n_0 | \hat{H}_1 | m_0 \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$|n_1\rangle = \sum_{m \neq n} \frac{\langle m_0 | \hat{H}_1 | n_0 \rangle}{E_n^{(0)} - E_m^{(0)}} |m_0\rangle.$$

Problem 8.16: Degenerate Time Independent Perturbation Theory. Consider the same setup as the previous problem except now there may be repeats among the eigenvalues of $\hat{H}_0$. Because of this, the eigenvectors of $\hat{H}_0$ are not uniquely defined (as linear combinations of eigenvectors with the same eigenvalue remain an eigenvector). But, only certain choices of eigenvectors allow the ε series to exist and precisely which choice is necessary is dependent upon $\hat{H}_1$. Assume that we see choose the phase of $|n_0\rangle$ so that $\langle n_0 | n_1 \rangle = 0$.

(a) Show that:

$$E_n^{(1)} = \langle n_0 | \hat{H}_1 | n_0 \rangle.$$

- (b) Show that for $m \neq n$ and $E_m^{(0)} \neq E_n^{(0)}$:

$$\langle m_0 | n_1 \rangle = \frac{\langle m_0 | \hat{H}_1 | n_0 \rangle}{E_n^{(0)} - E_m^{(0)}}.$$

- (c) Show that for $m \neq n$ and $E_m^{(0)} = E_n^{(0)}$:

$$\langle m_0 | \hat{H}_1 | n_0 \rangle = 0.$$

Explain that this implies that the unperturbed eigenvectors must be selected so that the perturbation $\hat{H}_1$ is diagonalized on each eigenspace of $\hat{H}_0$. Often this is enough to fully specify the proper choice of unperturbed eigenvectors. However, if there exist n, m so that $E_n^{(0)} = E_m^{(0)}$ and $E_n^{(1)} = E_m^{(1)}$ then the degeneracy is said not to be lifted at first order and the proper choice of unperturbed eigenvectors is still not determined. In that case one must keep going to higher orders until enough conditions are placed to fully specify the unperturbed eigenvectors.

- (d) Show that:

$$|n_1\rangle = \sum_{\substack{E_m^{(0)} \neq E_n^{(0)}}} \frac{\langle m_0 | \hat{H}_1 | n_0 \rangle}{E_n^{(0)} - E_m^{(0)}} |m_0\rangle + \sum_{\substack{m \neq n \\ E_m^{(0)} = E_n^{(0)}}} \sum_{\substack{E_k^{(0)} \neq E_n^{(0)}}} \frac{\langle m_0 | \hat{H}_1 | k_0 \rangle \langle k_0 | \hat{H}_1 | n_0 \rangle}{\langle n_0 | \hat{H}_1 | n_0 \rangle (E_n^{(0)} - E_k^{(0)})} |m_0\rangle$$

$$E_n^{(2)} = \sum_{\substack{E_m^{(0)} \neq E_n^{(0)}}} \frac{|\langle n_0 | \hat{H}_1 | m_0 \rangle|^2}{E_n^{(0)} - E_m^{(0)}}.$$

Problem 8.17: Time Dependent Perturbation Theory. Consider a system with a Hamiltonian operator of the form $\hat{H}(t) = \hat{H}_0 + \varepsilon \hat{H}_1(t)$ for a small parameter ε and $\hat{H}_0$ a time independent operator whose eigenvector problem we can solve exactly with orthonormal eigenvectors $|n\rangle$ and eigenvalues E_n . Importantly, note that in this question $|n\rangle$ and E_n are the eigenvectors and eigenvalues of $\hat{H}_0$ and we do not care about the eigenvectors or eigenvalues of $\hat{H}$. Define the coefficients $a_n(t)$ by:

$$a_n(t) = e^{\frac{i}{\hbar} E_n t} \langle n | \psi(t) \rangle.$$

Show that $|\psi(t)\rangle$ can be written as:

$$|\psi(t)\rangle = \sum_n e^{-\frac{i}{\hbar} E_n t} a_n(t) |n\rangle.$$

Further, show from the Schrödinger equation that $a_n(t)$ satisfies:

$$i\hbar \frac{da_n(t)}{dt} = \varepsilon \sum_m e^{\frac{i}{\hbar} (E_n - E_m)t} \langle n | \hat{H}_1(t) | m \rangle a_m(t).$$

Explain how this equation can be used to develop a series solution for $a_n(t)$ in powers of ε and thus can be used to approximately solve the original Schrödinger equation.

Problem 8.18: Fermi's Golden Rule (Approximate Form). Consider a perturbation $\hat{H}_1$ which “turns on” at time $t = 0$ and which is constant until a time $t = \tau$ at which point it is “turned off” ($\hat{H}_1$ is a non-zero constant operator for $0 < t < \tau$ and 0 otherwise) so that the total Hamiltonian is $\hat{H} = \hat{H}_0 + \varepsilon \hat{H}_1$. Suppose that the system begins at $t = 0$ in an eigenstate $|\iota\rangle$ of $\hat{H}_0$ with energy eigenvalue E_ι .

- (a) Show that the a_n coefficients of time dependent perturbation theory can be written as:

$$a_n(t) = \delta_{n\iota} + \varepsilon \delta a_n(t) + \mathcal{O}(\varepsilon^2)$$

where the $\delta a_n(t)$ coefficients satisfy:

$$\frac{d\delta a_n(t)}{dt} = -\frac{i}{\hbar} e^{\frac{i}{\hbar} (E_n - E_\iota)t} \langle n | \hat{H}_1 | \iota \rangle$$

- (b) Show that the $\delta a_n(t)$ are given by:

$$\delta a_n(t) = \frac{1 - e^{\frac{i}{\hbar} (E_n - E_\iota)t}}{E_n - E_\iota} \langle n | \hat{H}_1 | \iota \rangle.$$

(As written, this formula assumes $E_n \neq E_\iota$. Also find the correct formula for $E_n = E_\iota$ and show that the above formula correctly limits to that one in the $E_n \rightarrow E_\iota$ limit.)

- (c) Let $P_{\iota \rightarrow f}$ be the “transition intensity” for beginning in the eigenstate $|\iota\rangle$ of $\hat{H}_0$ at time $t = 0$ and ending

in the eigenstate $|f\rangle$ of $\hat{H}_0$ at time $t = \tau$ with $f \neq \iota$. That is, $P_{\iota \rightarrow f}$ is defined by:

$$P_{\iota \rightarrow f} = |\langle f | \psi(\tau) \rangle|^2.$$

Explain mathematically how $P_{\iota \rightarrow f}$ measures how close $|\psi(\tau)\rangle$ is to being $|f\rangle$, with a value of 1 indicating that they are identical and a value of 0 indicating that they are orthogonal. Show that to lowest order in perturbation theory:

$$P_{\iota \rightarrow f} = \frac{4\varepsilon^2 |\langle f | \hat{H}_1 | \iota \rangle|^2}{(E_f - E_\iota)^2} \sin^2 \left(\frac{(E_f - E_\iota)\tau}{2\hbar} \right) + \mathcal{O}(\varepsilon^3)$$

The finite time transition rate $\gamma_{\iota \rightarrow f}$ is defined by the rate of change of the transition intensity as we leave the perturbation on for slightly longer:

$$\gamma_{\iota \rightarrow f} = \frac{dP_{\iota \rightarrow f}}{d\tau}.$$

Show that:

$$\gamma_{\iota \rightarrow f} = \frac{2\varepsilon^2 |\langle f | \hat{H}_1 | \iota \rangle|^2}{\hbar(E_f - E_\iota)} \sin \left(\frac{E_f - E_\iota}{\hbar} \tau \right) + \mathcal{O}(\varepsilon^3).$$

(d) Show for an arbitrary smooth function $F(x)$ (by making the integral change of variables $y = \alpha x$) that:

$$\lim_{\alpha \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\sin(\alpha x)}{x} F(x) dx = F(0) \int_{-\infty}^{\infty} \frac{\sin x}{x} dx.$$

(e) Define the function $G(\beta)$ by:

$$G(\beta) = \int_0^{\infty} \frac{\sin x}{x} e^{-\beta x} dx.$$

Show that:

$$G(0) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\sin x}{x} dx, \quad \lim_{\beta \rightarrow \infty} G(\beta) = 0, \quad \frac{dG}{d\beta} = \int_0^{\infty} e^{-\beta x} \sin x dx.$$

In the expression for $\frac{dG}{d\beta}$, use the expression for $\sin(x)$ in terms of complex exponentials to show that:

$$\frac{dG}{d\beta} = -\frac{1}{\beta^2 + 1}.$$

Integrate this result and use our previous conditions to show:

$$\int_{-\infty}^{\infty} \frac{\sin x}{x} dx = \pi.$$

(f) Use the results of the previous two parts to show:

$$\lim_{\alpha \rightarrow \infty} \frac{\sin(\alpha x)}{x} = \pi \delta(x)$$

(g) Consider the long term behavior of the finite time transition rate $\gamma_{\iota \rightarrow f}$ for $\tau \rightarrow \infty$. Show using the result of the previous part that the long time transition rate (also simply called the transition rate) $\Gamma_{\iota \rightarrow f}$ is given by:

$$\Gamma_{\iota \rightarrow f} = \lim_{\tau \rightarrow \infty} \gamma_{\iota \rightarrow f} = \frac{2\pi}{\hbar} \varepsilon^2 |\langle f | \hat{H}_1 | \iota \rangle|^2 \delta(E_f - E_\iota) + \mathcal{O}(\varepsilon^3)$$

This formula is the approximate form of Fermi's Golden Rule. We see that it gives the lowest order in perturbation theory estimate of the stabilized rate at which a state nearly approximated by $|\iota\rangle$ transitions to a state nearly approximated by $|f\rangle$ under the perturbation $\varepsilon \hat{H}_1$. Later when we study transition rates in the context of scattering, we will find a more powerful version of Fermi's Golden Rule which gives the transition rate exactly.

Problem 8.19: Positive Operators.

(a) Let $\hat{\mathcal{O}}$ be a self-adjoint operator such that for all $|\psi\rangle \in \mathbb{H}$:

$$\langle \psi | \hat{\mathcal{O}} | \psi \rangle \geq 0.$$

Such an $\hat{\mathcal{O}}$ is called a nonnegative operator. Show that all of the eigenvalues of $\hat{\mathcal{O}}$ are nonnegative. Show that the above $\geq$ can be replaced by $>$ then all of the eigenvalues of $\hat{\mathcal{O}}$ are positive (such an operator is called a positive operator).

- (b) Show that if $\geq$ above cannot be replaced with $>$ then $\hat{O}$ must have 0 as an eigenvalue and that 0 is its least eigenvalue. Thus, show that for a self-adjoint operator $\hat{V}$ if v is the greatest real number such that:

$$\langle \psi | \hat{V} | \psi \rangle \geq v$$

for all $|\psi\rangle \in \mathbb{H}$ then v is an eigenvalue of $\hat{V}$ and v is the lowest eigenvalue of $\hat{V}$. An operator $\hat{V}$ for which such a v exists is said to be bounded below.

Problem 8.20: ★ The Baker–Campbell–Hausdorff formula. For operators $\hat{A}$ and $\hat{B}$ which do not commute:

$$e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{A}+\hat{B}}.$$

The product can be written as an exponential so that:

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{C}}$$

for some $\hat{C}$. The goal of this question is to find a formula for $\hat{C}$ (known as the BCH formula).

- (a) Consider the function $\hat{C}(\varepsilon)$ defined by:

$$e^{\hat{C}(\varepsilon)} = e^{\varepsilon \hat{A}} e^{\varepsilon \hat{B}}.$$

Taylor expand both sides in powers of ε to show:

$$\hat{C}(\varepsilon) = \varepsilon \hat{A} + \varepsilon \hat{B} + \frac{\varepsilon^2}{2} [\hat{A}, \hat{B}] + \frac{\varepsilon^3}{12} [\hat{A} - \hat{B}, [\hat{A}, \hat{B}]] + \mathcal{O}(\varepsilon^4).$$

- (b) The above series does not terminate for general operators and the exact expression for $\hat{C}$ is very complicated. However, assume the special case that:

$$[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0.$$

Show that in this case:

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A}, \hat{B}]}.$$

We call this the “simple” BCH formula.

Problem 8.21: The Wavefunction of Minimum Uncertainty is a Gaussian. Consider a quantum system in 1 spatial dimension. Due to the uncertainty theorem we know the minimum value possible for $\sigma_x \sigma_p$ among all wavefunctions in $\mathbb{H}$ is $\frac{\hbar}{2}$. In this question we will find all wavefunctions which achieve this minimum value.

- (a) Show that for all $|\psi\rangle$:

$$\sigma_p^2 + \frac{\hbar^2 \sigma_x^2}{4\ell^4} \geq \frac{\hbar^2}{2\ell^2} \quad \text{if } \ell = \sigma_x$$

and that the inequality becomes an equality if and only if $|\psi\rangle$ is a state of minimum uncertainty (meaning $\sigma_x \sigma_p = \frac{\hbar}{2}$). This is as simple as it seems.

- (b) Consider a state vector $|\psi\rangle$ with $\bar{x} = \langle \hat{x} \rangle$ and $\bar{p} = \langle \hat{p} \rangle$. Define the state vector $|\psi_0\rangle$ by:

$$|\psi_0\rangle = e^{-\frac{i}{\hbar} \bar{p} \hat{x} + \frac{i}{\hbar} \bar{x} \hat{p}} |\psi\rangle.$$

We call this transformation double-translation as it simultaneously performs a translation in position space and momentum space. Show that:

$$\langle \psi_0 | \hat{x} | \psi_0 \rangle = 0, \quad \langle \psi_0 | \hat{p} | \psi_0 \rangle = 0$$

and that the position and momentum spreads σ_x and σ_p computed using $|\psi_0\rangle$ match those computed using $|\psi\rangle$. Thus, show that every state of minimum uncertainty can be mapped to a state with minimum uncertainty and $\langle \hat{x} \rangle = 0, \langle \hat{p} \rangle = 0$.

- (c) Show using the dilation operator that given a minimum uncertainty state with position spread σ_x by applying $\hat{D}(\varepsilon)$ to it one achieves a minimum uncertainty state with position spread $e^\varepsilon \sigma_x$. Thus, explain that if one minimum uncertainty state exists then there exists a minimum uncertainty state for each value of σ_x .
- (d) Use the previous parts of this problem and the result of the previous problem to show that every

minimum uncertainty state is related by dilation and double-translation to a state $|\phi\rangle$ which satisfies:

$$\left(\hat{p}^2 + \frac{\hbar^2 \hat{x}^2}{4\ell^4}\right) |\phi\rangle = \frac{\hbar^2}{2\ell^2} |\phi\rangle$$

where ℓ is the position space width σ_x for $|\phi\rangle$. As well, explain that such $|\phi\rangle$ must be the minimum possible eigenvalue of $\hat{p}^2 + \frac{\hbar^2 \hat{x}^2}{4\ell^4}$.

- (e) Suppose $|\phi\rangle$ is as above. Show that $|\phi'\rangle$ defined by:

$$|\phi'\rangle = \left(\frac{\hat{x}}{2\ell} + \frac{i\ell}{\hbar}\hat{p}\right) |\phi\rangle$$

satisfies:

$$\left(\hat{p}^2 + \frac{\hbar^2 \hat{x}^2}{4\ell^4}\right) |\phi'\rangle = -\frac{\hbar^2}{2\ell^2} |\phi'\rangle.$$

Show using the results of the previous part that this must mean:

$$|\phi'\rangle = 0.$$

- (f) Show that the condition $|\phi'\rangle = 0$ when put into a position space differential equation for $|\phi\rangle$ means that $|\phi\rangle$ must satisfy:

$$\frac{\partial \phi}{\partial x} + \frac{x}{2\ell^2} \phi = 0.$$

Show that the solution to this once ϕ is normalized gives:

$$\phi(x) = \frac{e^{-\frac{x^2}{4\ell^2}}}{(2\pi\ell^2)^{\frac{1}{4}}}.$$

Thus, example how this demonstrates that every state of minimum uncertainty is related by dilation and double-translation to this Gaussian function. A wavefunction which is a decaying exponential of a quadratic polynomial in position space is called Gaussian. Show that all dilations and double-translations of ϕ remain Gaussian. Conclude that a wavefunction is a state of minimal uncertainty if and only if it is Gaussian.

Problem 8.22: ★ First Look at Coherent States. Consider a state of minimal uncertainty with $\sigma_x = \ell$, $\langle \hat{x} \rangle = q$, and $\langle \hat{p} \rangle = p$.

- (a) Show using the results of the previous question that the wavefunction for this state may be written as:

$$\psi(x) = \frac{1}{(2\pi\ell^2)^{\frac{1}{4}}} e^{-\frac{(x-q)^2}{4\ell^2} + \frac{i}{\hbar}px - \frac{iqp}{2\hbar}}.$$

To do so you should use the simple BCH formula. Define the state $|q, p\rangle \in \mathbb{H}$ as the state with this wavefunction:

$$\langle x|q, p\rangle = \psi(x).$$

Such a state is called a coherent state. Because coherent states are maximally localized in momentum space for a given amount of localization in position space, they are “maximally classical” (because for a wave packet to look like a classical point particle it must be effectively localized in position space and all parts of it must move with approximately the same velocity).

- (b) Show that the coherent states at fixed ℓ satisfy:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |q, p\rangle \langle q, p| \frac{dq dp}{2\pi\hbar} = \mathbb{1}.$$

This looks like a completeness relation but it should properly be called an over-completeness relation because the coherent states are **NOT** a basis. They are over-complete in the sense that they are not a linearly independent set. Explain how it is possible to fully determine an operator $\hat{O}$ from its coherent state matrix elements $\langle q, p|\hat{O}|q', p'\rangle$.

- (c) Show that the coherent states have the inner products:

$$\langle q, p|q', p'\rangle = e^{-\frac{(q-q')^2}{4\ell^2} - \frac{\ell^2(p-p')^2}{2\hbar^2} + \frac{i}{2\hbar}(qp' - q'p)}.$$

Thus, the coherent states are approximately orthogonal for significantly different (q, p) and (q', p') (where significantly different is determined by $\ell, \hbar$).

Problem 8.23: Time Reversal Pseudo-Operator and Time Reversal Symmetry. Let $\hat{\mathcal{K}}$ denote the simple time reversal pseudo-operator, defined so that (in some specific orthonormal basis $|n\rangle$):

$$\hat{\mathcal{K}}|\psi\rangle = |\psi^*\rangle.$$

In particular, this means:

$$\hat{\mathcal{K}}\left(\sum_n \psi_n |n\rangle\right) = \sum_n \psi_n^* |n\rangle.$$

The object $\hat{\mathcal{K}}$ is called a pseudo-operator because it is not complex linear.

- (a) Show that $\hat{\mathcal{K}}$ is complex “anti-linear” or conjugate linear, meaning that for complex numbers a and b and vectors in Hilbert space $|\psi_1\rangle$ and $|\psi_2\rangle$:

$$\hat{\mathcal{K}}(a|\psi_1\rangle + b|\psi_2\rangle) = a^* \hat{\mathcal{K}}|\psi_1\rangle + b^* \hat{\mathcal{K}}|\psi_2\rangle.$$

- (b) Show, using Wigner’s theorem, that if $\hat{\mathcal{T}}$ is a time reversal pseudo-operator, meaning the transformation $|\psi'\rangle = \hat{\mathcal{T}}|\psi\rangle$ is a time reversing transformation in quantum then there exists a unitary operator $\hat{V}$ so that $\hat{\mathcal{T}}$ can be written:

$$\hat{\mathcal{T}} = \hat{V} \hat{\mathcal{K}}.$$

Show that $\hat{\mathcal{T}}$ is also conjugate linear. Show that $\hat{\mathcal{T}}$ can be understood as a linear operator over the real numbers when $|\psi\rangle$ is broken up into real and imaginary components.

- (c) Show that:

$$\hat{\mathcal{T}}i\hat{\mathcal{T}}^{-1} = -i.$$

- (d) For an operator $\hat{\mathcal{O}}$, define the time reversed operator $\hat{\mathcal{O}}_{\mathcal{T}}$ as the operator which when acting on a time reversed state gives the time reversed behavior of $\hat{\mathcal{O}}$ acting on a non-time reversed state. Show that this means:

$$\hat{\mathcal{O}}_{\mathcal{T}}(\hat{\mathcal{T}}|\psi\rangle) = \hat{\mathcal{T}}(\hat{\mathcal{O}}\psi)$$

for all $|\psi\rangle$. Show further that this requires:

$$\hat{\mathcal{O}}_{\mathcal{T}} = \hat{\mathcal{T}} \hat{\mathcal{O}} \hat{\mathcal{T}}^{-1}.$$

- (e) Let $|n\rangle$ be an orthonormal basis of states which are invariant under time reversal: $\hat{\mathcal{T}}|n\rangle = |n\rangle$. Show that for any operator $\hat{\mathcal{O}}$, the matrix elements of the time reversed operator are related to the matrix elements of the original operator by:

$$\langle n|\hat{\mathcal{O}}_{\mathcal{T}}|n'\rangle = (\langle n|\hat{\mathcal{O}}|n'\rangle)^*.$$

- (f) Explain why, based on the time reversal properties of spatial position $\vec{x}$, it is natural to define:

$$\hat{\mathcal{T}}|\vec{x}\rangle = |\vec{x}\rangle.$$

Show that this implies:

$$\hat{\mathcal{T}}\hat{x}\hat{\mathcal{T}}^{-1} = \hat{x}, \quad \hat{\mathcal{T}}\hat{p}\hat{\mathcal{T}}^{-1} = -\hat{p}.$$

- (g) Show that if the Hamiltonian of a quantum system has time reversal symmetry then the Hamiltonian operator satisfies:

$$\hat{\mathcal{T}}\hat{H}\hat{\mathcal{T}}^{-1} = \hat{H}.$$

Suppose that $\hat{H}$ can be written solely as a function of the $\hat{x}$ and $\hat{p}$ operators and has time reversal symmetry. Show that this requires that $\hat{H}$ is an even function of $\hat{p}$.

8.6 Scalar Theory - The Galilean Schrödinger Equation

We are finally ready to look at our first explicit theory of matter without any point particles. Ultimately, we know we will have to consider quantum mechanics with Lorentz symmetry because we know the problems with Galilean symmetry, but it is very fruitful to learn about Galilean Quantum Mechanics first. Since all we are changing from GCM is that we are taking a wave theory of matter, we take as our assumptions exactly those of GCM with a single replacement:

Assumption :: GQMI - Matter is wave-like

A unit of matter is described by a matter field (also known as matter wave) called the wavefunction $\psi(t, \vec{x})$.

Assumption :: GQMII - Galilean boost symmetry

Isolated systems have symmetry under shifting the position of all objects at the same fixed rate (boosting the velocity) while keeping time unchanged.

Assumption :: GQMIII - Space is static and Euclidean

The background space on which fields are dynamical is not itself dynamical and is instead fixed without any curvature.

Assumption :: GQMIV: Parity Symmetry

Isolated systems have parity symmetry.

We first consider a scalar particle with no internal degrees of freedom so that $\mathbb{H} = \mathbb{H}_{\mathbb{S}}$. Recall from section 2.1 that the Poisson brackets for the classical Galilean theory are:

$$\{\vec{x}, \vec{G}\} = 0, \quad \{\vec{p}, \vec{G}\} = m\mathbb{1}, \quad \{\vec{v}, \vec{G}\} = \mathbb{1}. \quad (8.6.1)$$

Here $\vec{v}$ is the velocity and $\vec{G}$ is the generator of Galilean boosts at the time the boost is applied. We found that the classical position is given by $\langle \vec{x} \rangle$ and the classical momentum is given by $\langle \vec{p} \rangle$. We also know from Theorem 8.4 that as generators $\vec{v}$ and $\vec{G}$ must be expressible as $\langle \hat{v} \rangle$ and $\langle \hat{G} \rangle$ for some self-adjoint $\hat{v}$ and $\hat{G}$. Then, because we know that the Poisson brackets induce the same algebra onto the operators by Theorem 8.5:

$$[\hat{x}, \hat{G}] = 0, \quad [\hat{p}, \hat{G}] = i\hbar m\mathbb{1}, \quad [\hat{v}, \hat{G}] = i\hbar\mathbb{1}. \quad (8.6.2)$$

By the result of problem 8.11, $\hat{G}$ can be written as a function $t, \hat{x}, \hat{p}$. Because our $\hat{G}$ commutes with $\hat{x}$, it cannot depend on $\hat{p}$ (because $\hat{p}$ does not commute with $\hat{x}$). Therefore:

$$[\hat{x}, \hat{G}] = 0 \implies \hat{G} = \hat{G}(t, \hat{x}) \quad (8.6.3)$$

$$[\hat{p}, \hat{G}] = i\hbar m\mathbb{1} = m[\hat{x}, \hat{p}] \implies [\hat{p}, \hat{G} + m\hat{x}] = 0. \quad (8.6.4)$$

Similarly, because $\hat{G} + m\hat{x}$ commutes with $\hat{p}$, it cannot be a function of $\hat{x}$. Therefore, $\hat{G} + m\hat{x}$ can be a function of neither $\hat{x}$ nor $\hat{p}$ and so must be a function of only time times the identity:

$$\hat{G} = -m\hat{x} + \vec{a}(t)\mathbb{1}. \quad (8.6.5)$$

$$[\hat{v}, \hat{G}] = i\hbar\mathbb{1} \implies [\hat{v}, -m\hat{x} + \vec{a}\mathbb{1}] = [\hat{x}, \hat{p}] \quad (8.6.6)$$

$$\implies [\hat{x}, \hat{p} - m\hat{v}] = 0. \quad (8.6.7)$$

Yet again, because $\hat{p} - m\hat{v}$ commutes with $\hat{x}$ it cannot be a function of $\hat{p}$. Hence, there exists a function

$\hat{K}(t, \hat{x})$ so that:

$$\hat{p} - m\hat{v} = \hat{K} \implies \hat{v} = \frac{\hat{p} - \hat{K}(t, \hat{x})}{m}. \quad (8.6.8)$$

Now we will find an explicit relationship between the velocity operator and the Hamiltonian. By definition:

$$\langle \hat{v} \rangle = \frac{d\langle \hat{x} \rangle}{dt} = \frac{d}{dt} \langle \psi | \hat{x} | \psi \rangle = \frac{d\langle \psi |}{dt} \hat{x} | \psi \rangle + \langle \psi | \hat{x} \frac{d}{dt} | \psi \rangle \quad (8.6.9)$$

$$= -\frac{1}{i\hbar} \langle \psi | \hat{H} \hat{x} | \psi \rangle + \frac{1}{i\hbar} \langle \psi | \hat{x} \hat{H} | \psi \rangle = \langle \frac{1}{i\hbar} [\hat{x}, \hat{H}] \rangle \quad (8.6.10)$$

$$\implies \hat{v} = \frac{1}{i\hbar} [\hat{x}, \hat{H}] \quad (8.6.11)$$

where the last line follows because the previous must hold for all $|\psi\rangle$. Together (8.6.8) and (8.6.11) give:

$$\frac{1}{i\hbar} [\hat{x}, \hat{H}] = \frac{\hat{p} - \hat{K}(t, \hat{x})}{m}. \quad (8.6.12)$$

It is not obvious how to solve this equation for $\hat{H}$ in general. But, the general solution can be constructed from a reasonably guessed particular solution. Consider $\hat{H}_0$:

$$\hat{H}_0 = \frac{|\hat{p} - \hat{K}|^2}{2m} \quad (8.6.13)$$

$$\implies \frac{1}{i\hbar} [\hat{x}, \hat{H}_0] = \frac{1}{i\hbar} [\hat{x}, \frac{|\hat{p}|^2 - \hat{p} \cdot \hat{K} - \hat{K} \cdot \hat{p} + |\hat{K}|^2}{2m}] \quad (8.6.14)$$

$$= \frac{1}{2mi\hbar} [\hat{x}, |\hat{p}|^2] - \frac{1}{2mi\hbar} [\hat{x}, \hat{p}] \cdot \hat{K} - \frac{1}{2mi\hbar} \hat{K} \cdot [\hat{x}, \hat{p}] + 0 \quad (8.6.15)$$

$$= \frac{1}{2mi\hbar} ([\hat{x}, \hat{p}] \cdot \hat{p} + \hat{p} \cdot [\hat{x}, \hat{p}]) - \frac{1}{2mi\hbar} i\hbar \mathbb{1} \cdot \hat{K} - \frac{1}{2mi\hbar} \hat{K} \cdot i\hbar \mathbb{1} \quad (8.6.16)$$

$$= \frac{1}{2mi\hbar} (i\hbar \mathbb{1} \cdot \hat{p} + \hat{p} \cdot i\hbar \mathbb{1}) - \frac{\hat{K}}{m} \quad (8.6.17)$$

$$= \frac{\hat{p} - \hat{K}}{m}. \quad (8.6.18)$$

Hence $\hat{H}_0$ is a particular solution to equation (8.6.12). This particular solution was a reasonable guess because commuting with a function of $\hat{p}$ with $\hat{x}$ just takes the $\hat{p}$ derivative of that function and this $\hat{H}_0$ is an antiderivative of $\hat{v}$ with respect to $\hat{p}$. Now consider the difference between $\hat{H}$, a general solution, and $\hat{H}_0$:

$$\frac{1}{i\hbar} [\hat{x}, \hat{H} - \hat{H}_0] = \frac{1}{i\hbar} [\hat{x}, \hat{H}] - \frac{1}{i\hbar} [\hat{x}, \hat{H}_0] = 0. \quad (8.6.19)$$

So, $\hat{H} - \hat{H}_0$ cannot be a function of $\hat{p}$. This leaves $\hat{H}$ determined up to adding a function $\hat{U}(t, \hat{x})$:

$$\hat{H} = \frac{|\hat{p} - \hat{K}(t, \hat{x})|^2}{2m} + \hat{U}(t, \hat{x}). \quad (8.6.20)$$

Thus equation (8.6.20) is the general solution for the Hamiltonian operator consistent with our necessary symmetries. Now that we know the Hamiltonian operator for our theory, we can compute the equation of motion:

$$\mathcal{L} = i\hbar \langle \psi | \dot{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle \implies i\hbar |\dot{\psi}\rangle = \hat{H} |\psi\rangle \quad (8.6.21)$$

$$\implies i\hbar \langle \vec{x} | \dot{\psi} \rangle = \langle \vec{x} | \hat{H} | \psi \rangle = \langle \vec{x} | \left(\frac{|\hat{p} - \hat{K}(t, \hat{x})|^2}{2m} + \hat{U}(t, \hat{x}) \right) | \psi \rangle \quad (8.6.22)$$

$$\implies \boxed{i\hbar \frac{\partial \psi}{\partial t}(t, \vec{x}) = \left(-\frac{\hbar^2}{2m} \left(\nabla - \frac{i}{\hbar} \vec{K}(t, \vec{x}) \right)^2 + U(t, \vec{x}) \right) \psi(t, \vec{x}).} \quad (8.6.23)$$

Equation (8.6.23) is an extremely successful model, the Galilean Schrödinger equation. The Hamiltonian operator appearing here has a strikingly similar form to Theorem 2.1. However, at the moment we cannot justify associating the parameter m appearing here and the functions $\hat{U}$ and $\hat{K}$ with the classical mass and

potentials. To interpret these quantities we need to look at the classical limiting behavior of this equation.

Let us compute the dynamics of $\vec{x}_{\text{cl}}$ predicted by the Galilean Schrödinger equation:

$$\frac{d\langle\hat{\vec{x}}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{\vec{x}}, \hat{H}]\rangle = \frac{\langle\hat{\vec{p}}\rangle - \langle\hat{\vec{K}}\rangle}{m} \quad (8.6.24)$$

$$\frac{d^2\langle\hat{\vec{x}}\rangle}{dt^2} = \frac{1}{m}\frac{d\langle\hat{\vec{p}}\rangle}{dt} - \frac{1}{m}\frac{d\langle\hat{\vec{K}}\rangle}{dt} \quad (8.6.25)$$

$$\frac{d\langle\hat{\vec{p}}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{\vec{p}}, \hat{H}]\rangle \quad (8.6.26)$$

$$= \frac{1}{2mi\hbar}\left\langle[\hat{\vec{p}}, \hat{p}_a - \hat{K}_a](\hat{p}^a - \hat{K}^a) + (\hat{p}_a - \hat{K}_a)[\hat{\vec{p}}, \hat{p}^a - K^a]\right\rangle + \frac{1}{i\hbar}\langle[\hat{\vec{p}}, \hat{U}]\rangle \quad (8.6.27)$$

$$= \frac{1}{2}\left\langle\frac{\partial\hat{K}_a}{\partial\hat{x}}\hat{v}^a + \hat{v}^a\frac{\partial\hat{K}_a}{\partial\hat{x}}\right\rangle - \langle\nabla\hat{U}\rangle \quad (8.6.28)$$

$$\frac{d\langle\hat{\vec{K}}\rangle}{dt} = \frac{\partial\langle\hat{\vec{K}}\rangle}{\partial t} + \frac{1}{i\hbar}\langle[\hat{\vec{K}}, \hat{H}]\rangle = \frac{\partial\langle\hat{\vec{K}}\rangle}{\partial t} + \frac{1}{2}\left\langle\frac{\partial\hat{K}}{\partial\hat{x}^a}\hat{v}^a + \hat{v}^a\frac{\partial\hat{K}}{\partial\hat{x}^a}\right\rangle. \quad (8.6.29)$$

Collecting these together:

$$m\frac{d^2\langle\hat{\vec{x}}\rangle}{dt^2} = \left\langle-\frac{\partial\hat{\vec{K}}}{\partial t} - \nabla\hat{U}\right\rangle - \frac{1}{2}\left\langle(\nabla \times \hat{\vec{K}}) \times \hat{\vec{v}}\right\rangle + \frac{1}{2}\left\langle\hat{\vec{v}} \times (\nabla \times \hat{\vec{K}})\right\rangle. \quad (8.6.30)$$

This is satisfied exactly for all wavefunctions. Importantly, the operator summary of a function of an operator is **NOT** the same thing as that function of the operator summary. And so, in general this differential equation does not close (meaning it does not contain sufficient information to solve for $\vec{x}_{\text{cl}}$ from initial data about $\vec{x}_{\text{cl}}$ only). However, we can find what happens in the classical limit by considering a wavefunction which has approximately well defined position (meaning it is highly localized relative to experimental resolution) and approximately well defined velocity (meaning it is all moving together relative to experimental resolution). For a highly localized wavefunction:

$$\langle f(\hat{\vec{x}}) \rangle = \langle \psi | f(\hat{\vec{x}}) | \psi \rangle = \int_{\mathbb{S}} f(\vec{x}) |\psi|^2 d^3\vec{x} \approx f(\langle\hat{\vec{x}}\rangle) \int_{\mathbb{S}} |\psi|^2 d^3\vec{x} = f(\langle\hat{\vec{x}}\rangle) \langle \psi | \psi \rangle = f(\langle\hat{\vec{x}}\rangle). \quad (8.6.31)$$

This approximation is legitimate if ψ is highly localized because then the only significant contributions to the integral come from the region near $\langle\hat{\vec{x}}\rangle$ and if the function f does not vary much over this region then we can approximate its value anywhere on this region by its value at $\langle\hat{\vec{x}}\rangle$. This allows us to approximately move f outside of the integral. Making the same approximation that the velocity is approximately well defined and so can be approximately replaced by its operator summary $\frac{d\langle\hat{\vec{x}}\rangle}{dt}$, we then have that in the classical limit:

$$m\frac{d^2\langle\hat{\vec{x}}\rangle}{dt^2} \approx -\frac{\partial\vec{K}(t, \langle\hat{\vec{x}}\rangle)}{\partial t} - \nabla U(t, \langle\hat{\vec{x}}\rangle) - \frac{1}{2}(\nabla \times \vec{K}(t, \langle\hat{\vec{x}}\rangle) \times \frac{d\langle\hat{\vec{x}}\rangle}{dt}) + \frac{1}{2}\frac{d\langle\hat{\vec{x}}\rangle}{dt} \times (\nabla \times \vec{K}(t, \langle\hat{\vec{x}}\rangle)) \quad (8.6.32)$$

$$\implies m\ddot{\vec{x}}_{\text{cl}} \approx -\frac{\partial\vec{K}}{\partial t}(t, \vec{x}_{\text{cl}}) - \nabla U(t, \vec{x}_{\text{cl}}) + \dot{\vec{x}}_{\text{cl}} \times (\nabla \times \vec{K}(t, \vec{x}_{\text{cl}})) \quad (8.6.33)$$

Hence the center $\vec{x}_{\text{cl}}$ of a highly localized wavefunction approximately satisfies the classical equation of motion making the identification of m with the classical mass and U and $\vec{K}$ with the classical potentials. Again, in general no wavefunction exactly satisfies this equation of motion but if the wavefunction is sufficiently localized in position and velocity on the scale of our experiment then it satisfies this equation of motion to good enough accuracy to explain how the Galilean equation of motion was a successful macroscopic description of particles. Therefore, together we have:

Theorem 8.9: The Galilean Schrödinger Equation

In general, the Hamiltonian operator for a scalar Galilean Schrödinger wave is given by:

$$\hat{H} = \frac{|\hat{\vec{p}} - \vec{K}(t, \hat{\vec{x}})|^2}{2m} + \hat{U}(t, \hat{\vec{x}}) \quad (8.6.34)$$

where m is the mass of the wave and $U(t, \vec{x})$ and $\vec{K}(t, \vec{x})$ are the scalar and vector potentials experienced by the wave.

8.6.1 Interaction with Electromagnetism

In classical mechanics, when the potentials appearing in the Hamiltonian are due to electromagnetic fields, we identify $\vec{K} = q\vec{A}$ and $U = q\phi$ with q the electric charge of the body and ϕ and the $\vec{A}$ the scalar and vector potentials. This identification is still true in quantum mechanics because the potentials in the Hamiltonian operator correspond to the potentials in the classical Hamiltonian in the classical limit (as seen in equation (8.6.33)). Then, for an electrically charged wavefunction of charge q :

$$\hat{H} = \frac{|\hat{\vec{p}} - q\hat{\vec{A}}|^2}{2m} + q\hat{\phi} \quad (8.6.35)$$

where $\hat{\phi} = \phi(t, \vec{x})$ and $\hat{\vec{A}} = \vec{A}(t, \vec{x})$. We also know that the potentials are only actually defined up to the gauge transformation:

$$\vec{A}' = \vec{A} + \nabla f \quad \phi' = \phi - \frac{\partial f}{\partial t}. \quad (8.6.36)$$

If we insert these transformed potentials into the Hamiltonian operator, we arrive at the transformed Hamiltonian operator:

$$\hat{H}' = \frac{|\hat{\vec{p}} - q\hat{\vec{A}}'|^2}{2m} + q\hat{\phi}' = \frac{|\hat{\vec{p}} - q\hat{\vec{A}} - q\nabla f|^2}{2m} + q\hat{\phi} - q\frac{\partial f}{\partial t}. \quad (8.6.37)$$

In order for us to not violate the redundancy in the potentials, we need this transformed operator to be equivalent to our untransformed Hamiltonian operator up to symmetry transformation. Because the gauge transformation does not affect time, time is not reversed and so by Wigner's theorem there must exist a unitary operator $\hat{U}$ so that $\hat{H}'$ and $\hat{H}$ are related by:

$$\hat{H}' = \hat{U} \left(\hat{H} - i\hbar \frac{\partial}{\partial t} \right) \hat{U}^\dagger \quad (8.6.38)$$

and correspondingly this means the wavefunction is transformed by:

$$|\psi'\rangle = \hat{U}|\psi\rangle. \quad (8.6.39)$$

For a generic wavefunction and with a bit of algebra:

$$\langle \vec{x} | \left(\hat{U} \hat{H} \hat{U}^\dagger - i\hbar \hat{U} \frac{\partial \hat{U}^\dagger}{\partial t} \right) | \psi \rangle = -\frac{\hbar^2}{2m} \left(\nabla - i\frac{q}{\hbar} \vec{A} - i\frac{q}{\hbar} \nabla f \right)^2 \psi + q\phi\psi - q\frac{\partial f}{\partial t} \psi \quad (8.6.40)$$

$$= -\frac{\hbar^2}{2m} e^{i\frac{q}{\hbar}f(t, \vec{x})} \left(\nabla - i\frac{q}{\hbar} \vec{A} \right)^2 \left(e^{-i\frac{q}{\hbar}f} \psi \right) + q\phi e^{i\frac{q}{\hbar}f} e^{-i\frac{q}{\hbar}f} \psi - i\hbar e^{i\frac{q}{\hbar}f} \frac{\partial}{\partial t} \left(e^{-i\frac{q}{\hbar}f} \right) \psi \quad (8.6.41)$$

$$= \langle \vec{x} | \left(e^{i\frac{q}{\hbar}f} \hat{H} e^{-i\frac{q}{\hbar}f} - i\hbar e^{i\frac{q}{\hbar}f} \frac{\partial}{\partial t} \left(e^{-i\frac{q}{\hbar}f} \right) \right) | \psi \rangle. \quad (8.6.42)$$

Therefore:

$$\hat{U} = e^{i\frac{q}{\hbar}f} \quad (8.6.43)$$

$$\implies \psi'(t, \vec{x}) = e^{i\frac{q}{\hbar}f(t, \vec{x})} \psi(t, \vec{x}). \quad (8.6.44)$$

Our Lagrangian is then invariant under the combined transformation:

$$\psi'(t, \vec{x}) = e^{i\frac{q}{\hbar}f} \psi \quad \vec{A}' = \vec{A} + \nabla f, \quad \phi' = \phi - \frac{\partial f}{\partial t} \quad (8.6.45)$$

$$\implies \mathcal{L}' = i\hbar \langle \psi' | \dot{\psi}' \rangle - \langle \psi' | \hat{H}' | \psi' \rangle \quad (8.6.46)$$

$$= i\hbar \langle \psi | \hat{U}^\dagger \frac{d}{dt} (\hat{U} |\psi\rangle) - \langle \psi | \hat{U}^\dagger \left(\hat{U} \hat{H} \hat{U}^\dagger - i\hbar \hat{U} \frac{d\hat{U}^\dagger}{dt} \right) \hat{U} |\psi\rangle \quad (8.6.47)$$

$$= i\hbar \langle \psi | \hat{U}^\dagger \frac{d\hat{U}}{dt} |\psi\rangle + i\hbar \langle \psi | \hat{U}^\dagger \hat{U} |\dot{\psi}\rangle - \langle \psi | \hat{H} | \psi \rangle + i\hbar \langle \psi | \frac{d\hat{U}^\dagger}{dt} \hat{U} |\psi\rangle \quad (8.6.48)$$

$$= \mathcal{L} + i\hbar \langle \psi | \frac{d}{dt} (\hat{U}^\dagger \hat{U}) | \psi \rangle = \mathcal{L}. \quad (8.6.49)$$

So, the interacting theory of the wavefunction with the electromagnetic potentials still has exactly the same gauge symmetry. Under the gauge symmetry, ψ is multiplied by a spacetime dependent phase. The group of

complex numbers with magnitude 1 under the operation of multiplication is called $U(1)$ where U is for unitary and 1 is for 1 dimensional in the sense that you could think of a complex number as a 1×1 matrix. Thus, complex numbers of magnitude 1 are 1×1 unitary matrices. Further, this symmetry is a local symmetry in the sense that we can pick the phase independently at each point in space and time. Because of this, we say that this theory has a **local $U(1)$ gauge symmetry** and we call the potentials the $U(1)$ gauge field. Notice that while the gradient of ψ picks up an extra term under this transformation due to differentiating the phase, the combination of $\hat{p} - q\vec{A}$ does not. This motivates defining what is called the **gauge covariant derivative**:

$$\vec{\mathcal{D}}\psi \stackrel{\text{def}}{=} \left(\nabla - \frac{i}{\hbar} q \vec{A} \right) \psi \quad (8.6.50)$$

$$\implies (\vec{\mathcal{D}}\psi)' = \left(\nabla - \frac{i}{\hbar} q \vec{A}' \right) \psi' = \left(\nabla - \frac{i}{\hbar} q \vec{A} - \frac{i}{\hbar} q \nabla f \right) e^{\frac{iq}{\hbar} f} \psi = e^{\frac{iq}{\hbar} f} \vec{\mathcal{D}}\psi. \quad (8.6.51)$$

So, $\vec{\mathcal{D}}\psi$ transforms the same way ψ does under a gauge transformation. As well, we can define a gauge covariant time derivative with the same transformation property:

$$\mathcal{D}_t\psi \stackrel{\text{def}}{=} \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} q \phi \right) \psi \quad (8.6.52)$$

$$\implies (\mathcal{D}_t\psi)' = \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} q \phi' \right) \psi' = \left(\frac{\partial}{\partial t} + \frac{i}{\hbar} q \phi - \frac{i}{\hbar} q \frac{\partial f}{\partial t} \right) e^{\frac{iq}{\hbar} f} \psi = e^{\frac{iq}{\hbar} f} \mathcal{D}_t\psi. \quad (8.6.53)$$

With this our equation of motion can be written quite nicely as:

$$i\hbar\mathcal{D}_t\psi = -\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi. \quad (8.6.54)$$

The notation $\vec{\mathcal{D}}^2$ here means $\vec{\mathcal{D}} \cdot \vec{\mathcal{D}}$. This equation of motion is easy to remember as it is just the equation of motion for a free particle (meaning potentials vanishing) but all the derivatives are then replaced with gauge covariant derivatives.

We can write our Lagrangian explicitly in the position basis as:

$$\mathcal{L} = \int_{\mathbb{S}} \left(i\hbar\psi^*\dot{\psi} - \psi^* \left(\frac{(-i\hbar\nabla - q\vec{A})^2}{2m} + q\phi \right) \psi \right) d\mathbb{S} \quad (8.6.55)$$

$$= \int_{\mathbb{S}} \left(\frac{i}{2}\hbar\psi^*\dot{\psi} + \frac{i}{2}\hbar\dot{\psi}^*\psi - \psi^* \frac{-\hbar^2\nabla^2\psi + i\hbar q\nabla \cdot (\vec{A}\psi) + i\hbar q\vec{A} \cdot \nabla\psi + q^2|\vec{A}|^2\psi}{2m} \psi - q\psi^*\psi\phi \right) d\mathbb{S} \quad (8.6.56)$$

$$= \int_{\mathbb{S}} \left(\frac{i\hbar}{2}(\psi^*\dot{\psi} - \dot{\psi}^*\psi + 2\partial_t(\psi^*\psi)) - \frac{\hbar^2\nabla\psi^* \cdot \nabla\psi}{2m} + \frac{i\hbar q}{2m}(\nabla\psi^* \cdot \vec{A}\psi - \psi^*\vec{A} \cdot \nabla\psi) - \frac{q^2}{2m}|\vec{A}|^2|\psi|^2 - q|\psi|^2\phi \right) d\mathbb{S} \quad (8.6.57)$$

$$= \int_{\mathbb{S}} \left(\frac{i\hbar}{2}\psi^* \left(\dot{\psi} + \frac{i}{\hbar} q\phi\psi \right) - \frac{i\hbar}{2} \left(\dot{\psi}^* - \frac{i}{\hbar} q\phi\psi^* \right) \psi - \frac{\hbar^2 (\nabla + iq\vec{A})\psi^* \cdot (\nabla - iq\vec{A})\psi}{2m} \right) d\mathbb{S} + \frac{d}{dt}(i\hbar\langle\psi|\psi\rangle) \quad (8.6.58)$$

$$\simeq \int_{\mathbb{S}} \left(-\hbar\text{Im}(\psi^*\mathcal{D}_t\psi) - \frac{\hbar^2}{2m}|\vec{\mathcal{D}}\psi|^2 \right) d\mathbb{S}. \quad (8.6.59)$$

Therefore we have:

Theorem 8.10: Galilean Schrödinger Scalar with Gauge Theory

The Lagrangian density for a scalar Galilean Schrödinger field experiencing the electromagnetic potentials is:

$$\mathcal{L} = -\hbar\text{Im}(\psi^*\mathcal{D}_t\psi) - \frac{\hbar^2}{2m}|\vec{\mathcal{D}}\psi|^2 \quad (8.6.60)$$

where $\mathcal{D}_t\psi = (\partial_t + \frac{iq}{\hbar}\phi)\psi$ and $\vec{\mathcal{D}}\psi = (\nabla - \frac{iq}{\hbar}\vec{A})\psi$ are the gauge covariant derivatives. This theory has local U(1) symmetry:

$$\psi' = e^{\frac{iq}{\hbar}f(t,\vec{x})}\psi, \quad \vec{A}' = \vec{A} + \nabla f, \quad \phi' = \phi - \frac{\partial f}{\partial t}. \quad (8.6.61)$$

8.6.2 Gauge Transformation Geometry

The local U(1) symmetry has a very nice geometric interpretation. At each point in spacetime, $\psi(t, \vec{x})$ is a complex number. A complex number $a + ib$ may be viewed as a vector in the plane with coordinates (a, b) , thus identifying 1 and i with the unit vectors $(1, 0)$ and $(0, 1)$. Such a vector can also be understood as having a magnitude r and being rotated an angle θ counterclockwise from the vector $(1, 0)$. When two complex numbers are multiplied, the result has magnitude given by the product of their magnitudes and angle relative to $(1, 0)$ given by the sum of their individual angles. Thus, multiplying a complex number by $e^{i\theta}$ simply rotates that vector by an angle θ in the complex plane. So, our gauge transformation can be seen as us having the freedom to rotate $\psi(t, \vec{x})$ independently in the complex plane at each moment in time and point in space by an angle $\frac{q}{\hbar}f(t, \vec{x})$ provided we simultaneously change $\vec{A}$ and ϕ in the described way. Imagine a Hilbert space $\mathbb{V}$ isomorphic to the complex plane but with a copy at each time and point in space so that we have $\mathbb{V}(t, \vec{x})$. For each $(t, \vec{x})$, $\mathbb{V}(t, \vec{x})$ is then a two dimensional real vector space to which we can identify two orthonormal basis vectors $\vec{\xi}_1(t, \vec{x})$ and $\vec{\xi}_2(t, \vec{x})$:

$$\vec{\xi}_1 \cdot \vec{\xi}_1 = 1, \quad \vec{\xi}_1 \cdot \vec{\xi}_2 = 0, \quad \vec{\xi}_2 \cdot \vec{\xi}_2 = 1 \quad (8.6.62)$$

where these inner products are taken with both vectors at the same $(t, \vec{x})$ as for different $(t, \vec{x})$ the vectors are in different vector spaces and so their inner products are not defined. We can consider the wavefunction $\Psi(t, \vec{x})$ as being for each point in space and time an element of the corresponding vector space $\mathbb{V}(t, \vec{x})$. In that space it will have two real components $\psi_1(t, \vec{x})$ and $\psi_2(t, \vec{x})$ so that:

$$\Psi(t, \vec{x}) = \psi_1(t, \vec{x})\vec{\xi}_1(t, \vec{x}) + \psi_2(t, \vec{x})\vec{\xi}_2(t, \vec{x}). \quad (8.6.63)$$

Here we define ψ_1 and ψ_2 to be real and related to our usual complex valued wavefunction by:

$$\psi(t, \vec{x}) = \frac{\psi_1(t, \vec{x}) + i\psi_2(t, \vec{x})}{\sqrt{2}} \quad (8.6.64)$$

with the $\sqrt{2}$ just being a nice convention. Under our U(1) transformation:

$$\psi'(t, \vec{x}) = e^{\frac{iq}{\hbar}f(t, \vec{x})}\psi(t, \vec{x}) \quad (8.6.65)$$

$$\implies \frac{\psi'_1(t, \vec{x}) + i\psi'_2(t, \vec{x})}{\sqrt{2}} = \left(\cos\left(\frac{qf}{\hbar}\right) + i \sin\left(\frac{qf}{\hbar}\right) \right) \frac{\psi_1(t, \vec{x}) + i\psi_2(t, \vec{x})}{\sqrt{2}} \quad (8.6.66)$$

$$\implies \psi'_1 = \psi_1 \cos\left(\frac{qf}{\hbar}\right) - \psi_2 \sin\left(\frac{qf}{\hbar}\right), \quad \psi'_2 = \psi_1 \sin\left(\frac{qf}{\hbar}\right) + \psi_2 \cos\left(\frac{qf}{\hbar}\right). \quad (8.6.67)$$

Now you can see plainly that this is a rotation. We can invert these to identify:

$$\psi_1 = \psi'_1 \cos\left(\frac{qf}{\hbar}\right) + \psi'_2 \sin\left(\frac{qf}{\hbar}\right), \quad \psi_2 = -\psi'_1 \sin\left(\frac{qf}{\hbar}\right) + \psi'_2 \cos\left(\frac{qf}{\hbar}\right). \quad (8.6.68)$$

If under the U(1) transformation we also require our basis vectors $\vec{\xi}_1$ and $\vec{\xi}_2$ to transform so that the Ψ is unchanged we have:

$$\Psi' \stackrel{!}{=} \Psi \quad (8.6.69)$$

$$\implies \psi'_1 \vec{\xi}'_1 + \psi'_2 \vec{\xi}'_2 = \psi_1 \vec{\xi}_1 + \psi_2 \vec{\xi}_2 \quad (8.6.70)$$

$$= \psi'_1 \left(\cos\left(\frac{qf}{\hbar}\right) \vec{\xi}_1 - \sin\left(\frac{qf}{\hbar}\right) \vec{\xi}_2 \right) + \psi'_2 \left(\sin\left(\frac{qf}{\hbar}\right) \vec{\xi}_1 + \cos\left(\frac{qf}{\hbar}\right) \vec{\xi}_2 \right). \quad (8.6.71)$$

Because this holds regardless of the values of ψ'_1 and ψ'_2 :

$$\vec{\xi}'_1 = \cos\left(\frac{qf}{\hbar}\right) \vec{\xi}_1 - \sin\left(\frac{qf}{\hbar}\right) \vec{\xi}_2, \quad \vec{\xi}'_2 = \sin\left(\frac{qf}{\hbar}\right) \vec{\xi}_1 + \cos\left(\frac{qf}{\hbar}\right) \vec{\xi}_2. \quad (8.6.72)$$

In this view the gauge transformation is simply a change of basis of the internal space $\mathbb{V}(t, \vec{x})$. We transform our basis vectors $\vec{\xi}_1$ and $\vec{\xi}_2$ and components ψ_1 and ψ_2 together in such a way that the actual geometric object they contribute to, Ψ , is unchanged. The ability to choose our basis vectors independently at each point in time and space just means that there is no preferred basis of the internal space. Thus, gauge symmetry really just corresponds to an internal rotational symmetry within the internal space $\mathbb{V}$. We can identify here that the rotation angle applied on the internal space by a gauge transformation is just $\frac{qf}{\hbar}$. One can see immediately that our inner product conditions in (8.6.62) are preserved by gauge transformation, since it is just a rotation.

Now that we are thinking of the wavefunction at $(t, \vec{x})$ as an element of vector space $\mathbb{V}(t, \vec{x})$ where for each $(t, \vec{x})$ it is a different vector space, it is not meaningful to form linear combinations from $\Psi(t, \vec{x})$ at different values of $(t, \vec{x})$ from each other. (We are free to choose the basis elements at each $(t, \vec{x})$ and so adding Ψ 's at different $(t, \vec{x})$ mixes multiple independent choices of basis in a way that does not have any simple transformation property.) Consequently, it is not obvious how to define a meaningful notion of spatial or time derivative of Ψ . One would usually define a time derivative to be given by the difference quotient:

$$\frac{\partial \Psi}{\partial t} \stackrel{?}{=} \lim_{\varepsilon \rightarrow 0} \frac{\Psi(t + \varepsilon, \vec{x}) - \Psi(t, \vec{x})}{\varepsilon}. \quad (8.6.73)$$

However, $\Psi(t + \varepsilon, \vec{x}) \in \mathbb{V}(t + \varepsilon, \vec{x})$ while $\Psi(t, \vec{x}) \in \mathbb{V}(t, \vec{x})$ which are different vector spaces and so the difference $\Psi(t + \varepsilon, \vec{x}) - \Psi(t, \vec{x})$ is not actually defined and not apparently geometrically meaningful. This mathematically exactly like how in general relativity it is not meaningful to form linear combinations from tangent spaces at different spacetime points. The solution to this problem will also be exactly like in general relativity. In order to make a meaningful notion of the derivative we need to somehow put the two pieces of this difference in the same vector space. Let us assume we have some way of doing so. That is, let us assume we have a map $\Upsilon(\Psi, t, \vec{x}, t', \vec{x}')$ which acts on $\Psi(t, \vec{x}) \in \mathbb{V}(t, \vec{x})$ and gives us an element of $\mathbb{V}(t', \vec{x}')$. Such a map is also called a “parallel transport” as it gives a canonical way of “transporting” vectors from one place to another. Since we will use this map to define a derivative and a derivative only requires subtraction at nearby points, we only need this map to be able to transport between points $(t, \vec{x})$ and $(t', \vec{x}')$ which are sufficiently close to each other, not necessarily arbitrarily far away. Then, in a difference quotient we could use this map to transport $\Psi(t + \varepsilon, \vec{x})$ from $\mathbb{V}(t + \varepsilon, \vec{x})$ into a vector in $\mathbb{V}(t, \vec{x})$ so that we can define a derivative. Because this parallel transport acts on a vector space with an inner product, we require it respects the linearity of the vector space as well as its inner product in the sense that we demand the parallel transport be linear and that the inner product of two transported vectors is the same as the inner product of the untransported vectors (this is what is meant by the “parallel” in the parallel transport):

$$\Upsilon(a\vec{\xi}_1 + b\vec{\xi}_2, t, \vec{x}, t', \vec{x}') = a\Upsilon(\vec{\xi}_1, t, \vec{x}, t', \vec{x}') + b\Upsilon(\vec{\xi}_2, t, \vec{x}, t', \vec{x}') \quad (8.6.74)$$

$$\Upsilon(\Psi_1, t, \vec{x}, t', \vec{x}') \cdot \Upsilon(\Psi_2, t, \vec{x}, t', \vec{x}') = \Psi_1(t, \vec{x}) \cdot \Psi_2(t, \vec{x}). \quad (8.6.75)$$

Then, while the expression given in equation (8.6.73) is not defined, we can modify it to define the covariant time and space derivatives as the difference quotients with our parallel transported vectors:

$$\mathcal{D}_t \Psi \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(\Psi(t + \varepsilon, \vec{x}), t + \varepsilon, \vec{x}, t, \vec{x}) - \Psi(t, \vec{x})}{\varepsilon} \quad (8.6.76)$$

$$\mathcal{D}_a \Psi \stackrel{\text{def}}{=} \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(\Psi(t, \vec{x} + \varepsilon \vec{a}), t, \vec{x} + \varepsilon \vec{a}, t, \vec{x}) - \Psi(t, \vec{x})}{\varepsilon}. \quad (8.6.77)$$

Or, using our component expression for $\Psi(t, \vec{x})$:

$$\mathcal{D}_t \Psi = \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon\left(\sum_{n=1}^2 \psi_n(t + \varepsilon, \vec{x}) \vec{\xi}_n(t + \varepsilon, \vec{x}), t + \varepsilon, \vec{x}, t, \vec{x}\right) - \sum_{n=1}^2 \psi_n(t, \vec{x}) \vec{\xi}_n(t, \vec{x})}{\varepsilon} \quad (8.6.78)$$

$$= \sum_{n=1}^2 \lim_{\varepsilon \rightarrow 0} \left(\frac{\psi_n(t + \varepsilon, \vec{x}) - \psi_n(t, \vec{x})}{\varepsilon} \Upsilon(\vec{\xi}_n(t + \varepsilon, \vec{x}), t + \varepsilon, \vec{x}, t, \vec{x}) + \psi_n(t, \vec{x}) \frac{\Upsilon(\vec{\xi}_n(t + \varepsilon, \vec{x}), t + \varepsilon, \vec{x}, t, \vec{x}) - \vec{\xi}_n(t, \vec{x})}{\varepsilon} \right) \quad (8.6.79)$$

$$= \sum_{n=1}^2 \left(\frac{\partial \psi_n}{\partial t}(t, \vec{x}) \vec{\xi}_n(t, \vec{x}) + \psi_n(t, \vec{x}) \mathcal{D}_t \vec{\xi}_n \right). \quad (8.6.80)$$

Here we used that $\Upsilon(\vec{\xi}_n(t, \vec{x}), t, \vec{x}, t, \vec{x}) = \vec{\xi}_n(t, \vec{x})$ as when the initial and final points are the same no transport has occurred and thus Υ becomes just the identity map. The same calculation for spatial derivatives predictably gives:

$$\mathcal{D}_a \Psi = \sum_{n=1}^2 \left(\frac{\partial \psi_n}{\partial x^a}(t, \vec{x}) \vec{\xi}_n(t, \vec{x}) + \psi_n(t, \vec{x}) \mathcal{D}_a \vec{\xi}_n \right). \quad (8.6.81)$$

This notion of covariant derivative is the closest possible notion we can define to ordinary differentiation due to the need to somehow put the Ψ 's at different locations in the same vector space. We can see from the component expressions for the covariant derivative that because of linearity, if we know how to take the covariant derivative of the basis vectors we can immediately take the covariant derivative of Ψ . Thinking about the covariant derivative of the basis vectors:

$$\mathcal{D}_t \vec{\xi}_n = \lim_{\varepsilon \rightarrow 0} \frac{\Upsilon(\vec{\xi}_n(t + \varepsilon, \vec{x}), t + \varepsilon, \vec{x}, t, \vec{x}) - \vec{\xi}_n(t, \vec{x})}{\varepsilon} \quad (8.6.82)$$

we can see that the difference quotient is the difference of two vectors in $\mathbb{V}(t, \vec{x})$ and so is a vector in $\mathbb{V}(t, \vec{x})$. Thus, the covariant derivative of any of the basis vectors in $\mathbb{V}(t, \vec{x})$ is also in $\mathbb{V}(t, \vec{x})$ and thus can be expressed, for some coefficients, as a linear combination of the basis vectors of $\mathbb{V}(t, \vec{x})$:

$$\mathcal{D}_t \vec{\xi}_n = \sum_{m=1}^2 \Gamma_{nt}^m(t, \vec{x}) \vec{\xi}_m(t, \vec{x}), \quad \mathcal{D}_a \vec{\xi}_n = \sum_{m=1}^2 \Gamma_{na}^m(t, \vec{x}) \vec{\xi}_m(t, \vec{x}). \quad (8.6.83)$$

These Γ_{nt}^m , Γ_{na}^m are called the “connection coefficients”, in precise analogy with general relativity. Because the connection coefficients specify how to differentiate the basis vectors and doing so specifies the covariant derivative fully, these connection coefficients allow us to “connect” the internal spaces at different points and times. $\mathcal{D}_t \Psi$ (or $\mathcal{D}_a \Psi$) is an element of $\mathbb{V}(t, \vec{x})$ and so we can identify the components $\mathcal{D}_t \psi_1$ and $\mathcal{D}_t \psi_2$ as:

$$\mathcal{D}_t \Psi = (\mathcal{D}_t \psi_1) \vec{\xi}_1 + (\mathcal{D}_t \psi_2) \vec{\xi}_2, \quad \mathcal{D}_a \Psi = (\mathcal{D}_a \psi_1) \vec{\xi}_1 + (\mathcal{D}_a \psi_2) \vec{\xi}_2 \quad (8.6.84)$$

$$\implies \mathcal{D}_t \psi_1 = \frac{\partial \psi_1}{\partial t} + \Gamma_{1t}^1 \psi_1 + \Gamma_{2t}^1 \psi_2, \quad \mathcal{D}_a \psi_1 = \frac{\partial \psi_1}{\partial x^a} + \Gamma_{1a}^1 \psi_1 + \Gamma_{2a}^1 \psi_2 \quad (8.6.85)$$

$$\implies \mathcal{D}_t \psi_2 = \frac{\partial \psi_2}{\partial t} + \Gamma_{1t}^2 \psi_1 + \Gamma_{2t}^2 \psi_2, \quad \mathcal{D}_a \psi_2 = \frac{\partial \psi_2}{\partial x^a} + \Gamma_{1a}^2 \psi_1 + \Gamma_{2a}^2 \psi_2 \quad (8.6.86)$$

Because our parallel transformation map preserves the inner product, it preserves the orthonormality of our basis vectors and thus the $\vec{\xi}_n(t', \vec{x}')$ are simply some linear combination of the $\Upsilon(\vec{\xi}_n(t, \vec{x}), t, \vec{x}, t', \vec{x}')$ which preserves the inner product:

$$\vec{\xi}_1(t', \vec{x}') = \alpha(t, \vec{x}, t', \vec{x}') \Upsilon(\vec{\xi}_1) + \beta(t, \vec{x}, t', \vec{x}') \Upsilon(\vec{\xi}_2) \quad (8.6.87)$$

$$\vec{\xi}_2(t', \vec{x}') = \gamma(t, \vec{x}, t', \vec{x}') \Upsilon(\vec{\xi}_1) + \lambda(t, \vec{x}, t', \vec{x}') \Upsilon(\vec{\xi}_2). \quad (8.6.88)$$

Then:

$$\vec{\xi}_1(t', \vec{x}') \cdot \vec{\xi}_1(t', \vec{x}') = \alpha^2 + \beta^2 \stackrel{!}{=} 1. \quad (8.6.89)$$

So, we can define an angle $\theta(t, \vec{x}, t', \vec{x}')$ such that:

$$\alpha = \cos \theta, \quad \beta = -\sin \theta. \quad (8.6.90)$$

The remaining orthonormality conditions then give:

$$\vec{\xi}_1(t', \vec{x}') \cdot \vec{\xi}_2(t', \vec{x}') = \alpha\gamma + \lambda\beta \stackrel{!}{=} 0 \implies \gamma = \lambda \tan \theta \quad (8.6.91)$$

$$\vec{\xi}_2(t', \vec{x}') \cdot \vec{\xi}_2(t', \vec{x}') = \gamma^2 + \lambda^2 = \frac{\lambda^2}{\cos^2 \theta} \stackrel{!}{=} 1 \implies \lambda = \pm \cos \theta. \quad (8.6.92)$$

When $t' = t$ and $\vec{x}' = \vec{x}$ we should have $\alpha = \lambda = 1$ and $\beta = \gamma = 0$ as in the case no transportation has occurred. From here we see that $\alpha = \pm \lambda$ and so because the parallel transport must be continuous in order for us to define differentiation we need to take $\lambda = \alpha$ (as $\lambda = \alpha$ when no transportation occurs and there is no way to change continuously from $\lambda = \alpha$ to $\lambda = -\alpha$ if $\alpha \neq 0$) and thus:

$$\vec{\xi}_1(t', \vec{x}') = \cos \theta \Upsilon(\vec{\xi}_1) - \sin \theta \Upsilon(\vec{\xi}_2) \quad (8.6.93)$$

$$\vec{\xi}_2(t', \vec{x}') = \sin \theta \Upsilon(\vec{\xi}_1) + \cos \theta \Upsilon(\vec{\xi}_2). \quad (8.6.94)$$

As well, we then have that $\theta(t, \vec{x}, t, \vec{x}) = 0$. Using the difference quotient definition of the covariant derivative:

$$\mathcal{D}_t \xi_1 = - \left. \frac{\partial \theta}{\partial t'} \right|_{(t', \vec{x}')=(t, \vec{x})} \vec{\xi}_2, \quad \mathcal{D}_a \xi_1 = - \left. \frac{\partial \theta}{\partial x'^a} \right|_{(t', \vec{x}')=(t, \vec{x})} \vec{\xi}_2 \quad (8.6.95)$$

$$\mathcal{D}_t \xi_2 = \left. \frac{\partial \theta}{\partial t'} \right|_{(t', \vec{x}')=(t, \vec{x})} \vec{\xi}_1, \quad \mathcal{D}_a \xi_2 = \left. \frac{\partial \theta}{\partial x'^a} \right|_{(t', \vec{x}')=(t, \vec{x})} \vec{\xi}_1. \quad (8.6.96)$$

Let us define then:

$$\phi(t, \vec{x}) = - \frac{\hbar}{q} \left. \frac{\partial \theta}{\partial t'} (t, \vec{x}, t', \vec{x}') \right|_{(t', \vec{x}')=(t, \vec{x})}, \quad A_a(t, \vec{x}) = \left. \frac{\hbar}{q} \frac{\partial \theta}{\partial x'^a} (t, \vec{x}, t', \vec{x}') \right|_{(t', \vec{x}')=(t, \vec{x})} \quad (8.6.97)$$

so that:

$$\mathcal{D}_t \xi_1 = \frac{q}{\hbar} \phi(t, \vec{x}) \vec{\xi}_2, \quad \mathcal{D}_a \xi_1 = - \frac{q}{\hbar} A_a(t, \vec{x}) \vec{\xi}_2 \quad (8.6.98)$$

$$\mathcal{D}_t \xi_2 = - \frac{q}{\hbar} \phi(t, \vec{x}) \vec{\xi}_1, \quad \mathcal{D}_a \xi_2 = \frac{q}{\hbar} A_a(t, \vec{x}) \vec{\xi}_1. \quad (8.6.99)$$

Then, we can actually see that our connection coefficients are given by:

$$\begin{pmatrix} \Gamma^1_{1t} & \Gamma^1_{2t} \\ \Gamma^2_{1t} & \Gamma^2_{2t} \end{pmatrix} = \frac{q}{\hbar} \phi(t, \vec{x}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} \Gamma^1_{1a} & \Gamma^1_{2a} \\ \Gamma^2_{1a} & \Gamma^2_{2a} \end{pmatrix} = - \frac{q}{\hbar} A_a(t, \vec{x}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (8.6.100)$$

The component expressions for our covariant derivative then become:

$$\mathcal{D}_t \psi_1 = \frac{\partial \psi_1}{\partial t} - \frac{q}{\hbar} \phi \psi_2, \quad \mathcal{D}_a \psi_1 = \frac{\partial \psi_1}{\partial x^a} + \frac{q}{\hbar} A_a \psi_2 \quad (8.6.101)$$

$$\mathcal{D}_t \psi_2 = \frac{\partial \psi_2}{\partial t} + \frac{q}{\hbar} \phi \psi_1, \quad \mathcal{D}_a \psi_2 = \frac{\partial \psi_2}{\partial x^a} - \frac{q}{\hbar} A_a \psi_1. \quad (8.6.102)$$

Computing then the covariant derivative for the complex wavefunction ψ defined in (8.6.64) gives:

$$\mathcal{D}_t \psi = \frac{\partial \psi}{\partial t} + i \frac{q}{\hbar} \phi \psi, \quad \mathcal{D}_a \psi = \frac{\partial \psi}{\partial x^a} - i \frac{q}{\hbar} A_a \psi \quad (8.6.103)$$

which is precisely the original definition of gauge covariant differentiation. As such, we can understand the scalar and vector potentials as defining the connection on the internal space on which Ψ lives, the complex wavefunction ψ as the component representation of Ψ , and the gauge transformation as a local change of basis on the internal space.

Consider the definitions given above for the scalar and vector potentials when a gauge transformation is applied. Combining how the basis vectors transform under a gauge transformation and how they are parallel transported,

$$\begin{pmatrix} \vec{\xi}'_1(t', \vec{x}') \\ \vec{\xi}'_2(t', \vec{x}') \end{pmatrix} = \begin{pmatrix} \cos\left(\frac{qf'}{\hbar}\right) & -\sin\left(\frac{qf'}{\hbar}\right) \\ \sin\left(\frac{qf'}{\hbar}\right) & \cos\left(\frac{qf'}{\hbar}\right) \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\left(\frac{qf}{\hbar}\right) & \sin\left(\frac{qf}{\hbar}\right) \\ -\sin\left(\frac{qf}{\hbar}\right) & \cos\left(\frac{qf}{\hbar}\right) \end{pmatrix} \begin{pmatrix} \Upsilon(\vec{\xi}'_1(t, \vec{x})) \\ \Upsilon(\vec{\xi}'_2(t, \vec{x})) \end{pmatrix} \quad (8.6.104)$$

$$= \begin{pmatrix} \cos\left(\theta + \frac{q}{\hbar} f(t', \vec{x}') - \frac{q}{\hbar} f(t, \vec{x})\right) & -\sin\left(\theta + \frac{q}{\hbar} f(t', \vec{x}') - \frac{q}{\hbar} f(t, \vec{x})\right) \\ \sin\left(\theta + \frac{q}{\hbar} f(t', \vec{x}') - \frac{q}{\hbar} f(t, \vec{x})\right) & \cos\left(\theta + \frac{q}{\hbar} f(t', \vec{x}') - \frac{q}{\hbar} f(t, \vec{x})\right) \end{pmatrix} \begin{pmatrix} \Upsilon(\vec{\xi}'_1(t, \vec{x})) \\ \Upsilon(\vec{\xi}'_2(t, \vec{x})) \end{pmatrix}. \quad (8.6.105)$$

Above $f' = f(t', \vec{x}')$ and $f = f(t, \vec{x})$ as a shorthand. Therefore under a gauge transformation:

$$\theta'(t, \vec{x}, t', \vec{x}') = \theta(t, \vec{x}, t', \vec{x}') + \frac{q}{\hbar} f(t', \vec{x}') - \frac{q}{\hbar} f(t, \vec{x}). \quad (8.6.106)$$

Automatically from (8.6.97):

$$\phi'(t, \vec{x}) = \phi(t, \vec{x}) - \frac{\partial f}{\partial t}, \quad \vec{A}'(t, \vec{x}) = \vec{A}(t, \vec{x}) + \nabla f \quad (8.6.107)$$

which is again our familiar gauge transformation for the potentials.

The scalar and vector potentials are determined by the connection coefficients $\Gamma^m_{n\mu}$ which are in turn determined by the parallel transport map Υ . Therefore, the scalar and vector potentials really just tell us geometric information about how to move between the different $\mathbb{V}(t, \vec{x})$ as we change $(t, \vec{x})$. The collection of vector spaces $\mathbb{V}(t, \vec{x})$ among all $(t, \vec{x})$ together with the parallel transport map is called a vector bundle $\mathcal{V}$. ϕ and $\vec{A}$ are said to provide the connection on that vector bundle. Because we can now literally see the gauge transformation properties of the potentials as arising entirely from our ability to freely choose

our basis vectors for $\mathbb{V}(t, \vec{x})$ at each $(t, \vec{x})$, we can further see that the outdated view that one sometimes encounters that the potentials are unphysical is as ridiculous as claiming that all vectors are unphysical because their components are basis dependent. The components of all vectors are not uniquely defined because I can choose my coordinate axes to be whatever I want! Similarly, the potentials are not uniquely defined because I can choose the axes of $\mathbb{V}(t, \vec{x})$ to be whatever I want. But, not uniquely defined is not the same as unphysical. While the x component v_x of a vector $\vec{v}$ is not uniquely defined it does contain information that may be physical as it is necessary to compute $|\vec{v}|$ which is uniquely defined under changes of your coordinate axes. Similarly, while the numerical value of the potentials at a particular $(t, \vec{x})$ is not uniquely defined, the set of values of the potentials carries all of the physical information of electromagnetism! Altogether, the electromagnetic potentials are exactly mathematically analogous to the Christoffel symbols of general relativity. The only difference is that in general relativity the space $\mathbb{V}(t, \vec{x})$ is the tangent space of the spacetime manifold while in electromagnetism it is a copy of the complex plane.

One may be worried that there is more to the geometry of the vector bundle $\mathcal{V}$ than what is in the connection. However, knowing the connection is actually enough to determine the entire parallel transport map. Consider a path $(t(\lambda), \vec{x}(\lambda))$ parameterized by a real parameter λ through spacetime. Given a vector $\vec{v} \in \mathbb{V}(t(\lambda), \vec{x}(\lambda))$ at a particular λ , we can define a new vector $\vec{v}'$ at $\mathbb{V}(t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon))$ for small ε by parallel transporting $\vec{v}$ slightly:

$$\vec{v}' = \Upsilon(\vec{v}, t(\lambda), \vec{x}(\lambda), t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon)). \quad (8.6.108)$$

If we call $\vec{v}$ now $\vec{v}(\lambda)$ we can use the above to define a new vector $\vec{v}(\lambda + \varepsilon) \in \mathbb{V}(t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon))$ as how $\vec{v}$ is parallel transported. Parallel transporting from $(t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon))$ to $(t(\lambda), \vec{x}(\lambda))$ is the inverse of parallel transporting from $(t(\lambda), \vec{x}(\lambda))$ to $(t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon))$. So, parallel transporting both sides above back to to $(t(\lambda), \vec{x}(\lambda))$:

$$\Upsilon(\vec{v}(\lambda + \varepsilon), t(\lambda + \varepsilon), \vec{x}(\lambda + \varepsilon), t(\lambda), \vec{x}(\lambda)) = \vec{v}(\lambda). \quad (8.6.109)$$

Now this is always an equation within $\mathbb{V}(t(\lambda), \vec{x}(\lambda))$ and so we can differentiate both sides with respect to ε . Using our definition of covariant differentiation, we have:

$$\sum_{n=1}^2 \left(\frac{dv_n}{d\lambda} \vec{\xi}_n + v_n \left(\frac{dt}{d\lambda} \mathcal{D}_t \vec{\xi}_n + \frac{dx^a}{d\lambda} \mathcal{D}_a \vec{\xi}_n \right) \right) = 0. \quad (8.6.110)$$

In analogy with (8.6.64) we can define the complex function $v(\lambda)$ by:

$$v(\lambda) = \frac{v_1(\lambda) + iv_2(\lambda)}{\sqrt{2}} \quad (8.6.111)$$

which then contains full information about $\vec{v}(\lambda)$. In terms of the potentials then, the parallel transport equation for v becomes:

$$\frac{dv}{d\lambda} = i \frac{q}{\hbar} \left(-\frac{dt}{d\lambda} \phi + \frac{dx^a}{d\lambda} A_a \right) v(\lambda). \quad (8.6.112)$$

This differential equation thus determines the parallel transport of our arbitrary vector along an arbitrary curve. Conveniently, this differential equation can be solved directly. Let γ be a path through spacetime given by a curve $(t(\lambda), \vec{x}(\lambda))$. Let v_0 be the complex value of our vector at the initial point on γ and let v_f be the complex value of our vector at the final point on γ when v_0 has been parallel transported along γ . Then, define the angle $\theta[\gamma]$:

$$\theta[\gamma] = \frac{q}{\hbar} \int_{\gamma} \left(-\frac{dt}{d\lambda} \phi(t(\lambda), \vec{x}(\lambda)) + \frac{d\vec{x}}{d\lambda} \cdot \vec{A}(t(\lambda), \vec{x}(\lambda)) \right) d\lambda. \quad (8.6.113)$$

The solution to the parallel transport equation is then:

$$v_f = e^{i\theta[\gamma]} v_0. \quad (8.6.114)$$

Therefore under parallel transport the vector transported simply picks up a phase given by the above integral. For a general path of finite size this phase generically depends on the whole path and not simply the end points. Because of this, the parallel transport map $\Upsilon(v, t, \vec{x}, t', \vec{x}')$ as written before is only defined for $(t, \vec{x})$ and $(t', \vec{x}')$ which are within a small neighborhood of each other. This is perfectly alright as for all calculations so far we have only used Υ for when $(t, \vec{x})$ and $(t', \vec{x}')$ differed by ε . In general the parallel transport map should be written $\Upsilon(v)[\gamma]$ for a path $\gamma(\lambda) = (t(\lambda), \vec{x}(\lambda))$ which begins at $(t, \vec{x})$ and ends at $(t', \vec{x}')$. Similarly, the angle previously written as $\theta(t, \vec{x}, t', \vec{x}')$ should in general be replaced by the above $\theta[\gamma]$. Using that angle we find that the parallel transport map along an arbitrary curve of finite length which starts at $(t, \vec{x})$ and

ends at $(t', \vec{x}')$ is given by:

$$\xi_1(t', \vec{x}') = \cos(\theta[\gamma])\Upsilon(\xi_1(t, \vec{x}))[\gamma] - \sin(\theta[\gamma])\Upsilon(\xi_2(t, \vec{x}))[\gamma] \quad (8.6.115)$$

$$\xi_2(t', \vec{x}') = \sin(\theta[\gamma])\Upsilon(\xi_1(t, \vec{x}))[\gamma] + \cos(\theta[\gamma])\Upsilon(\xi_2(t, \vec{x}))[\gamma]. \quad (8.6.116)$$

For a wavefunction $\psi(t, \vec{x})$ considered along a path $(t(\lambda), \vec{x}(\lambda))$, the λ derivative of ψ is not gauge invariant. Instead, it is useful to define covariant total λ derivative:

$$\frac{D\psi}{D\lambda} = \frac{d\psi}{d\lambda} + i\frac{q}{\hbar} \frac{dt}{d\lambda} \phi\psi - i\frac{q}{\hbar} \frac{d\vec{x}}{d\lambda} \cdot \vec{A}\psi = \frac{dt}{d\lambda} \mathcal{D}_t\psi + \frac{d\vec{x}}{d\lambda} \cdot \vec{\mathcal{D}}\psi. \quad (8.6.117)$$

With this we can see that the parallel transport equation is that a parallel transported vector's covariant total λ derivative vanishes:

$$\frac{Dv}{D\lambda} = 0. \quad (8.6.118)$$

In general relativity, parallel transporting a vector around a small loop tells us about the curvature of spacetime within that loop. By exactly the same thinking, in electromagnetism, parallel transporting a vector in $\mathcal{V}$ around a small loop tells us about the curvature of the electromagnetic vector bundle within that loop. Suppose we consider a small rectangle formed by transporting in the one direction, then a second, backward back along the first, and then backward back along the second. This is precisely the structure discussed in (1.11.25) and (7.5.13). We can see above in the parallel transport equation that the gauge covariant derivative in a direction generates parallel transport in that direction (because the spacetime we are working with at the moment is flat we don't need the final correction to close the loop needed in (7.5.13)). So, we know that the change in our vector parallel transporting along such a small rectangle will be given by the commutator of covariant derivatives in the two different directions. Therefore, the commutator of covariant derivatives at $(t, \vec{x})$ gives us a notion of the local curvature of the vector bundle $\mathcal{V}$ at $(t, \vec{x})$. Directly computing:

$$[\mathcal{D}_t, \mathcal{D}_a]\psi = \left(\frac{\partial}{\partial t} + i\frac{q}{\hbar}\phi\right) \left(\frac{\partial\psi}{\partial x^a} - i\frac{q}{\hbar}A_a\psi\right) - \left(\frac{\partial}{\partial x^a} - i\frac{q}{\hbar}A_a\right) \left(\frac{\partial\psi}{\partial t} + i\frac{q}{\hbar}\phi\psi\right) \quad (8.6.119)$$

$$= -i\frac{q}{\hbar} \left(\frac{\partial A_a}{\partial t} + \frac{\partial\phi}{\partial x^a}\right) \psi \quad (8.6.120)$$

$$= i\frac{q}{\hbar} E_a(t, \vec{x})\psi \quad (8.6.121)$$

$$[\mathcal{D}_a, \mathcal{D}_b]\psi = \left(\frac{\partial}{\partial x^a} - i\frac{q}{\hbar}A_a\right) \left(\frac{\partial\psi}{\partial x^b} - i\frac{q}{\hbar}A_b\psi\right) - \left(\frac{\partial}{\partial x^b} - i\frac{q}{\hbar}A_b\right) \left(\frac{\partial\psi}{\partial x^a} - i\frac{q}{\hbar}A_a\psi\right) \quad (8.6.122)$$

$$= -i\frac{q}{\hbar} \left(\frac{\partial A_b}{\partial x^a} - \frac{\partial A_a}{\partial x^b}\right) \psi \quad (8.6.123)$$

$$= -i\frac{q}{\hbar} \epsilon_{ab}^c B_c(t, \vec{x})\psi. \quad (8.6.124)$$

The electric and magnetic field precisely give the local curvature of $\mathcal{V}$ at $(t, \vec{x})$! The magnetic field is the curvature of $\mathcal{V}$ in spatial directions and the electric field is the curvature of $\mathcal{V}$ in the mixture of time and spatial directions. Both gravity and electromagnetism are extremely geometric theories. The Christoffel symbols in gravity are directly analogous to the potentials in electromagnetism while the Riemann curvature tensor in gravity is directly analogous to the electric and magnetic fields. In another perspective, we can view the parallel transport transformation for different paths as a Lie group of continuous transformations. Then, the covariant derivatives are a basis for the Lie algebra that generates the group. The commutator of the covariant derivatives thus gives us the structure constants of the algebra and so we see that the structure constants of parallel transport are precisely the curvature (the electric and magnetic fields) of $\mathcal{V}$.

8.6.3 Charge Conservation

The Lagrangian density in theorem 8.10 contains interactions with the electromagnetic potentials. Recall from chapter 3 when we first started looking for a Lagrangian for the potentials that the interacting part of the Lagrangian was given by equation (3.1.17):

$$\mathcal{L}_{\text{int}} = \int_{\mathbb{S}} (\vec{J} \cdot \vec{A} - \rho\phi) d\mathbb{S}. \quad (8.6.125)$$

From this we can identify:

$$\rho = -\frac{\delta \mathcal{L}_{\text{int}}}{\delta \phi}, \quad \vec{J} = \frac{\delta \mathcal{L}_{\text{int}}}{\delta \vec{A}^T}. \quad (8.6.126)$$

Using our Lagrangian density:

$$\mathcal{L} = i\hbar \psi^* \dot{\psi} - \frac{\hbar^2 \nabla \psi^* \cdot \nabla \psi}{2m} + \frac{i\hbar q}{2m} \nabla \psi^* \cdot \vec{A} \psi - \frac{i\hbar q}{2m} \psi^* \vec{A} \cdot \nabla \psi - \frac{q^2}{2m} |\vec{A}|^2 \psi^* \psi - q|\psi|^2 \phi \quad (8.6.127)$$

$$\implies \rho = -\frac{\delta \mathcal{L}_{\text{int}}}{\delta \phi} = -\frac{\partial \mathcal{L}}{\partial \phi} = q|\psi|^2 \quad (8.6.128)$$

$$\implies \vec{J} = \frac{\delta \mathcal{L}_{\text{int}}}{\delta \vec{A}^T} = \frac{\partial \mathcal{L}}{\partial \vec{A}^T} = \frac{i\hbar q}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) - \frac{q^2}{m} \vec{A} |\psi|^2. \quad (8.6.129)$$

Using the gauge covariant derivative, we can rewrite $\vec{J}$ in a nice way to find:

$$\rho(t, \vec{x}) = q|\psi(t, \vec{x})|^2, \quad \vec{J}(t, \vec{x}) = \frac{q\hbar}{m} \text{Im} \left(\psi^* \vec{\mathcal{D}} \psi \right). \quad (8.6.130)$$

We can immediately see that these charge and current densities are gauge invariant:

$$\rho' = q|\psi'|^2 = q \left| e^{i\frac{q}{\hbar} f} \psi \right|^2 = q|\psi|^2 = \rho \quad (8.6.131)$$

$$\vec{J}' = \frac{q\hbar}{m} \text{Im} \left(\psi'^* \vec{\mathcal{D}} \psi' \right) = \frac{q\hbar}{m} \text{Im} \left(e^{-i\frac{q}{\hbar} f} \psi^* e^{i\frac{q}{\hbar} f} \vec{\mathcal{D}} \psi \right) = \frac{q\hbar}{m} \text{Im} (\psi^* \vec{\mathcal{D}} \psi) = \vec{J}. \quad (8.6.132)$$

Equation (8.6.130) gives that $q|\psi|^2$ is the charge density of ψ and confirms that q is in fact the total charge of the wavefunction:

$$\text{Total Charge} = \int_{\mathbb{S}} \rho d\mathbb{S} = \int_{\mathbb{S}} q|\psi|^2 d\mathbb{S} = q \langle \psi | \psi \rangle = q. \quad (8.6.133)$$

Because we have expressions now for the charge density and current densities, we had better hope they satisfy the continuity equation. From our previous study of gauge invariance we know actually that it is guaranteed that they do from gauge symmetry. But, it is still nice to compute it explicitly:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = \frac{\partial}{\partial t} (q\psi^* \psi) + \nabla \cdot \left(\frac{i\hbar q}{2m} (\psi (\vec{\mathcal{D}} \psi)^* - \psi^* \vec{\mathcal{D}} \psi) \right) \quad (8.6.134)$$

$$= \frac{q}{i\hbar} \psi^* \left(i\hbar \mathcal{D}_t \psi + \frac{\hbar^2}{2m} \mathcal{D}^2 \psi \right) - \frac{q}{i\hbar} \left(-i\hbar \mathcal{D}_t \psi^* + \frac{\hbar^2}{2m} \mathcal{D}^2 \psi^* \right) \psi \quad (8.6.135)$$

$$= 0. \quad (8.6.136)$$

Hence we see that our charge density and current density do satisfy the continuity equation, exactly as they must.

With our formula for the charge density we can find a nice formula for the electric dipole moment of the wavefunction:

$$\vec{\rho} = \int_{\mathbb{S}} \rho \vec{x} d\mathbb{S} = \int_{\mathbb{S}} q|\psi|^2 \vec{x} d\mathbb{S} = q \langle \psi | \hat{\vec{x}} | \psi \rangle = q \langle \hat{\vec{x}} \rangle. \quad (8.6.137)$$

As well, we can find a nice formula for the magnetic dipole moment:

$$\vec{\mu} = \frac{1}{2} \int_{\mathbb{S}} \vec{x} \times \vec{J} d\mathbb{S} = \frac{q\hbar}{2m} \text{Im} \int_{\mathbb{S}} \vec{x} \times (\psi^* \vec{\mathcal{D}} \psi) d\mathbb{S} = \frac{q\hbar}{2m} \epsilon^a{}_b{}^c \vec{\tau}_a \text{Im} \int_{\mathbb{S}} x^b \psi^* \mathcal{D}_c \psi d\mathbb{S} \quad (8.6.138)$$

$$= \frac{q\hbar}{4im} \epsilon^a{}_b{}^c \vec{\tau}_a \int_{\mathbb{S}} x^b \left(\psi^* \partial_c \psi - i\frac{q}{\hbar} \psi^* A_c \psi - \partial_c \psi^* \psi - i\frac{q}{\hbar} A_c \psi^* \psi \right) d\mathbb{S} \quad (8.6.139)$$

$$= \frac{q\hbar}{4im} \epsilon^a{}_b{}^c \vec{\tau}_a \int_{\mathbb{S}} x^b \left(\psi^* \partial_c \psi - 2i\frac{q}{\hbar} \psi^* A_c \psi + \psi^* \partial_c \psi + \delta_c^b \psi^* \psi \right) d\mathbb{S} \quad (8.6.140)$$

$$= \frac{q\hbar}{2im} \epsilon^a{}_b{}^c \vec{\tau}_a \int_{\mathbb{S}} \psi^* x^b \left(\partial_c \psi - i\frac{q}{\hbar} A_c \psi \right) d\mathbb{S} \quad (8.6.141)$$

$$= \frac{q\hbar}{2im} \langle \psi | \hat{\vec{x}} \times \hat{\vec{\mathcal{D}}} | \psi \rangle \quad (8.6.142)$$

$$= \frac{q}{2m} \langle \hat{\vec{x}} \times (-i\hbar \hat{\vec{\mathcal{D}}}) \rangle. \quad (8.6.143)$$

The operator $\hat{\vec{x}} \times (-i\hbar \hat{\vec{\mathcal{D}}})$ has a definite physical interpretation. To see it, let us look at the total angular

momentum of our system. Because $\psi(t, \vec{x})$ is a scalar field, under a rotation by a rotation matrix $\hat{R}$:

$$\psi'(t', \vec{x}') = \psi(t, \vec{x}) \implies \psi'(t, \vec{x}) = \psi(t, \hat{R}^{-1} \vec{x}). \quad (8.6.144)$$

Differentiating both sides with respect to the rotation angle θ^a near $\theta = 0$:

$$\left. \frac{d\psi}{d\theta^a} \right|_{\theta=0} = -\epsilon_{ab}^{c} \frac{\partial \psi}{\partial x^c}. \quad (8.6.145)$$

Therefore:

$$\left. \frac{d|\psi\rangle}{d\theta^a} \right|_{\theta=0} = -\frac{i}{\hbar} \epsilon_{abc} \hat{x}^b \hat{p}^c |\psi\rangle. \quad (8.6.146)$$

The generator of rotations (and thus the angular momentum) of just the wavefunction is given by Noether's theorem (or its special case, theorem 8.4):

$$L_a = \langle \pi | \left. \frac{d|\psi\rangle}{d\theta^a} \right|_{\theta=0} = \langle \psi | \epsilon_{abc} \hat{x}^b \hat{p}^c | \psi \rangle \quad (8.6.147)$$

$$\implies \vec{L} = \langle \psi | \vec{\hat{L}} | \psi \rangle = \langle \psi | (\hat{\vec{x}} \times \hat{\vec{p}}) | \psi \rangle \quad (8.6.148)$$

$$\implies \vec{\hat{L}} = \hat{\vec{x}} \times \hat{\vec{p}}. \quad (8.6.149)$$

Here we have defined the orbital angular momentum operator $\hat{\vec{x}} \times \hat{\vec{p}}$. As we will see in a moment this $\vec{L}$ is only the free angular momentum of the wavefunction, meaning neglecting angular momentum due to its interactions with other fields such as electromagnetism. This angular momentum is the orbital angular momentum because it all comes from changing the evaluation point $\vec{x}$ and not from intrinsic changes in the direction of ψ (because ψ is a scalar under rotations, its direction does not change at all).

To derive the total angular momentum of the interacting theory we have to use the action for the fully interacting theory (and thus include the Maxwell terms in our Lagrangian density in theorem 8.10). Then, Noether's theorem gives the total angular momentum:

$$J_a = \langle \pi | \left. \frac{d|\psi\rangle}{d\theta^a} \right|_{\theta=0} + \int_{\mathbb{S}} \vec{P}_A \cdot \left. \frac{d\vec{A}}{d\theta^a} \right|_{\theta=0} d\mathbb{S}. \quad (8.6.150)$$

There is no surface term because the Lagrangian density is invariant under rotations. Under a rotation the vector potential transforms as:

$$\vec{A}'(t, \vec{x}') = \hat{R} \vec{A}(t, \vec{x}) \implies \vec{A}'(t, \vec{x}) = \hat{R} \vec{A}(t, \hat{R}^{-1} \vec{x}) \quad (8.6.151)$$

$$\implies \left. \frac{d\vec{A}}{d\theta^a} \right|_{\theta=0} = \left. \frac{d\hat{R}}{d\theta^a} \right|_{\theta=0} \vec{A} + \frac{\partial \vec{A}}{\partial x^b} \left. \frac{d(\hat{R}^{-1} \vec{x})^b}{d\theta^a} \right|_{\theta=0} \quad (8.6.152)$$

$$= \epsilon_a^{bc} A_b \vec{t}_c - \epsilon_{ab}^{c} x^b \frac{\partial \vec{A}}{\partial x^c}. \quad (8.6.153)$$

Then using Gauss' law and doing some calculation:

$$J_a = \langle (\hat{\vec{x}} \times \hat{\vec{p}})_a \rangle + \int_{\mathbb{S}} (-\vec{E}) \cdot \left(\epsilon_a^{bc} A_b \vec{t}_c - \epsilon_{ab}^{c} x^b \frac{\partial \vec{A}}{\partial x^c} \right) d\mathbb{S} \quad (8.6.154)$$

$$= \langle (\hat{\vec{x}} \times \hat{\vec{p}})_a \rangle + \int_{\mathbb{S}} \left((\vec{E} \times \vec{A})_a + \epsilon_{ab}^{c} x^b \vec{E} \cdot \frac{\partial \vec{A}}{\partial x^c} \right) d\mathbb{S} + \int_{\mathbb{S}} \nabla \cdot \vec{E} \epsilon_{ab}^{c} x^b A_c d\mathbb{S} - \int_{\mathbb{S}} q|\psi|^2 (\vec{x} \times \vec{A})_a d\mathbb{S} \quad (8.6.155)$$

$$= \langle (\hat{\vec{x}} \times (\hat{\vec{p}} - q\vec{A}))_a \rangle + \int_{\mathbb{S}} \left((\vec{E} \times \vec{A})_a + \epsilon_{ab}^{c} x^b \vec{E} \cdot \frac{\partial \vec{A}}{\partial x^c} + \epsilon_{ab}^{c} x^b A_c \frac{\partial E^d}{\partial x^d} \right) d\mathbb{S} \quad (8.6.156)$$

$$= \langle (\hat{\vec{x}} \times (-i\hbar \vec{\nabla}))_a \rangle + \int_{\mathbb{S}} \epsilon_{ab}^{c} x^b E^d \left(\frac{\partial A_d}{\partial x^c} - \frac{\partial A_c}{\partial x^d} \right) d\mathbb{S}. \quad (8.6.157)$$

So, we see that the total angular momentum is given as:

$$\vec{J} = \langle (\hat{\vec{x}} \times (-i\hbar \vec{\nabla})) \rangle + \int_{\mathbb{S}} \vec{x} \times (\vec{E} \times \vec{B}) d\mathbb{S}. \quad (8.6.158)$$

The second integral is exactly the angular momentum we identified in chapter 4 as the electromagnetic angular momentum and the first term is the free angular momentum we identified previously except with $\hat{\vec{p}}$

replaced by the gauge invariant combination $\hat{\vec{p}} - q\hat{\vec{A}}$. Thus, we can identify that the total orbital angular momentum of the wavefunction, including its contribution due to interacting with electromagnetism as:

$$\vec{L} = \langle \hat{\vec{x}} \times (-i\hbar\hat{\vec{\nabla}}) \rangle \quad (8.6.159)$$

with the previous formula (equation (8.6.148)) holding in the case of no vector potential. So, the magnetic dipole moment of the wavefunction is given by:

$$\vec{\mu} = \frac{q\vec{L}}{2m}. \quad (8.6.160)$$

Exercises

Problem 8.24: Free Quantum Wave. Consider a free Galilean Schrödinger wave (meaning $U = 0$ and $\vec{K} = 0$) in d spatial dimensions.

(a) Show that the free Schrödinger equation becomes:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi.$$

(b) Fourier transform the free Schrödinger equation and solve it in Fourier space. Then, Fourier transform it back into position space to show that the general solution to the free Schrödinger equation is given by:

$$\psi(t, \vec{x}) = \int_{\mathbb{S}} \left(\frac{m}{2\pi i \hbar t} \right)^{\frac{d}{2}} e^{\frac{im}{2\hbar t} |\vec{x} - \vec{x}'|^2} \psi(0, \vec{x}') d^d \vec{x}'.$$

(c) Let $\vec{x}_{cl} = \langle \hat{\vec{x}} \rangle$, $\vec{p}_{cl} = \langle \hat{\vec{p}} \rangle$. Show that they exactly satisfy the equations of motion:

$$\frac{d\vec{x}_{cl}}{dt} = \frac{\vec{p}_{cl}}{m}, \quad \frac{d\vec{p}_{cl}}{dt} = 0$$

for all wavefunctions ψ and that these are solved by the classical solutions:

$$\vec{x}_{cl}(t) = \vec{x}_{cl}(0) + \frac{\vec{p}_{cl}(0)}{m}t, \quad \vec{p}_{cl}(t) = \vec{p}_{cl}(0).$$

Thus, the center of mass of a free quantum wave packet moves exactly classically.

(d) Define:

$$X^{ab} = \langle (\hat{x}^a - \mathbb{1}x_{cl}^a)(\hat{x}^b - \mathbb{1}x_{cl}^b) \rangle, \quad P_{ab} = \langle (\hat{p}_a - \mathbb{1}p_{cl,a})(\hat{p}_b - \mathbb{1}p_{cl,b}) \rangle, \\ C^a{}_b = \frac{1}{2} \langle ((\hat{x}^a - \mathbb{1}x_{cl}^a)(\hat{p}_b - \mathbb{1}p_{cl,b}) + (\hat{p}_b - \mathbb{1}p_{cl,b})(\hat{x}^a - \mathbb{1}x_{cl}^a)) \rangle.$$

So, X^{ab} is the matrix of position correlations, P_{ab} is the matrix of momentum correlations, and $C^a{}_b$ is the matrix of position-momentum correlations. Show that these exactly satisfy the equations of motion:

$$\frac{dX^{ab}}{dt} = \frac{C^{ab} + C^{ba}}{m}, \quad \frac{dC^{ab}}{dt} = \frac{P^{ab}}{m}, \quad \frac{dP^{ab}}{dt} = 0.$$

Finally then show that these are solved by:

$$X^{ab}(t) = X^{ab}(0) + \frac{C^{ab}(0) + C^{ba}(0)}{m}t + \frac{P^{ab}(0)}{m^2}t^2, \\ C^{ab}(t) = C^{ab}(0) + \frac{P^{ab}(0)}{m}t, \quad P_{ab}(t) = P_{ab}(0).$$

(e) Consider a single spatial dimension ($d = 1$) for simplicity and an initial wavefunction which is a coherent state of position space width ℓ . Show that the position space spread at later times is:

$$\sigma_x(t) = \ell \sqrt{1 + \left(\frac{\hbar t}{2m\ell^2} \right)^2}.$$

Thus show that after a long time the wave spread grows linearly with t .

Problem 8.25: ★ Double-Slit Experiment Revisited. Consider the setup of the double-slit experiment with an otherwise free Galilean quantum wave passing through two slits on its way to a screen.

(a) First consider a single slit at the origin. Away from the origin $\psi(t, \vec{x})$ will satisfy the free Schrödinger equation. Thus, the problem has spherical symmetry about this origin and so whatever is produced by

the source at the origin we model $\psi(t, \vec{x})$ as being a function of t, r only. Let $\phi(t, r)$ be defined by:

$$\phi(t, r) = r\psi.$$

Show that $\phi(t, r)$ satisfies:

$$\frac{\partial \phi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \phi}{\partial r^2}.$$

Now assume the incoming wave to the source has angular frequency ω and that the momentum of the outgoing solution should be directed outward from the origin (the wave is leaving the slit). Show that for some complex number ξ :

$$\psi(t, \vec{x}) = \frac{\xi}{r} e^{i\sqrt{\frac{2m\omega}{\hbar}} r - i\omega t}.$$

This is the simplest model of the outgoing wave from the slit; this functional form is called a spherical wave.

- (b) Now let us consider two slits, one placed at $\vec{x}_1 = (0, \frac{s}{2}, 0)$ and the other at $\vec{x}_2 = (0, -\frac{s}{2}, 0)$, and a screen at $z = d$. Show that the combined solution is:

$$\psi(t, \vec{x}) = \frac{\xi_1 e^{ik|\vec{x}-\vec{x}_1| - i\omega t}}{|\vec{x} - \vec{x}_1|} + \frac{\xi_2 e^{ik|\vec{x}-\vec{x}_2| - i\omega t}}{|\vec{x} - \vec{x}_2|}$$

where $k = \sqrt{\frac{2m\omega}{\hbar}}$. Show further that on the screen:

$$\psi(t, 0, y, d) = e^{ik\left(d + \frac{s^2}{8d} + \frac{y^2}{2d}\right) - i\omega t} d \left(\xi_1 e^{-\frac{iksy}{2d}} + \xi_2 e^{\frac{iksy}{2d}} \right) + \mathcal{O}\left(\frac{1}{d^2}\right).$$

- (c) The screen is able to measure impinging charges and so is sensitive to $|\psi|^2$ (as $\rho = q|\psi|^2$). Let $\mathcal{I} = |\psi|^2$ define the intensity of the incident wave and show that on the screen:

$$\mathcal{I} = \frac{1}{d^2} \left(|\xi_1|^2 + |\xi_2|^2 + 2\text{Re} \left(\xi_1^* \xi_2 e^{\frac{iksy}{d}} \right) \right) + \text{H.O.T.}$$

where the higher order terms fall off like $\frac{1}{d^3}$ or faster.

- (d) Assume that the slits are equally spaced from the incoming wave source so that the components of the wave which reach each slit have equal magnitude and are in phase. Thus, show that $\xi_1 = \xi_2$ and let $A = |\xi_1|$. Show that the intensity pattern on the screen becomes:

$$\mathcal{I} = \frac{4A^2}{d^2} \cos^2 \left(\frac{ksy}{2d} \right) + \text{H.O.T.}$$

This is precisely the same intensity pattern we first found when we described the wave result of the double-slit experiment!

- (e) Now assume that there is a detector at one of the slits (choose the second one for this part). Such a detector interacts with the incoming wave as it passes through, adding a local perturbation to the Hamiltonian operator. Argue using what we have found about adiabatic invariance in quantum mechanics that if this local perturbation is brief then it will cause the wave passing through the detector slit to maintain its magnitude but pick up a phase which depends very sensitively on the details of the detector. Thus, we can model the presence of the detector by setting ξ_2 and ξ_1 to be related by a randomly oscillating phase:

$$\xi_2 = e^{i\varphi(t)} \xi_1.$$

Show that now the time averaged resulting intensity pattern is:

$$\mathbb{T}(\mathcal{I}) = \frac{1}{d^2} (|\xi_1|^2 + |\xi_2|^2) + \text{H.O.T.}$$

Explain how this is the intensity pattern predicted from an incoming beam of classical particles. Thus, classical behavior can also often be recovered when there is **decoherence** between the phases of different components in a quantum system. (Decoherence here was our modeling of the detector interaction as the introduction of a rapidly changing phase, essentially random due to the unmodeled detector degrees of freedom.)

Problem 8.26: Wave in an impenetrable box. Consider a Galilean Schrödinger wave which is in an impenetrable box of side length ℓ , meaning $\vec{K} = 0$ and $U = 0$ inside the box and ∞ outside the box. For

simplicity, consider only one spatial dimension.

- (a) Show that all finite energy eigenstates of the Hamiltonian operator must satisfy:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi, \quad \psi(0) = \psi(\ell) = 0$$

where E is the energy eigenvalue corresponding to ψ . (Outside of the interval $0 \leq x \leq \ell$ the box enforces $\psi(t, x) = 0$, so all formulas in this question are assumed only to hold on the inside of the box.)

- (b) Solve the eigenvector problem to show that the energy eigenstates are labeled by $n \in \{1, 2, 3, \dots\}$ and that once normalized are given by:

$$\psi_n(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi x}{\ell}\right), \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2m\ell^2}.$$

- (c) Show that the solution to the Schrödinger equation for arbitrary initial conditions is given by:

$$\psi(t, x) = \sum_{n=1}^{\infty} A_n e^{-\frac{i n^2 \pi^2 \hbar t}{2m\ell^2}} \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi x}{\ell}\right)$$

where the A_n coefficients are given by:

$$A_n = \int_0^\ell \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi x}{\ell}\right) \psi(0, x) dx.$$

- (d) Notice that the eigenvalues of the Hamiltonian operator for this system are discrete. It is a very common error to say “the energy of the particle in a box is discretized” in quantum mechanics. This error is made by those who do not understand the difference between the energy (the conserved quantity due to time translation symmetry, given by $E = \mathcal{H} = \langle \psi | \hat{H} | \psi \rangle$) and an eigenvalue of $\hat{H}$. Show that the interpretation of the eigenvalues of $\hat{H}$ is that $\frac{E_n}{\hbar}$ gives the angular frequency of eigenstate n and that the actual energy E of the wave is in general not an eigenvalue of $\hat{H}$ and can take any continuous value greater than or equal to E_1 .

Problem 8.27: Wave in a penetrable box. Consider a Galilean Schrödinger wave which is in an penetrable box of side length ℓ , meaning $\vec{K} = 0$ and $U = 0$ inside the box and ε outside the box. For simplicity, consider only one spatial dimension.

- (a) Show that the eigenstates of the Hamiltonian operator must satisfy:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} &= E\psi & (0 < x < \ell) \\ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} &= (E - \varepsilon)\psi & (x < 0 \text{ or } x > \ell) \end{aligned}$$

where E is the energy eigenvalue corresponding to ψ .

- (b) Consider eigenstates of the Hamiltonian operator which decay to 0 far away from the box. Show that for some constants $\kappa > 0$, A , B , C , D :

$$\psi(x) = \begin{cases} Ae^{\kappa x}, & x < 0 \\ Be^{ix\sqrt{\frac{2m\varepsilon}{\hbar^2} - \kappa^2}} + Ce^{-ix\sqrt{\frac{2m\varepsilon}{\hbar^2} - \kappa^2}}, & 0 < x < \ell \\ De^{-\kappa x}, & x > \ell. \end{cases}$$

- (c) Show using the boundary conditions at the box walls that:

$$B = \left(1 - \frac{i\kappa}{k}\right) \frac{A}{2}, \quad C = \left(1 + \frac{i\kappa}{k}\right) \frac{A}{2}, \quad D = e^{\kappa\ell} \left(\cos k\ell + \frac{k}{\kappa} \sin k\ell\right) A$$

where:

$$k = \sqrt{\frac{2m\varepsilon}{\hbar^2} - \kappa^2}.$$

Don't waste your time normalizing the solution. Further show that due to the boundary conditions the possible values of k are the discrete values satisfying:

$$\tan k\ell = \frac{k\sqrt{\frac{2m\varepsilon}{\hbar^2} - k^2}}{k^2 - \frac{m\varepsilon}{\hbar^2}}.$$

Some people are very surprised when they learn quantum mechanics to see that the wave in the box is not fully contained in the box (ψ is not zero outside). There is no reason to be surprised; that is how waves work and the exact same thing happens in electromagnetism. They are confused because they are imagining a point-particle, but no such point-particle exists here to be found.

- (d) Consider eigenstates of the Hamiltonian operator which do not decay to 0 far away from the box. Show that they take the form:

$$\psi(x) = \begin{cases} Ae^{ikx} + rAe^{-ikx}, & x < 0 \\ \frac{\sqrt{k^2 + \delta^2} + k}{2\sqrt{k^2 + \delta^2}} t A e^{i(k - \sqrt{k^2 + \delta^2})\ell} e^{i\sqrt{k^2 + \delta^2}x} + \frac{\sqrt{k^2 + \delta^2} - k}{2\sqrt{k^2 + \delta^2}} t A e^{i(k + \sqrt{k^2 + \delta^2})\ell} e^{-i\sqrt{k^2 + \delta^2}x}, & 0 < x < \ell \\ tAe^{ikx}, & x > \ell. \end{cases}$$

Here k is a real parameter, A is a coefficient, and:

$$\begin{aligned} \delta &= \sqrt{\frac{2m\varepsilon}{\hbar^2}}, \\ r &= \frac{i\delta^2 \tan(\ell\sqrt{k^2 + \delta^2})}{2k\sqrt{k^2 + \delta^2} - i(2k^2 + \delta^2) \tan(\ell\sqrt{k^2 + \delta^2})}, \\ t &= \frac{k\sqrt{k^2 + \delta^2} e^{-ik\ell}}{k\sqrt{k^2 + \delta^2} \cos(\ell\sqrt{k^2 + \delta^2}) - i(k^2 + \frac{\delta^2}{2}) \sin(\ell\sqrt{k^2 + \delta^2})}. \end{aligned}$$

- (e) Recall the definitions of reflection and transmission coefficients at an interface in electromagnetism. Show that r and t given above correspond to the reflection and transmission coefficients of this system when a wavepacket is sent toward from the box from far away to the left (for $k > 0$). Show that in this case these coefficients satisfy:

$$|r|^2 + |t|^2 = 1.$$

Later we will prove that this must hold very generally, not simply for this system.

Problem 8.28: Bloch's Theorem. Spatially periodic Hamiltonian operators occur in many applications (a crystalline material for example will produce a periodic potential). Let $V(x)$ be an analytic function which decays to 0 sufficiently quickly for large $|x|$ and consider the Hamiltonian operator in 1 spatial dimension:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_{n \in \mathbb{Z}} V(\hat{x} - n\ell \mathbb{1})$$

for a constant ℓ .

- (a) Define the lattice translation operator:

$$\hat{T} = e^{-\frac{i}{\hbar} \ell \hat{p}}.$$

Show that $\hat{T}$ is unitary and that this system has symmetry under the transformation $|\psi'\rangle = \hat{T}|\psi\rangle$.

- (b) Show that a general eigenstate of $\hat{T}$ takes the form:

$$|\psi\rangle = \sum_{n \in \mathbb{Z}} c_n |p_n\rangle$$

for some coefficients c_n and where $|p_n\rangle$ are momentum eigenstates with momentum eigenvalue:

$$p_n = \hbar k + \frac{2\pi\hbar n}{\ell}$$

and $0 \leq k < \frac{2\pi}{\ell}$. Show that $\hat{T}$ and $\hat{H}$ are simultaneously diagonalizable and use this to explain that there exists a choice of the c_n so that $|\psi\rangle$ is also an eigenstate of $\hat{H}$.

- (c) Prove Bloch's theorem: the eigenfunctions of a spatially periodic Hamiltonian operator can be written in the form:

$$\psi(x) = e^{-ikx} u(x)$$

where $0 \leq k < \frac{2\pi}{\ell}$ and $u(x)$ has the same periodicity as the Hamiltonian operator.

Problem 8.29: Amplitude and Phase Variables. Define the real valued fields $n(t, \vec{x})$ and $S(t, \vec{x})$ by:

$$\psi(t, \vec{x}) = \sqrt{n(t, \vec{x})} e^{\frac{i}{\hbar} S(t, \vec{x})}.$$

- (a) Show that the Lagrangian density in theorem 8.10 can be written in these coordinates as:

$$\mathcal{L} = -n \left(\dot{S} + q\phi + \frac{|\nabla S - q\vec{A}|^2}{2m} \right) - \frac{\hbar^2 |\nabla n|^2}{8mn}.$$

Show that this Lagrangian density produces the equations of motion:

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(n \frac{\nabla S - q\vec{A}}{m} \right) = 0, \quad \frac{\partial S}{\partial t} + q\phi + \frac{|\nabla S - q\vec{A}|^2}{2m} + \frac{\hbar^2}{8mn^2} (|\nabla n|^2 - 2n\nabla^2 n) = 0.$$

Notice that the first is a continuity equation velocity $\vec{v} = \frac{\nabla S - q\vec{A}}{m}$ and the second is almost the Hamilton-Jacobi equation for a classical charge particle's canonical action S .

- (b) Assume that $\frac{\hbar \nabla n}{n}$ is everywhere small compared to $\nabla S - q\vec{A}$. Explain that this means that we assume $|\psi|^2$ is approximately steady on the length scale of the gauge invariant fluctuations of the phase of ψ . Show that under these circumstances the above equations of motion have a smooth $\hbar \rightarrow 0$ limit and reduce exactly the continuity equation for a classical number density n of charge and that S becomes the canonical action for a classical charged particle. Compare this with problem 6.13. Because $\hbar \rightarrow 0$ formally represents the classical limit, it is common to consider a series solution for n and S in powers of $\hbar$ with the lowest order solutions being these classical results. That series solution is known as the Wentzel–Kramers–Brillouin (WKB) approximation.

Problem 8.30: ★ The Aharonov-Bohm Effect. Consider a double-slit experiment with the same setup as in problem 8.25 except that now between the two slits is a closed impenetrable solenoid of cross sectional area $\mathbb{A}$ with a uniform magnetic field of magnitude B pointing in the x direction inside it.

- (a) Show that it is possible to choose the gauge of $\vec{A}$ so that the part of the wave that passes through the top slit is always in a region of $\vec{A} = 0$. Show that it is possible to choose instead the gauge so that the corresponding result is true for the bottom slit. Show that it is not possible to pick the gauge so that this is true for both of them.
- (b) Show that a gauge invariant phase difference is accumulated between the parts of the wave from each slit. Use equation (8.6.113) to show that the phase difference is:

$$\theta = -\frac{qB\mathbb{A}}{\hbar}.$$

Show under the assumptions of problem 8.25(d) that this produces the new interference pattern:

$$\mathcal{I} = \frac{4A^2}{d^2} \cos^2 \left(\frac{ksy}{2d} - \frac{qB\mathbb{A}}{2\hbar} \right) + \mathcal{O} \left(\frac{1}{d^3} \right).$$

This spatially shifts the interference pattern detected on the screen and is known as the Aharonov-Bohm effect. We see that even though the wavefunction is only nonzero in regions of space with $\vec{E} = 0$ and $\vec{B} = 0$ it is still affected by electromagnetism. This is to be expected because the Schrödinger equation depends directly on $\vec{A}$ and ϕ , not only on $\vec{E}$ or $\vec{B}$. The observation of this effect serves as experimental proof that the potentials are physical as in this experiment they are directly interacted with⁸.

Problem 8.31: ★ Generator of Gauge Transformations. Show using equation (4.6.19) that the generator of gauge transformations for the Schrödinger equation is:

$$G = - \int f(t, \vec{x}) (q|\psi|^2 + \nabla \cdot \vec{P}_A) d^3\vec{x}.$$

Further, show that the resulting gauge transformation property produced by this generator is:

$$\left. \frac{d\phi}{d\varepsilon} \right|_{\varepsilon=0} = -\frac{\partial f}{\partial t}, \quad \left. \frac{d\vec{A}}{d\varepsilon} \right|_{\varepsilon=0} = \{\vec{A}, G\} = \nabla f, \quad \left. \frac{d\vec{P}_A}{d\varepsilon} \right|_{\varepsilon=0} = \{\vec{P}_A, G\} = 0, \quad \left. \frac{d\psi}{d\varepsilon} \right|_{\varepsilon=0} = \{\psi, G\} = \frac{iq}{\hbar} f(t, \vec{x}) \psi.$$

⁸Historically there was a lot of incorrect fuss over this result and it was suggested that instead this was proof that quantum mechanics is non-local. The thinking here was that we assume $\psi, \vec{A}, \phi$ are unphysical but $|\psi|^2, \vec{E}, \vec{B}$ are physical because they are gauge invariant. There is no local equation of motion that can couple $|\psi|^2, \vec{E}, \vec{B}$ which is equivalent to the Schrödinger equation and so since they experimentally are coupled, this must mean quantum mechanics is not local. This is ridiculous because the Schrödinger equation is entirely local as a field theory. This silliness stemmed from a dislike of the potentials which has since been rendered incompatible with a basic understanding of field theory. In the modern day there are many experiments in which the potentials are directly essential.

Show that when integrated these produce the correct gauge transformation property for each of these quantities.

Problem 8.32: ★ The Quantum Harmonic Oscillator (QHOI) - Creation and Annihilation Operators. Consider a Galilean Schrödinger wave in 1 spatial dimension subject to the harmonic oscillator potential so that:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

for constants m and ω .

- (a) We found in equation (8.2.3) a useful coordinate transformation for a harmonic oscillator. Taking that transformation as inspiration, define the “annihilation operator”:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}.$$

Show that $\hat{a}$ is not self-adjoint and is not a normal operator. In particular, show that:

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

Therefore, by the spectral theorem $\hat{a}$ cannot be diagonalized by an orthonormal basis of eigenvectors.

- (b) Show that $\hat{H}$ can be expressed in terms of $\hat{a}$ by:

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \mathbb{1} \right).$$

Define the number operator $\hat{N}$ by:

$$\hat{N} = \hat{a}^\dagger \hat{a}.$$

Show that $\hat{N}$ is self-adjoint.

- (c) Let $|\psi\rangle$ be an eigenstate of $\hat{N}$ with eigenvalue λ . Show that $|\psi\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $\hbar\omega(\lambda + \frac{1}{2})$. Further, show that $\hat{a}|\psi\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $\lambda - 1$ and that $\hat{a}^\dagger|\psi\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $\lambda + 1$. Because $\hat{a}$ lowers the eigenvalue of $\hat{N}$ it is called the annihilation operator (or lowering operator) and because $\hat{a}^\dagger$ raises the eigenvalue of $\hat{N}$ it is called the creation operator (or raising operator).
- (d) Let $|\psi\rangle$ be a normalized eigenstate of $\hat{N}$ with eigenvalue λ . By considering the norm of $\hat{a}|\psi\rangle$, show that $\lambda \geq 0$.
- (e) Use the results of the previous two parts to show that there exists a normalized eigenstate $|\phi\rangle$ of $\hat{N}$ with eigenvalue $\lambda \geq 0$ such that $\hat{a}|\phi\rangle = 0$. Show further that this $|\phi\rangle$ has eigenvalue $\lambda = 0$.
- (f) Show that the $|\phi\rangle$ described in the previous part in position space satisfies the differential equation:

$$\frac{\partial\phi}{\partial x} + \frac{m\omega x}{\hbar}\phi = 0.$$

Solve this equation for ϕ and normalize it. Show that:

$$\phi(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}.$$

Call this state $|0\rangle = |\phi\rangle$ because its $\hat{N}$ eigenvalue is 0.

- (g) Show that all of the eigenstates of $\hat{N}$ are given by:

$$|n\rangle = C_n (\hat{a}^\dagger)^n |0\rangle$$

for some coefficients C_n and that $\hat{N}$ has only nonrepeated eigenvalues given by $\{0, 1, 2, 3, 4, \dots\}$. Because $\hat{a}$ and $\hat{a}^\dagger$ allow the lowering and raising of eigenvalues of $\hat{N}$ in integer amounts, the two of them as a pair are sometimes called ladder operators.

- (h) Show that once normalized:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle, \quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

Show that these $|n\rangle$ are orthonormal as expected and that because they are a complete set of eigenstates of $\hat{N}$, they satisfy the completeness relation:

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{1}.$$

(i) Show that in position space:

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega x^2}{2\hbar}}$$

where $H_n(z)$ is the n^{th} Hermite polynomial defined by:

$$H_n(z) = (-1)^n e^{z^2} \left(\frac{\partial}{\partial z} \right)^n e^{-z^2}.$$

Show that $H_n(z)$ is a polynomial in z of degree n . Plot $\psi_n(x)$ as a function of x for several different n .

Notice that $\psi_n(x)$ always decays for large $|x|$ and has $n+1$ bumps.

(j) Show that the $|n\rangle$ are the complete set of eigenstates of $\hat{H}$ and that $\hat{H}$ has the associated eigenvalues:

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right).$$

Use the familiar fact that the Hamiltonian may be shifted by a constant with no physical consequences and the interpretation of $\frac{E_n}{\hbar}$ as the angular frequencies of the system to show that the quantum harmonic oscillator can be thought of as having angular frequencies coming in integer multiples of the classical frequency ω . Use the silver-bullet solution to show that the time evolution of the QHO is given by:

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2})\omega t} |n\rangle \langle n|\psi(0)\rangle.$$

(k) Let $\ell = \sqrt{\frac{\hbar}{2m\omega}}$ and recall the definition of a coherent state in terms of ℓ . Show that coherent states may be written:

$$|q, p\rangle = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} |0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

where α has been defined by:

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}} q + \frac{i}{\sqrt{2m\omega\hbar}} p.$$

To do this you should use the simple BCH formula. As well, show that coherent states are eigenstates of $\hat{a}$ with eigenvalue α :

$$\hat{a}|q, p\rangle = \alpha|q, p\rangle.$$

Problem 8.33: ★ QHOII - Moment Evolution Equations. Consider again the quantum harmonic oscillator. Define the first and second order moments of the wavefunction:

$$\bar{x} = \langle \hat{x} \rangle, \quad \bar{p} = \langle \hat{p} \rangle, \quad \sigma_x^2 = \langle \hat{x}^2 \rangle - \bar{x}^2, \quad \sigma_{xp} = \frac{\langle (\hat{x}\hat{p} + \hat{p}\hat{x}) \rangle}{2} - \bar{x}\bar{p}, \quad \sigma_p^2 = \langle \hat{p}^2 \rangle - \bar{p}^2.$$

(a) Show these exactly satisfy the equations of motion:

$$\begin{aligned} \frac{d\bar{x}}{dt} &= \frac{\bar{p}}{m}, & \frac{d\bar{p}}{dt} &= -m\omega^2 \bar{x}, \\ \frac{d\sigma_x^2}{dt} &= \frac{2}{m} \sigma_{xp}, & \frac{d\sigma_{xp}}{dt} &= \frac{\sigma_p^2}{m} - m\omega^2 \sigma_x^2, & \frac{d\sigma_p^2}{dt} &= -2m\omega^2 \sigma_{xp}. \end{aligned}$$

(b) Solve those equations of motion to show that:

$$\begin{aligned} \bar{x}(t) &= \bar{x}(0) \cos \omega t + \frac{\bar{p}(0)}{m\omega} \sin \omega t, & \bar{p}(t) &= \bar{p}(0) \cos \omega t - m\omega \bar{x}(0) \sin \omega t, \\ \sigma_x^2(t) &= \sigma_x^2(0) \cos^2(\omega t) + \frac{2\sigma_{xp}(0)}{m\omega} \sin(\omega t) \cos(\omega t) + \frac{\sigma_p^2(0)}{m^2\omega^2} \sin^2(\omega t), \\ \sigma_{xp}(t) &= \sigma_{xp}(0) \cos(2\omega t) + \frac{\sigma_p^2(0) - m^2\omega^2 \sigma_x^2(0)}{2m\omega} \sin(2\omega t), \\ \sigma_p^2(t) &= \sigma_p^2(0) \cos^2(\omega t) - 2m\omega \sigma_{xp}(0) \sin(\omega t) \cos(\omega t) + m^2\omega^2 \sigma_x^2(0) \sin^2(\omega t). \end{aligned}$$

Interpret what these tell you about how the quantum harmonic oscillator wave sloshes around.

- (c) Show that the active picture operators $\hat{x}_A(t)$ and $\hat{p}_A(t)$ satisfy:

$$\frac{d\hat{x}_A}{dt} = \frac{\hat{p}_A}{m}, \quad \frac{d\hat{p}_A}{dt} = -m\omega^2\hat{x}_A$$

and that these are solved by (taking $t_0 = 0$):

$$\hat{x}_A(t) = \hat{x} \cos \omega t + \frac{\hat{p}}{m\omega} \sin \omega t, \quad \hat{p}_A(t) = \hat{p} \cos \omega t - m\omega \hat{x} \sin \omega t.$$

- (d) Define the normalized central moments $N_{k,n}$ by:

$$N_{k,n} = (m\omega)^{\frac{k-n}{2}} \langle \text{Sym}((\hat{x} - \bar{x}\mathbb{1}); k, (\hat{p} - \bar{p}\mathbb{1}); n) \rangle.$$

Show that their time dependence is given by:

$$N_{k,n} = \sum_{l=0}^k \sum_{m=0}^n (-1)^m \binom{k}{l} \binom{n}{m} \cos^{k+n-l-m}(\omega t) \sin^{l+m}(\omega t) N_{k-l+m, n+l-m}(0).$$

Interpret what this tells you about how the quantum harmonic oscillator wave sloshes around.

Problem 8.34: ★ QHOIII - Evolution of Coherent States and Evolutor. Consider again the quantum harmonic oscillator. Use the results of the previous quantum harmonic oscillator problems.

- (a) Show that if the initial state vector is a coherent state $|q_0, p_0\rangle$ with $\ell = \sqrt{\frac{\hbar}{2m\omega}}$ then the second order moments of the wavefunction satisfy for all t :

$$\sigma_x^2(t) = \frac{\hbar}{2m\omega}, \quad \sigma_{xp}(t) = 0, \quad \sigma_p^2(t) = \frac{\hbar m\omega}{2}.$$

Use this and the fact that a state of minimal uncertainty is necessarily a coherent state to show that for all t the wavefunction is of the form:

$$|\psi(t)\rangle = e^{i\varphi(t)} |q(t), p(t)\rangle$$

for some real functions $\varphi(t), q(t), p(t)$.

- (b) Show that $\varphi(t), q(t), p(t)$ satisfy:

$$\dot{\varphi} = -\frac{\omega}{2}, \quad \dot{q} = \frac{p}{m}, \quad \dot{p} = -m\omega^2 q.$$

Solve these to show that:

$$\varphi(t) = -\frac{\omega t}{2}, \quad q(t) = q_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t), \quad p(t) = p_0 \cos(\omega t) - m\omega q_0 \sin(\omega t).$$

- (c) Now consider a wavefunction with arbitrary initial conditions and use that the coherent states are an over-complete set to show that:

$$\psi(t, x) = \int_{-\infty}^{\infty} U(t, x, x') \psi(0, x') dx'$$

where $U(t, x, x')$ called the evolutor is given in terms of the time evolution operator by:

$$U(t, x, x') = \langle x | \hat{U}(t) | x' \rangle = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega t)}} e^{-\frac{m\omega((x^2 + x'^2) \cos(\omega t) - 2xx')}{2i\hbar \sin(\omega t)}}.$$

Thus, this evolutor fully solves the quantum harmonic oscillator.

- (d) Consider a classical harmonic oscillator with the same value of m and ω as our quantum oscillator. Let $S(t, x, x')$ be the value of its action along the classical trajectory with initial condition x' at time 0 and final condition x at time t . Show that:

$$S(t, x, x') = \frac{m\omega((x^2 + x'^2) \cos(\omega t) - 2xx')}{2 \sin(\omega t)}.$$

Use this to show that the evolutor for the quantum harmonic oscillator may be written exactly as:

$$U(t, x, x') = \frac{1}{\sqrt{2\pi i \hbar}} \sqrt{-\frac{\partial^2 S}{\partial x \partial x'}} e^{\frac{i}{\hbar} S(t, x, x')}.$$

Problem 8.35: ★ QHOIV - Driven Oscillations. Consider yet again the quantum harmonic oscillator.

- (a) Assume that a linear force $F(t)$ is applied to the oscillator. Show that this can be modeled by the

Hamiltonian operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - F(t)\hat{x}.$$

- (b) Show that under such driven oscillations, a coherent state still remains coherent and so has solution of the form:

$$|\psi(t)\rangle = e^{i\varphi(t)}|q(t), p(t)\rangle.$$

Show that φ, q, p satisfy:

$$\dot{\varphi} = -\frac{\omega}{2} + \frac{q(t)F(t)}{2\hbar}, \quad \dot{q} = \frac{p}{m}, \quad \dot{p} = -m\omega^2 q + F(t).$$

Solve these to show that:

$$\begin{aligned} q(t) &= q(0) \cos(\omega t) + \frac{p(0)}{m\omega} \sin(\omega t) + \frac{1}{m\omega} \int_0^t F(t') \sin(\omega(t-t')) dt' \\ p(t) &= p(0) \cos(\omega t) - m\omega q(0) \sin(\omega t) + \int_0^t F(t') \cos(\omega(t-t')) dt' \\ \varphi(t) &= -\frac{\omega t}{2} + \frac{1}{2\hbar} \int_0^t q(t') F(t') dt'. \end{aligned}$$

- (c) Following the steps used for the free quantum harmonic oscillator, show that the evolver for the driven quantum harmonic oscillator is:

$$\begin{aligned} U(t, x, x') &= \langle x | \hat{U}(t) | x' \rangle \\ &= \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega t)}} e^{-\frac{m\omega((x-Q)^2 + x'^2) \cos(\omega t) - 2(x-Q)x'}{2i\hbar \sin(\omega t)} + \frac{im\omega}{\hbar} x \dot{Q} - \frac{im\omega}{2\hbar} Q \dot{Q} + \frac{i}{2\hbar} \int_0^t Q(t') F(t') dt'} \end{aligned}$$

where $Q(t)$ is defined by:

$$Q(t) = \int_0^t \frac{F(t')}{m\omega} \sin(\omega(t-t')) dt'.$$

- (d) Consider a classical harmonic oscillator with the same value of m and ω as our quantum oscillator experiencing the same linear force $F(t)$ so that its Hamiltonian is given by:

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - F(t)x.$$

Let $S(t, x, x')$ be the value of its action along the classical trajectory with initial condition x' at time 0 and final condition x at time t . Show that:

$$S(t, x, x') = \frac{m\omega(((x-Q)^2 + x'^2) \cos(\omega t) - 2(x-Q)x')}{2 \sin(\omega t)} + mx\dot{Q} - \frac{1}{2}mQ\dot{Q} + \frac{1}{2} \int_0^t Q(t') F(t') dt'.$$

Use this to show that the evolver for the driven quantum harmonic oscillator may be written exactly as:

$$U(t, x, x') = \frac{1}{\sqrt{2\pi i \hbar}} \sqrt{-\frac{\partial^2 S}{\partial x \partial x'}} e^{\frac{i}{\hbar} S(t, x, x')}.$$

Problem 8.36: ★ QHOV - Multivariable Oscillator. Consider a quantum system of d coupled quantum harmonic oscillators with undriven Hamiltonian operator $\hat{H}_0$ experiencing a linear force $F_a(t)$ so that the driven system has Hamiltonian operator:

$$\hat{H} = \hat{H}_0 - F_a(t)\hat{x}^a.$$

Consider as well the classical system with the Hamiltonian $\mathcal{H}$ given by replacing $\hat{x}$ and $\hat{p}$ in $\hat{H}$ with classical x and p . Let $S(t, x, x')$ be the value of that classical system's action along the classical trajectory with initial condition x' at time 0 and final condition x at time t . Define the Van Vleck matrix V as having components:

$$V_{ab}(t, x, x') = -\frac{1}{2\pi i \hbar} \frac{\partial^2 S}{\partial x^a \partial x'^b}.$$

The determinant of this matrix is called the Van Vleck determinant. Show that the evolver for the general quantum harmonic oscillator system may be written exactly as:

$$U(t, x, x') = \langle x | \hat{U} | x' \rangle = e^{\frac{i}{\hbar} S(t, x, x')} \sqrt{\det V}.$$

Problem 8.37: Landau Levels. Consider a Schrödinger wave with electric charge q in a uniform magnetic field $\vec{B}$. For convenience, define your coordinates so that $\vec{B}$ points in the z direction with magnitude B . Show that one may choose the gauge of the vector potential so that $\vec{A}$ is given by:

$$\vec{A} = Bx\vec{e}_y.$$

Show that the Hamiltonian operator of the system in this gauge becomes:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{(\hat{p}_y - qBx)^2}{2m} + \frac{\hat{p}_z^2}{2m}.$$

Show that the eigenvectors (up to a normalization factor) and eigenvalues of the Hamiltonian operator are labeled by a nonnegative integer n and real numbers k_y, k_z by:

$$\psi_{nk_yk_z}(x, y, z) = Ne^{ik_y y + ik_z z} \Psi_n \left(x - \frac{\hbar k_y}{m\omega} \right)$$

$$E_{nk_yk_z} = \hbar\omega \left(n + \frac{1}{2} \right) + \frac{\hbar^2 k_z^2}{2m}$$

where $\omega = \frac{qB}{m}$ is called the cyclotron frequency and $\Psi_n(x)$ is the n^{th} quantum harmonic oscillator eigenfunction for an oscillator of mass m and frequency ω .

8.7 Angular Momentum

The most important and common internal degree of freedom is spin. When we discussed rigid bodies, we found that the total angular momentum of the body decomposed into the sum of a term due to the center of mass of the body orbiting about a location in space (which we called orbital angular momentum) and a term due to the orientation of the object changing about its center of mass (which we called spin angular momentum). The same idea of decomposition exists in quantum mechanics. There is orbital angular momentum due to the wavefunction flowing about around a location in space. The wavefunction can also have at each location in space an orientation in its internal space which rotates under spatial rotations. The generator of such transformations on the internal space is the spin angular momentum⁹. The orientation of the wavefunction on its internal space is called the polarization of the wavefunction and the angular momentum corresponding to the changing of the polarization is called the spin. In this section we will discuss representations of angular momentum in quantum mechanics.

Under a rotation of the wavefunction, the different components will get rotated in some way and thus become some linear combination of each other. As well, due to rotating the space, the underlying point of evaluation will be rotated as well. So, let $\hat{R}$ be the rotation so that $\vec{x}' = \hat{R}\vec{x}$ is the rotated point. The rotated wavefunction $\psi'^a(t, \vec{x}')$ will then be related to the unrotated wavefunction by:

$$\psi'^a(t, \vec{x}') = V^a_b(\theta) \psi^b(t, \vec{x}) \quad (8.7.1)$$

$$\implies \psi'^a(t, \vec{x}) = V^a_b(\theta) \psi^b(t, \hat{R}^{-1}\vec{x}). \quad (8.7.2)$$

for some coefficients $V^a_b(\theta)$ which depend on the rotation applied. Then, if we say that the wavefunction has D components and orthonormal basis vectors for the internal space $|n\rangle$ where n goes from 1 to D , we can write the wavefunction as:

$$|\psi\rangle = \sum_{n=1}^D \int_{\mathbb{S}} \psi^n(t, \vec{x}) |\vec{x}\rangle \otimes |n\rangle d^3\vec{x} = \sum_{n=1}^D \int_{\mathbb{S}} \psi^n(t, \vec{x}) |\vec{x}, n\rangle d^3\vec{x} \quad (8.7.3)$$

where we have introduced the notation:

$$|\vec{x}, n\rangle = |\vec{x}\rangle \otimes |n\rangle. \quad (8.7.4)$$

Differentiating equation (8.7.2) at the identity with respect to the rotation angles:

$$\mathcal{D}_b \psi^a(t, \vec{x}) = \left. \frac{d}{d\theta^b} \left(V^a_c \psi^c(t, \hat{R}^{-1}\vec{x}) \right) \right|_{\theta=0} = (\mathcal{D}_b V^a_c) \psi^c(t, \vec{x}) - \delta^a_c \frac{\partial \psi^c}{\partial x^d}(t, \vec{x}) \mathcal{D}_b x^d \quad (8.7.5)$$

$$= -\frac{\partial \psi^a}{\partial x^d} \epsilon^d_{bc} x^c + (\mathcal{D}_b V^a_c) \psi^c(t, \vec{x}) = -\epsilon_{bc}^d x^c \frac{\partial \psi^a}{\partial x^d} + (\mathcal{D}_b V^a_c) \psi^c(t, \vec{x}). \quad (8.7.6)$$

Then, we have:

$$\mathcal{D}_a |\psi\rangle = \sum_{n=1}^D \int_{\mathbb{S}} \mathcal{D}_a \psi^n(t, \vec{x}) |\vec{x}, n\rangle d^3\vec{x} = \sum_{n=1}^D \int_{\mathbb{S}} \left(-\epsilon_{ab}^c x^b \frac{\partial \psi^n}{\partial x^c} + (\mathcal{D}_a V^n_b) \psi^b(t, \vec{x}) \right) |\vec{x}, n\rangle d^3\vec{x} \quad (8.7.7)$$

$$= \sum_{n=1}^D \int_{\mathbb{S}} |\vec{x}, n\rangle \left(-\epsilon_{ab}^c x^b \frac{\partial}{\partial x^c} \langle \vec{x}, n| + \sum_{m=1}^D (\mathcal{D}_a V^n_m) \langle \vec{x}, m| \right) d^3\vec{x} |\psi\rangle \quad (8.7.8)$$

$$= - \left(\sum_{n=1}^D |n\rangle \langle n| \right) \otimes \epsilon_{ab}^c \hat{x}^b \int_{\mathbb{S}} |\vec{x}\rangle \frac{\partial}{\partial x^c} \langle \vec{x}| d^3\vec{x} |\psi\rangle + \left(\sum_{n=1}^D \mathcal{D}_a V^n_m |n\rangle \langle m| \right) \otimes \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d^3\vec{x} |\psi\rangle \quad (8.7.9)$$

$$= -\mathbb{1}_{\text{int}} \otimes \epsilon_{ab}^c \hat{x}^b \frac{i}{\hbar} \hat{p}_c |\psi\rangle + \left(\sum_{n=1}^D \mathcal{D}_a V^n_m |n\rangle \langle m| \right) \otimes \mathbb{1}_{\mathbb{S}} |\psi\rangle \quad (8.7.10)$$

⁹It is a very common error among quantum mechanics books to say that spin has no classical analog. This is entirely wrong but is a second-order error (it is a wrong result derived from a more basic error). The first-order error which is the parent of this mistake is the belief that the quantum mechanics of a single particle is about a single *point-particle*. Hopefully by now you understand why that belief is fundamentally misguided and know that quantum mechanics of a single particle is about the dynamics of an extended wave-packet. It is true that point particles do not have any spin (spin is finitely proportional to the moment of inertia which itself scales like the squared radius of the body, so 0 in the point case) but neither the classical mechanics of spinning bodies nor quantum mechanics of a particle have anything to do with point particles.

$$= -\frac{i}{\hbar}(\hat{x} \times \hat{p})_a |\psi\rangle + \left(\sum_{n=1}^{D,D} \mathcal{D}_a V^n_m |n\rangle \langle m| \right) |\psi\rangle. \quad (8.7.11)$$

In the last line we have applied a common abuse of notation. If $\hat{A}$ is an operator in Hilbert space $\mathbb{H}_1$ and $\mathbb{1}$ is the identity on Hilbert space $\mathbb{H}_2$, when acting the operator $\hat{A} \otimes \mathbb{1}$ on a vector $|\psi\rangle$ in the Hilbert space $\mathbb{H}_1 \otimes \mathbb{H}_2$, it is common to write $\hat{A}|\psi\rangle$ even though more rigorously $\hat{A} \otimes \mathbb{1}|\psi\rangle$ is intended.

From the change in $|\psi\rangle$ under a rotation, we have that the generator of rotations (the total angular momentum J_a) of the wavefunction is given by equation (8.4.5) as:

$$J_a = i\hbar \langle \psi | \mathcal{D}_a | \psi \rangle = i\hbar \langle \psi | \left(-\frac{i}{\hbar}(\hat{x} \times \hat{p})_a |\psi\rangle + \left(\sum_{n=1}^{D,D} \mathcal{D}_a V^n_m |n\rangle \langle m| \right) |\psi\rangle \right) \quad (8.7.12)$$

$$= \langle \psi | (\hat{x} \times \hat{p})_a | \psi \rangle + \langle \psi | \left(-\frac{i}{\hbar} \right) \left(\sum_{n=1}^{D,D} \mathcal{D}_a V^n_m |n\rangle \langle m| \right) |\psi\rangle. \quad (8.7.13)$$

From this we can extract the definition of the total angular momentum operator as:

$$\vec{J} = \langle \psi | \hat{J} | \psi \rangle \quad (8.7.14)$$

$$\hat{J} = \hat{x} \times \hat{p} - \frac{i}{\hbar} \sum_{n=1}^{D,D} \mathcal{D} V^n_m |n\rangle \langle m|. \quad (8.7.15)$$

Thus, the total angular momentum operator decomposes into a part that acts only on the spatial degrees of freedom called the orbital angular momentum operator:

$$\hat{L} = \hat{x} \times \hat{p} \quad (8.7.16)$$

and a part that acts only on rotating the components of the wavefunction (the internal degrees of freedom), called the spin angular momentum operator:

$$\hat{S} = -\frac{i}{\hbar} \sum_{n=1}^{D,D} \mathcal{D} V^n_m |n\rangle \langle m|. \quad (8.7.17)$$

So, we have $\hat{J} = \hat{L} + \hat{S}$ just as in Theorem 8.5. Consequently, we have that:

$$\vec{J} = \langle \hat{J} \rangle, \quad \vec{L} = \langle \hat{L} \rangle, \quad \vec{S} = \langle \hat{S} \rangle \quad (8.7.18)$$

$$\vec{J} = \vec{L} + \vec{S}. \quad (8.7.19)$$

We found in (2.4.58) that angular momentum must satisfy the $\mathfrak{so}(3)$ algebra:

$$\{J_a, J_b\} = \epsilon_{ab}^c J_c. \quad (8.7.20)$$

Consequently, due to Theorem 8.5 we must have:

$$[\hat{J}_a, \hat{J}_b] = i\hbar \epsilon_{ab}^c \hat{J}_c. \quad (8.7.21)$$

We will call this the $\mathfrak{su}(2)$ algebra (wait! What? Why isn't it called the $\mathfrak{so}(3)$ algebra?? What gives? Don't worry. We will explain by the end of the section). By direct computation, the orbital angular momentum operator $\hat{L} = \hat{x} \times \hat{p}$ we found already satisfies

$$[\hat{L}_a, \hat{L}_b] = i\hbar \epsilon_{ab}^c \hat{L}_c. \quad (8.7.22)$$

As can be seen directly from their definitions, because the orbital angular momentum operator acts only on the spatial degrees of freedom of $|\psi\rangle$ and the spin angular momentum operator acts only on the internal degrees of freedom of $|\psi\rangle$, they commute automatically. So:

$$[\hat{L}_a, \hat{S}_b] = 0. \quad (8.7.23)$$

Then, because $\hat{J}_a = \hat{L}_a + \hat{S}_a$, in order for $\hat{J}_a$ to satisfy the $\mathfrak{su}(2)$ algebra, $\hat{S}_a$ must satisfy it as well:

$$[\hat{S}_a, \hat{S}_b] = i\hbar \epsilon_{ab}^c \hat{S}_c. \quad (8.7.24)$$

Hence the spin operators for any quantum system must satisfy this canonical commutation relation. As well, from Theorem 8.5, $\hat{J}_a$, $\hat{L}_a$, and $\hat{S}_a$ must all be self-adjoint.

8.7.1 Representations of SU(2)

We will now classify all of the ways in which the $\mathfrak{su}(2)$ algebra can be satisfied and the SU(2) group can be represented. To do so, we will use J but because all of the results follow from the algebra, everything applies for L and S as well until noted otherwise. Representations of a Lie algebra can be classified as reducible or as irreducible. A representation is irreducible if there is no subset of that representation which is itself a nontrivial representation of the algebra. A representation is reducible if there is such a subset. For example, 3x3 rotation matrices form an irreducible representation of the group SO(3). There is no subset of those matrices which is also a representation of SO(3) (except the identity matrix which gives a trivial representation of SO(3)). The 3x3 rotation matrices represent how a single vector is rotated. An ordered pair of 3x3 rotation matrices represents how two separate vectors are rotated. That ordered pair of 3x3 rotation matrices forms a reducible representation of the group SO(3) (the ordered pair $(\hat{R}_1, \hat{R}_2)$ can be reduced into $(\hat{R}_1, \mathbb{1})$, $(\mathbb{1}, \hat{R}_2)$ which are both irreducible representations). So, we only need to understand all irreducible representations of a group or algebra and can build the reducible representations by just combinations of the irreducible ones.

Now turning to irreducible representations of SU(2), for convenience define the operators:

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \quad \hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y. \quad (8.7.25)$$

It is useful to note that $\hat{J}^2$ is self-adjoint automatically and that $\hat{J}_{-} = \hat{J}_{+}^{\dagger}$. As well:

$$[\hat{J}^2, \hat{J}_a] = [\hat{J}_b \hat{J}^b, \hat{J}_a] = \hat{J}_b [\hat{J}^b, \hat{J}_a] + [\hat{J}_b, \hat{J}_a] \hat{J}^b \quad (8.7.26)$$

$$= \hat{J}^b i\hbar\epsilon_{ba}{}^c \hat{J}_c + i\hbar\epsilon_{ba}{}^c \hat{J}_c \hat{J}^b = -i\hbar\epsilon_a{}^{bc} \hat{J}_b \hat{J}_c + i\hbar\epsilon_a{}^{bc} \hat{J}_b \hat{J}_c = 0. \quad (8.7.27)$$

Hence $\hat{J}^2$ commutes with the angular momentum along any particular axis. By convention when discussing angular momentum, we give special designation to the z axis in notation but in application the z axis is for this reason always defined to be whatever axis the problem in question natural designates as special. From equation (8.7.27) we conclude in particular that:

$$[\hat{J}^2, \hat{J}_z] = 0. \quad (8.7.28)$$

Because $\hat{J}^2$ and $\hat{J}_z$ are self-adjoint, they are diagonalizable by the spectral theorem and because they commute they are simultaneously diagonalizable. Hence, we can find a simultaneous eigenbasis of these operators which we shall call $|j, m\rangle$. Here j labels the eigenvalue of $\hat{J}^2$ and m labels the eigenvalue of $\hat{J}_z$. When I say “labels” I don’t mean that j and m are necessarily equal to the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$, simply that there will be an invertible map between j and the eigenvalue of $\hat{J}^2$ and between m and the eigenvalue of $\hat{J}_z$. We will choose that map for convenience as we continue. In particular, we choose $\hbar m$ to be the eigenvalue of $\hat{J}_z$ but we will call the eigenvalue of $\hat{J}^2$ $\lambda(j)$ which will be specified later. Because $\hat{J}_a$ are all self-adjoint, they all have real eigenvalues and hence $\hat{J}_a^2$ are all nonnegative operators. Therefore,

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \quad (8.7.29)$$

$$\implies \langle \hat{J}^2 \rangle = \langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z^2 \rangle \geq \langle \hat{J}_z^2 \rangle \quad (8.7.30)$$

for all $|\psi\rangle$. In particular, for our eigenstates:

$$\langle j, m | \hat{J}_z^2 | j, m \rangle = \langle j, m | \hbar^2 m^2 | j, m \rangle = \hbar^2 m^2, \quad \langle j, m | \hat{J}^2 | j, m \rangle = \langle j, m | \lambda(j) | j, m \rangle = \lambda(j) \quad (8.7.31)$$

$$\implies \hbar^2 m^2 \leq \lambda(j). \quad (8.7.32)$$

Hence the eigenvalues of $\hat{J}_z$ are bounded at least this strongly by the eigenvalues of $\hat{J}^2$. From the definitions of $\hat{J}_{\pm}$, a short calculation gives:

$$[\hat{J}^2, \hat{J}_{\pm}] = 0 \quad (8.7.33)$$

$$[\hat{J}_z, \hat{J}_{\pm}] = \pm \hbar \hat{J}_{\pm}. \quad (8.7.34)$$

Now consider the action of $\hat{J}_{\pm}$ on the $|j, m\rangle$ eigenstates:

$$\hat{J}_z |j, m\rangle = \hbar m |j, m\rangle \quad (8.7.35)$$

$$\implies \hat{J}_{\pm} \hat{J}_z |j, m\rangle = \hbar m \hat{J}_{\pm} |j, m\rangle \quad (8.7.36)$$

$$\implies (\hat{J}_\pm \hat{J}_z - \hat{J}_z \hat{J}_\pm + \hat{J}_z \hat{J}_\pm) |j, m\rangle = \hbar m \hat{J}_\pm |j, m\rangle \quad (8.7.37)$$

$$\implies -[\hat{J}_z, \hat{J}_\pm] |j, m\rangle + \hat{J}_z \hat{J}_\pm |j, m\rangle = \hbar m \hat{J}_\pm |j, m\rangle \quad (8.7.38)$$

$$\implies \hat{J}_z (\hat{J}_\pm |j, m\rangle) = \hbar(m \pm 1) \hat{J}_\pm |j, m\rangle. \quad (8.7.39)$$

Therefore, $\hat{J}_\pm |j, m\rangle$ is an eigenstate of $\hat{J}_z$ with eigenvalue $\hbar(m \pm 1)$. Completing the same with $\hat{J}^2$:

$$\hat{J}^2 |j, m\rangle = \lambda(j) |j, m\rangle \quad (8.7.40)$$

$$\implies \hat{J}_\pm \hat{J}^2 |j, m\rangle = \lambda(j) \hat{J}_\pm |j, m\rangle \quad (8.7.41)$$

$$\implies \hat{J}^2 \hat{J}_\pm |j, m\rangle = \lambda(j) \hat{J}_\pm |j, m\rangle. \quad (8.7.42)$$

Hence $\hat{J}_\pm |j, m\rangle$ is an eigenstate of $\hat{J}^2$ with eigenvalue $\lambda(j)$. With these two facts together, we conclude that up to normalization $N_\pm(j, m)$:

$$\hat{J}_\pm |j, m\rangle = N_\pm(j, m) |j, m \pm 1\rangle. \quad (8.7.43)$$

We can see that $\hat{J}_+$ acts as a raising operator, increasing m at fixed j , and that $\hat{J}_-$ acts as a lowering operator, decreasing m at fixed j . It appears that we can keep raising or lowering the eigenvalues of $\hat{J}_z$ indefinitely using $\hat{J}_\pm$. However, because $\hbar^2 m^2 \leq \lambda$ by equation (8.7.32) this raising and lowering must terminate if pushing further would cause this bound to be violated. So, we can only raise or lower m a finite amount. However, if we are to only be able to raise m a finite amount, there must be some m_+ so that attempting to raise it any further causes the right hand side of equation (8.7.43) to go to 0 (else we could solve for the higher m state appearing on that side). So, there must exist an m_+ so that $\hat{J}_+ |j, m_+\rangle = 0$. Similarly if we are only able to lower m a finite amount, there must be some m_- so that $\hat{J}_- |j, m_-\rangle = 0$. Starting with $|j, m_-\rangle$ and iteratively applying the raising operator must eventually give 0 which is precisely the condition which defines m_+ . However, iteratively applying the raising operator will only increment by m_- by 1 each time. Hence, by incrementing m_- by 1 sufficiently one reaches m_+ and therefore $m_+ - m_-$ is a positive integer. (You may argue that there may be two different values of m_+ . However, having two such branches would then give two families of eigenvectors $|j, m\rangle$ which do not mix under the algebra and so would give us a reducible representation.) Further, because we go through one state for each m , we have $m_+ - m_- + 1$ eigenvectors for $\hat{J}_z$ at fixed j . So the dimension $D(j)$ of the subspace of the vector space with a particular value of j is $D(j) = m_+ - m_- + 1$.

Now rewrite $\hat{J}^2$ in terms of the $\hat{J}_\pm$ operators instead of $\hat{J}_x$ and $\hat{J}_y$ and use the commutation relation between $\hat{J}_+$ and $\hat{J}_-$:

$$[\hat{J}_+, \hat{J}_-] = [\hat{J}_x + i\hat{J}_y, \hat{J}_x - i\hat{J}_y] = i[\hat{J}_y, \hat{J}_x] - i[\hat{J}_x, \hat{J}_y] = i(-i\hbar)\hat{J}_z - i(i\hbar)\hat{J}_z = 2\hbar\hat{J}_z \quad (8.7.44)$$

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \implies \hat{J}_x = \frac{\hat{J}_+ + \hat{J}_-}{2}, \quad \hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i} \quad (8.7.45)$$

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \quad (8.7.46)$$

$$= \left(\frac{\hat{J}_+ + \hat{J}_-}{2} \right)^2 + \left(\frac{\hat{J}_+ - \hat{J}_-}{2i} \right)^2 + \hat{J}_z^2 \quad (8.7.47)$$

$$= \frac{\hat{J}_+^2 + \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ + \hat{J}_-^2}{4} - \frac{\hat{J}_+^2 - \hat{J}_+ \hat{J}_- - \hat{J}_- \hat{J}_+ + \hat{J}_-^2}{4} + \hat{J}_z^2 \quad (8.7.48)$$

$$= \frac{\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+}{2} + \hat{J}_z^2 \quad (8.7.49)$$

$$= \hat{J}_+ \hat{J}_- - \hbar\hat{J}_z + \hat{J}_z^2 = \hat{J}_- \hat{J}_+ + \hbar\hat{J}_z + \hat{J}_z^2. \quad (8.7.50)$$

Now let us act these relationships on our eigenstates $|j, m_\pm\rangle$.

$$\hat{J}^2 |j, m_+\rangle = \hat{J}_- \hat{J}_+ |j, m_+\rangle + \hbar\hat{J}_z |j, m_+\rangle + \hat{J}_z^2 |j, m_+\rangle \quad (8.7.51)$$

$$\implies \lambda(j) |j, m_+\rangle = 0 + \hbar^2 m_+ |j, m_+\rangle + \hbar^2 m_+^2 |j, m_+\rangle = \hbar^2 m_+ (m_+ + 1) |j, m_+\rangle \quad (8.7.52)$$

$$\implies \lambda(j) = \hbar^2 m_+ (m_+ + 1) \quad (8.7.53)$$

$$\hat{J}^2 |j, m_-\rangle = \hat{J}_+ \hat{J}_- |j, m_-\rangle - \hbar\hat{J}_z |j, m_-\rangle + \hat{J}_z^2 |j, m_-\rangle \quad (8.7.54)$$

$$\implies \lambda(j) |j, m_-\rangle = 0 - \hbar^2 m_- |j, m_-\rangle + \hbar^2 m_-^2 |j, m_-\rangle = \hbar^2 m_- (m_- - 1) |j, m_-\rangle \quad (8.7.55)$$

$$\implies \lambda(j) = \hbar^2 m_- (m_- - 1). \quad (8.7.56)$$

Hence we have two expression for λ . Equating them:

$$\hbar^2 (m_+^2 + m_+) = \hbar^2 (m_-^2 - m_-) \quad (8.7.57)$$

$$\implies (m_+ + m_-)(m_+ - m_- + 1) = 0 \quad (8.7.58)$$

$$\implies D(j)(m_+ + m_-) = 0 \quad (8.7.59)$$

$$D(j) \neq 0 \implies m_- = -m_+. \quad (8.7.60)$$

$D(j)$ is never 0 because even if the internal space is trivial so that there is only 1 single state in it, $D = 1$. We now define $j = m_+ = -m_-$. Then, following from our previously found relationship between the dimension of the representation and $m_{\pm}$:

$$D(j) = m_+ - m_- + 1 = 2j + 1 \implies j = \frac{D - 1}{2}. \quad (8.7.61)$$

Hence the value j comes in half-integers (because D comes in natural numbers). For D as 1, 2, 3 we have j as 0, 1/2, 1 and so on. That is, j comes in discrete values (which is necessitated by the algebra). These different values of j give what are called different representations of the angular momentum and some common ones are named. In the case that we are discussing spin angular momentum in particular, we write s instead of j and systems with $s = 0$ are called spin-0 or scalars, systems with $s = 1/2$ are called spin-1/2 or spinors (although spinor is sometimes used for any half-integer spin), systems with $s = 1$ are called spin-1 or vectors. Because $D = 2s + 1$ gives the dimension of the angular momentum space at fixed s , different fields with different spins have different spin spaces. From equation (8.7.53), $\lambda = \hbar^2 j(j + 1)$. Therefore, we have that the angular momentum eigenvectors are given by:

$$\hat{J}^2 |j, m\rangle = \hbar^2 j(j + 1) |j, m\rangle \quad (8.7.62)$$

$$\hat{J}_z |j, m\rangle = \hbar m |j, m\rangle \quad -j \leq m \leq j. \quad (8.7.63)$$

We can now compute the normalization factors $N_{\pm}$ to get exact expressions for the raising and lowering operators.

$$\hat{J}_{\pm} |j, m\rangle = N_{\pm}(j, m) |j, m \pm 1\rangle \quad (8.7.64)$$

$$\implies \|\hat{J}_+ |j, m\rangle\|^2 = \|N_+(j, m) |j, m + 1\rangle\|^2 \quad (8.7.65)$$

$$\implies \langle j, m | \hat{J}_+^\dagger \hat{J}_+ |j, m\rangle = |N_+(j, m)|^2 \langle j, m + 1 | j, m + 1 \rangle \quad (8.7.66)$$

$$\implies \langle j, m | \hat{J}_- N_+(j, m) |j, m + 1\rangle = N_+^*(j, m) N_+(j, m) \quad (8.7.67)$$

$$\implies N_+(j, m) \langle j, m | N_-(j, m + 1) |j, m\rangle = N_+^*(j, m) N_+(j, m) \quad (8.7.68)$$

$$\implies N_-(j, m + 1) = N_+^*(j, m). \quad (8.7.69)$$

Now using the commutator between $\hat{J}_+$ and $\hat{J}_-$:

$$\hat{J}_- \hat{J}_+ |j, m\rangle = \hat{J}_- N_+(j, m) |j, m + 1\rangle = N_+(j, m) N_-(j, m + 1) |j, m\rangle = |N_+(j, m)|^2 |j, m\rangle \quad (8.7.70)$$

$$\hat{J}_+ \hat{J}_- |j, m\rangle = \hat{J}_+ N_-(j, m) |j, m - 1\rangle = N_-(j, m) N_+(j, m - 1) |j, m\rangle = |N_+(j, m - 1)|^2 |j, m\rangle \quad (8.7.71)$$

$$\implies [\hat{J}_+, \hat{J}_-] |j, m\rangle = (|N_+(j, m - 1)|^2 - |N_+(j, m)|^2) |j, m\rangle \quad (8.7.72)$$

$$\implies 2\hbar \hat{J}_z |j, m\rangle = (|N_+(j, m - 1)|^2 - |N_+(j, m)|^2) |j, m\rangle \quad (8.7.73)$$

$$\implies 2\hbar^2 m |j, m\rangle = (|N_+(j, m - 1)|^2 - |N_+(j, m)|^2) |j, m\rangle \quad (8.7.74)$$

$$\implies 2\hbar^2 m = |N_+(j, m - 1)|^2 - |N_+(j, m)|^2. \quad (8.7.75)$$

We know that $N_+(j, j) = 0$ because the $|j, j\rangle$ state when raised must go to 0 by definition. Now take equation (8.7.75) and sum from $m = l$ to $m = j$:

$$2\hbar^2 \sum_{m=l}^j m = \sum_{m=l}^j |N_+(j, m - 1)|^2 - \sum_{m=l}^j |N_+(j, m)|^2 \quad (8.7.76)$$

$$\implies 2\hbar^2 \sum_{m=0}^{j-l} (m + l) = |N_+(j, l - 1)|^2 + \sum_{m=l+1}^j |N_+(j, m - 1)|^2 - \sum_{m=l}^{j-1} |N_+(j, m)|^2 - |N_+(j, j)|^2 \quad (8.7.77)$$

$$\Rightarrow 2\hbar^2 \sum_{m=0}^{j-l} m + 2l \sum_{m=0}^{j-l} 1 = |N_+(j, l-1)|^2 + \sum_{m=l}^{j-1} |N_+(j, m)|^2 - \sum_{m=l}^{j-1} |N_+(j, m)|^2 - 0 \quad (8.7.78)$$

$$\Rightarrow 2\hbar^2 \frac{(j-l)(j-l+1)}{2} + 2\hbar^2 l(j-l+1) = |N_+(j, l-1)|^2 \quad (8.7.79)$$

$$\Rightarrow |N_+(j, l-1)|^2 = \hbar^2(j+l)(j-l+1) \quad (8.7.80)$$

$$\Rightarrow |N_+(j, m)|^2 = \hbar^2(j+m+1)(j-m) = \hbar^2(j(j+1) - m(m+1)) \quad (8.7.81)$$

$$\Rightarrow N_+ = \hbar e^{i\varphi(j,m)} \sqrt{j(j+1) - m(m+1)}. \quad (8.7.82)$$

Here the phases are undetermined because the phase of eigenvectors is set only by convention even after normalization. Returning to the raising operation, we see we can define the eigenvectors so that this phase vanishes:

$$\hat{J}_+ |j, m\rangle = \hbar e^{i\varphi(j,m)} \sqrt{j(j+1) - m(m+1)} |j, m+1\rangle. \quad (8.7.83)$$

The phase factor can be absorbed into the definition of the eigenvector on the right hand side and so is unnecessary. Now that N_+ is real by convention, N_- is also real by equation (8.7.69). Hence, the complete action of the raising and lowering operators on the eigenstates is given by:

$$\hat{J}_{\pm} |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle. \quad (8.7.84)$$

Now that we know exactly how the $\hat{J}_z$ and raising and lower operators act, we can find explicit forms for all of the angular momentum operators.

Here we will split our discussion into considering spin and orbital angular momenta separately. For spin angular momentum, if the wavefunction has D components which all mutually become linear combinations of each other under rotations we have found that it is described by spin $s = \frac{D-1}{2}$. Then, because $\hat{S}_z$ is self-adjoint and therefore normal, its orthonormal eigenvectors form a basis for the spin space. This allows us to use the completeness relation:

$$\left(\sum_{l=-s}^s |s, l\rangle \langle s, l| \right) |s, m\rangle = \sum_{l=-s}^s |s, l\rangle \langle s, l | s, m\rangle = \sum_{l=-s}^s |s, l\rangle \delta_{lm} = |s, m\rangle \quad (8.7.85)$$

$$\Rightarrow \sum_{l=-s}^s |s, l\rangle \langle s, l| = \mathbb{1}. \quad (8.7.86)$$

Beginning with the $\hat{S}^2$ operator:

$$\hat{S}^2 |s, m\rangle = \hbar^2 s(s+1) |s, m\rangle \quad (8.7.87)$$

$$\Rightarrow \hat{S}^2 \sum_{m=-s}^s |s, m\rangle \langle s, m| = \hbar^2 s(s+1) \sum_{m=-s}^s |s, m\rangle \langle s, m| \quad (8.7.88)$$

$$\Rightarrow \hat{S}^2 = \hbar^2 s(s+1) \mathbb{1}. \quad (8.7.89)$$

The next easiest is $\hat{S}_z$:

$$\hat{S}_z |s, m\rangle = \hbar m |s, m\rangle \quad (8.7.90)$$

$$\Rightarrow \hat{S}_z \sum_{m=-s}^s |s, m\rangle \langle s, m| = \sum_{m=-s}^s \hbar m |s, m\rangle \langle s, m| \quad (8.7.91)$$

$$\Rightarrow \hat{S}_z = \sum_{m=-s}^s \hbar m |s, m\rangle \langle s, m|. \quad (8.7.92)$$

The raising and lower operators are slightly nastier because they are not diagonal:

$$\hat{S}_+ |s, m\rangle = \hbar \sqrt{s(s+1) - m(m+1)} |s, m+1\rangle \quad (8.7.93)$$

$$\Rightarrow \hat{S}_+ \sum_{m=-s}^s |s, m\rangle \langle s, m| = \sum_{m=-s}^s \hbar \sqrt{s(s+1) - m(m+1)} |s, m+1\rangle \langle s, m| \quad (8.7.94)$$

$$\Rightarrow \hat{S}_+ = \sum_{m=-s}^{s-1} \hbar \sqrt{s(s+1) - m(m+1)} |s, m+1\rangle \langle s, m| \quad (8.7.95)$$

$$\hat{S}_-|s, m\rangle = \hbar\sqrt{s(s+1) - m(m-1)}|s, m-1\rangle \quad (8.7.96)$$

$$\Rightarrow \hat{S}_- \sum_{m=-s}^s |s, m\rangle\langle s, m| = \sum_{m=-s}^s \hbar\sqrt{s(s+1) - m(m-1)}|s, m-1\rangle\langle s, m| \quad (8.7.97)$$

$$\Rightarrow \hat{S}_- = \sum_{m=-s+1}^s \hbar\sqrt{s(s+1) - m(m-1)}|s, m-1\rangle\langle s, m|. \quad (8.7.98)$$

Finally we can use these to complete the $\hat{S}_x$ and $\hat{S}_y$ operators:

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} \quad (8.7.99)$$

$$= \frac{\hbar}{2} \sum_{m=-s}^{s-1} \sqrt{s(s+1) - m(m+1)}|s, m+1\rangle\langle s, m| + \frac{\hbar}{2} \sum_{m=-s+1}^s \sqrt{s(s+1) - m(m-1)}|s, m-1\rangle\langle s, m| \quad (8.7.100)$$

$$= \sum_{m=-s}^{s-1} \hbar\sqrt{s(s+1) - m(m+1)} \frac{|s, m+1\rangle\langle s, m| + |s, m\rangle\langle s, m+1|}{2} \quad (8.7.101)$$

$$\hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} \quad (8.7.102)$$

$$= \frac{\hbar}{2i} \sum_{m=-s}^{s-1} \sqrt{s(s+1) - m(m+1)}|s, m+1\rangle\langle s, m| - \frac{\hbar}{2i} \sum_{m=-s+1}^s \sqrt{s(s+1) - m(m-1)}|s, m-1\rangle\langle s, m| \quad (8.7.103)$$

$$= \sum_{m=-s}^{s-1} \hbar\sqrt{s(s+1) - m(m+1)} \frac{|s, m+1\rangle\langle s, m| - |s, m\rangle\langle s, m+1|}{2i}. \quad (8.7.104)$$

Hence we can compute the spin matrices in general and in principle have all of the setup for use with any spin s .

Theorem 8.11: Spin Representation Theorem

The spin angular momentum of a wavefunction in quantum mechanics is given by $S_a = \langle \hat{S}_a \rangle$ where $\hat{S}_a$ are internal self-adjoint operators called the spin operators which satisfy the $\mathfrak{su}(2)$ commutation relations:

$$[\hat{S}_a, \hat{S}_b] = i\hbar\epsilon_{abc}\hat{S}_c. \quad (8.7.105)$$

The spin operators have irreducible representations labeled by s , the total spin, which takes values $0, 1/2, 1, 3/2, 2, \dots$ determined by the eigenvalue of the $\hat{S}^2$ operator as:

$$\hat{S}^2|\psi\rangle = (\hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2)|\psi\rangle = \hbar^2 s(s+1)|\psi\rangle. \quad (8.7.106)$$

The representation of spin s has dimension $D = 2s + 1$ and is spanned by the orthonormal states $|s, m\rangle$, $-s \leq m \leq s$, defined by:

$$\hat{S}^2|s, m\rangle = \hbar^2 s(s+1)|s, m\rangle, \quad \hat{S}_z|s, m\rangle = \hbar m|s, m\rangle. \quad (8.7.107)$$

In terms of these states, the spin operators have the explicit forms:

$$\hat{S}_x = \sum_{m=-s}^{s-1} \hbar\sqrt{s(s+1) - m(m+1)} \frac{|s, m+1\rangle\langle s, m| + |s, m\rangle\langle s, m+1|}{2} \quad (8.7.108)$$

$$\hat{S}_y = \sum_{m=-s}^{s-1} \hbar\sqrt{s(s+1) - m(m+1)} \frac{|s, m+1\rangle\langle s, m| - |s, m\rangle\langle s, m+1|}{2i} \quad (8.7.109)$$

$$\hat{S}_z = \sum_{m=-s}^s \hbar m|s, m\rangle\langle s, m|. \quad (8.7.110)$$

One interesting fact of note comes from considering a rotation about any particular axis by 2π . Take it to be the z axis for convenience. By equation (8.7.2), we can see that the V^a_b appearing there are simply the components of the operator $\hat{U}_{\text{int}}$ appearing in equation (8.4.47). Thus, we have that:

$$\hat{U}_{\text{int}}(\theta) = e^{-\frac{i}{\hbar}\theta\hat{S}_z} \quad (8.7.111)$$

for a z axis rotation by θ from Theorem 8.4. We can compute this matrix exponential explicitly by using the fact that $\hat{S}_z$ is diagonal:

$$\hat{U}_{\text{int}}(\theta)|s, m\rangle = e^{-\frac{i}{\hbar}\theta\hat{S}_z}|s, m\rangle = e^{-\frac{i}{\hbar}\theta\hbar m}|s, m\rangle = e^{-im\theta}|s, m\rangle \quad (8.7.112)$$

$$\implies \hat{U}_{\text{int}}(\theta) \sum_{m=-s}^s |s, m\rangle\langle s, m| = \sum_{m=-s}^s e^{-im\theta}|s, m\rangle\langle s, m| \quad (8.7.113)$$

$$\implies \hat{U}_{\text{int}}(\theta) = \sum_{m=-s}^s e^{-im\theta}|s, m\rangle\langle s, m|. \quad (8.7.114)$$

In particular for a rotation by 2π this becomes:

$$\hat{U}_{\text{int}}(2\pi) = \sum_{m=-s}^s e^{-2\pi im}|s, m\rangle\langle s, m|. \quad (8.7.115)$$

If s is an integer then so is m . $e^{-2\pi im}$ for all integer m is just 1. If s is an integer plus a half then so is m . $e^{-2\pi im}$ for all half-integers m is just -1 . These can both be captured $(-1)^{2s}$ which is 1 for s and integer and -1 for s a half more than an integer. Therefore, this can be simplified as:

$$\hat{U}_{\text{int}}(2\pi) = \sum_{m=-s}^s (-1)^{2s}|s, m\rangle\langle s, m| = (-1)^{2s} \mathbb{1} \quad (8.7.116)$$

$$\implies V^a_b = (-1)^{2s}\delta^a_b. \quad (8.7.117)$$

Then, under a rotation by 2π , equation (8.7.2) becomes:

$$\psi'^a(t, \vec{x}) = (-1)^{2s}\delta^a_b\psi^b(t, \vec{x}) = (-1)^{2s}\psi^a(t, \vec{x}) \quad (8.7.118)$$

$$\implies |\psi'\rangle = (-1)^{2s}|\psi\rangle. \quad (8.7.119)$$

Here $\vec{x}'$ has simply been replaced by $\vec{x}$ because under a 2π rotation any point in space returns to that same point. So, we see under such a rotation the wavefunction may or may not pick up a minus sign, depending on its spin. One may be surprised that such a sign can appear as a 2π rotation ought to return the world back to the way it was. Those who aren't careful treat the possibility of a minus sign on $|\psi\rangle$ after a 2π rotation as one of the great mysteries of quantum mechanics, proof that it can never be understood. It is true that you cannot understand quantum mechanics if you ignore how quantum mechanics works. Recall that the overall phase of the wavefunction is meaningless and this minus sign can just be viewed as accumulating an overall phase of π . In particular, $|\psi'\rangle$ and $|\psi\rangle$ here produce all of the same operator summaries:

$$\langle\psi'|\hat{G}|\psi'\rangle = (-\langle\psi|)\hat{G}(-|\psi\rangle) = \langle\psi|\hat{G}|\psi\rangle \quad (8.7.120)$$

and so because these are the quantities which we relate to experiment, this phase is meaningless. All generators of all the physical properties of the system are returned exactly to what they were after a 2π rotation, exactly as you would expect. This sign means nothing physically, but it does have consequences mathematically. Due to this minus sign, it actually takes a rotation by 4π to return the wavefunction back to itself in general. This is the essence of the difference between $\text{SO}(3)$ and $\text{SU}(2)$. The group $\text{SO}(3)$ only has representations which return to themselves after a 2π rotation (and thus only have integer s) whereas $\text{SU}(2)$ allows for half-integer s . These half-integer representations are allowed because $|\psi\rangle$ and $-|\psi\rangle$ correspond to the same physical state.

The commutation relations satisfied by the angular momentum operators in equation (8.7.21) define what is called the $\text{su}(2)$ algebra. Looking at the lowest dimensional representation of those commutators, $D = 1$, we see from Theorem 8.11 that:

$$s = 0 \implies \hat{S}_x = \hat{S}_y = \hat{S}_z = 0. \quad (8.7.121)$$

These operators do in fact satisfy the commutation relations trivially and so this representation is called the trivial representation. The smallest representation which satisfies the commutation relations without just simply making all of the operators 0 is for $D = 2$ and consequently $s = \frac{1}{2}$. Then, we see from Theorem 8.11

that:

$$s = \frac{1}{2} \implies \hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.7.122)$$

These are called the fundamental representation of the $\mathfrak{su}(2)$ Lie algebra for being the smallest non-trivial representation. These are all 2x2 self-adjoint matrices with 0 trace and so the rotations they create on the internal space are 2x2 unitary matrices:

$$\hat{U}_{\text{int}} = e^{-\frac{i}{\hbar}(\theta_x \hat{S}_x + \theta_y \hat{S}_y + \theta_z \hat{S}_z)} \implies \hat{U}^\dagger = e^{\frac{i}{\hbar}(\theta_x \hat{S}_x + \theta_y \hat{S}_y + \theta_z \hat{S}_z)} = \hat{U}^{-1}. \quad (8.7.123)$$

As well, because these $\hat{S}_a$ are traceless, the determinant of $\hat{U}_{\text{int}}$ is automatically 1. This can be shown by using that the determinant of a diagonalizable matrix is given by the product of its eigenvalues and the trace is given by the sum of its eigenvalues:

$$\det(\hat{U}_{\text{int}}) = \det\left(e^{-\frac{i}{\hbar}\theta^a \hat{S}_a}\right) = \prod_n \lambda_n = \prod_n e^{\ln \lambda_n} = e^{\sum_n \ln \lambda_n} = e^{\text{Tr}(\ln \hat{U})} = e^{\text{Tr}(-\frac{i}{\hbar}\theta^a \hat{S}_a)} = e^0 = 1. \quad (8.7.124)$$

Thus, the Lie group made by the internal rotations is the Lie group of 2x2 Unitary matrices of determinant 1. So, it is said to be the Special (meaning determinant 1) Unitary group of 2x2 matrices also known as $\text{SU}(2)$. All of the other angular momentum representations are just different representations of $\text{SU}(2)$. When we originally started studying rotations we were considering 3x3 rotation matrices and found that they satisfied the same commutation relations. The group of 3x3 rotation matrices is called the Special Orthogonal group of 3x3 matrices also known as $\text{SO}(3)$. Because the commutation relations are the same, the Lie algebras of $\text{SU}(2)$ and $\text{SO}(3)$ are the same. However, the Lie groups are not quite the same. As we found $\text{SU}(2)$ matrices require a 4π rotation to return to the identity whereas $\text{SO}(3)$ matrices only require a 2π rotation. In fact, for every $\text{SO}(3)$ matrix there are two $\text{SU}(2)$ matrices which correspond to it (a particular matrix and its negative). So, the Lie group $\text{SU}(2)$ is the “double-cover” of $\text{SO}(3)$ as there is a map from $\text{SU}(2)$ into $\text{SO}(3)$ which preserves the commutation relations but it is 2-to-1, not 1-to-1. Since we tend to think in 3 dimensions rather than 2x2 matrices, we also call the group of rotations as given here by $\text{SU}(2)$ as the group $\text{Spin}(3)$.

$\text{SU}(2)$ or $\text{Spin}(3)$ has several nice properties that $\text{SO}(3)$ does not. One of particular help is that $\text{SU}(2)$ is simply connected, while $\text{SO}(3)$ is not simply connected. A 3x3 rotation matrix is determined by a unit vector $\vec{n}$ as the axis of rotation and a magnitude θ as the angle of rotation. We only ever need to define rotations with magnitude $\leq \pi$ because a rotation by an angle of greater than π is equivalent to a rotation in the opposite direction by an angle less than π . With this, we can visualize $\text{SO}(3)$ as a ball in 3 spatial dimensions of radius π . Every point in the ball specifies θ by its distance from the origin and $\vec{n}$ as the unit vector from the origin to that point. However, antipodal points on this ball (meaning points which are directly opposite each other, like the north pole and the south pole) actually correspond to the same rotation. A rotation in the z direction by π is the same as a rotation in the $-z$ direction by π . So, $\text{SO}(3)$ is really like a ball of radius π with antipodal points identified with each other. One can consider a path running directly from the north pole of the ball to the south pole. This path is technically a closed loop because the north and south poles are the same rotation. However, there is no way to continuously deform this closed loop within the ball so that it shrinks down to a single point. Because of this, $\text{SO}(3)$ is not simply connected. However, $\text{SU}(2)$ is the double-cover of $\text{SO}(3)$. $\text{SU}(2)$ can instead be thought of as two balls of radius π where the north pole of one ball is identified with the south pole of the other (and similarly so for each antipodal point pair). In this two ball picture, every closed loop can be continuously deformed to a point, and so $\text{SU}(2)$ is simply connected.

8.7.2 Spherical Harmonics

Let us now study the angular momentum commutation relations with specific attention to orbital angular momentum. To do so it is nicest to use spherical coordinates (r, θ, φ) . Then, the orbital angular momentum operators become:

$$\langle \vec{x} | \hat{L}_x | \psi \rangle = \langle \vec{x} | (\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) | \psi \rangle = -i\hbar \left(y \frac{\partial \psi}{\partial z} - z \frac{\partial \psi}{\partial y} \right) = i\hbar \left(\sin \varphi \frac{\partial \psi}{\partial \theta} + \frac{\cos \varphi}{\tan \theta} \frac{\partial \psi}{\partial \varphi} \right) \quad (8.7.125)$$

$$\langle \vec{x} | \hat{L}_y | \psi \rangle = \langle \vec{x} | (\hat{z} \hat{p}_x - \hat{x} \hat{p}_z) | \psi \rangle = -i\hbar \left(z \frac{\partial \psi}{\partial x} - x \frac{\partial \psi}{\partial z} \right) = i\hbar \left(-\cos \varphi \frac{\partial \psi}{\partial \theta} + \frac{\sin \varphi}{\tan \theta} \frac{\partial \psi}{\partial \varphi} \right) \quad (8.7.126)$$

$$\langle \vec{x} | \hat{L}_z | \psi \rangle = \langle \vec{x} | (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) | \psi \rangle = -i\hbar \left(x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x} \right) = -i\hbar \frac{\partial \psi}{\partial \varphi}. \quad (8.7.127)$$

As well, $\hat{L}^2$ becomes after a bit of effort:

$$\langle \vec{x} | \hat{L}^2 | \psi \rangle = -\hbar^2 \left(\frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial \psi}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \varphi^2} \right) \quad (8.7.128)$$

So, if we define the $\hat{r} = \sqrt{\hat{x}^2 + \hat{y}^2 + \hat{z}^2}$, we can immediately see that $\hat{r}$ commutes with all 3 $\hat{L}_a$ because they contain no r derivatives when put into coordinates. Because they commute, we can find a simultaneous eigenbasis. In fact, at fixed r , ψ is only a function of θ and φ and so at fixed r we can define the Hilbert space of functions of (θ, φ) $\mathbb{H}_\Omega$. This is the space of functions on the sphere (which we can take by definition to be the unit sphere). Let $Y_\alpha(\theta, \varphi)$ be an orthonormal basis of such functions. Then, $\psi(t, \vec{x})$ at fixed r can necessarily be written as a linear combination of them. For different values of r and t the coefficients of linear combination will be different and so for some coefficients $R_\alpha(t, r)$ we have:

$$\psi(t, \vec{x}) = \sum_\alpha R_\alpha(t, r) Y_\alpha(\theta, \varphi). \quad (8.7.129)$$

Our angular momentum operators then can be considered as operators on only $\mathbb{H}_\Omega$. Then, if we have $|l, m\rangle$ as the eigenvectors of the angular momentum operators in that space:

$$\hat{L}^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle, \quad \hat{L}_z |l, m\rangle = \hbar m |l, m\rangle. \quad (8.7.130)$$

Letting $Y_{lm}(\theta, \varphi)$ be the corresponding wavefunctions (called the spherical harmonics):

$$\langle \vec{x} | \hat{L}^2 |l, m\rangle = -\hbar^2 \left(\frac{\partial^2 Y_{lm}}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial Y_{lm}}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{lm}}{\partial \varphi^2} \right) = \hbar^2 l(l+1) Y_{lm} \quad (8.7.131)$$

$$\implies \frac{\partial^2 Y_{lm}}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial Y_{lm}}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_{lm}}{\partial \varphi^2} + l(l+1) Y_{lm} = 0. \quad (8.7.132)$$

$$\langle \vec{x} | \hat{L}_z |l, m\rangle = -i\hbar \frac{\partial Y_{lm}}{\partial \varphi} = \hbar m Y_{lm} \quad (8.7.133)$$

$$\implies \frac{\partial Y_{lm}}{\partial \varphi} = im Y_{lm}. \quad (8.7.134)$$

The last of these conditions gives:

$$\frac{1}{Y_{lm}} \frac{\partial Y_{lm}}{\partial \varphi} = im \implies Y_{lm}(\theta, \varphi) = e^{im\varphi} P_{lm}(\theta) \quad (8.7.135)$$

for some $P_{lm}(\theta)$. The wavefunction given in equation (8.7.134) is differentiable. In order to be differentiable it must first be continuous. Because the points identified at $\varphi = 0$ and $\varphi = 2\pi$ for fixed r and θ exactly the same point in space, this requires:

$$\psi(t, r, \theta, 2\pi) = \psi(t, r, \theta, 0). \quad (8.7.136)$$

Consequently, the Y_{lm} must satisfy the same condition as they are a particular choice of wavefunction:

$$Y_{lm}(\theta, 2\pi) = Y_{lm}(\theta, 0) \implies e^{2\pi im} P_{lm}(\theta) = P_{lm}(\theta) \implies e^{2\pi im} = 1. \quad (8.7.137)$$

This condition is only true for integer m . Therefore **while half-integer angular momentum is perfectly allowed for spin, for orbital angular momentum only the integer eigenvalues are allowed** by the boundary conditions. Then, equation (8.7.131) becomes:

$$\frac{\partial^2 P_{lm}}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial P_{lm}}{\partial \theta} + \left(l(l+1) - \frac{m^2}{\sin^2 \theta} \right) P_{lm} = 0. \quad (8.7.138)$$

We can solve this differential equation for the $P_{lm}(\theta)$ by using our $\hat{L}_\pm$ operators. By definition:

$$\hat{J}_+ |l, l\rangle = 0 \implies \langle \vec{x} | (\hat{J}_x + i\hat{J}_y) |l, l\rangle = 0 \implies i\hbar e^{i\varphi} \left(\frac{1}{\tan \theta} \frac{\partial Y_{ll}}{\partial \varphi} - i \frac{\partial Y_{ll}}{\partial \theta} \right) = 0 \quad (8.7.139)$$

$$\implies \frac{\partial P_{ll}}{\partial \theta} = \frac{l}{\tan \theta} P_{ll} \quad (8.7.140)$$

$$\implies \frac{\partial}{\partial \theta} (\ln P_{ll} - l \ln \sin \theta) = 0 \quad (8.7.141)$$

$$\implies P_{ll}(\theta) = N \sin^l \theta \quad (8.7.142)$$

for some normalization factor N . We can set this normalization factor by considering our normalization of the wavefunctions $Y_{lm}(\theta, \varphi)$. Because we are considering them on the sphere, we normalize them on the unit

sphere:

$$\langle l, m | l, m \rangle = \int_{\Omega} Y_{lm}^*(\theta, \varphi) Y_{lm}(\theta, \varphi) d\Omega = \int_0^{\pi} \int_0^{2\pi} |Y_{lm}(\theta, \varphi)|^2 \sin \theta d\varphi d\theta \stackrel{!}{=} 1 \quad (8.7.143)$$

In particular, for Y_{ll} this becomes:

$$1 = \int_0^{\pi} \int_0^{2\pi} |N e^{il\varphi} \sin^l \theta|^2 \sin \theta d\varphi d\theta = |N|^2 \int_0^{\pi} d\varphi \int_0^{\pi} \sin^{2l+1} \theta d\theta \quad (8.7.144)$$

$$= 2\pi |N|^2 \int_0^{\pi} \sin^{2l+1} \theta d\theta = 2\pi |N|^2 2^{2l+1} \frac{l!^2}{(2l+1)!} \quad (8.7.145)$$

$$\Rightarrow |N| = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}}. \quad (8.7.146)$$

Here we have used the integral identity:

$$\int_0^{\pi} \sin^{2l+1} \theta d\theta = 2^{2l+1} \frac{l!^2}{(2l+1)!} \quad (8.7.147)$$

which is proven in the homework. By convention, we choose N to be real and to have sign so that it is positive for even l and negative for odd l so then:

$$Y_{ll}(\theta, \varphi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{il\varphi} \sin^l \theta. \quad (8.7.148)$$

From equation (8.7.84) then we have:

$$|l, m-1\rangle = \frac{1}{\hbar \sqrt{l(l+1) - m(m-1)}} \hat{L}_- |l, m\rangle \quad (8.7.149)$$

$$\Rightarrow Y_{l(m-1)} = \frac{1}{\hbar \sqrt{l(l+1) - m(m-1)}} i\hbar e^{-i\varphi} \left(\frac{1}{\tan \theta} \frac{\partial Y_{lm}}{\partial \varphi} + i \frac{\partial Y_{lm}}{\partial \theta} \right) \quad (8.7.150)$$

$$\Rightarrow P_{l(m-1)}(\theta) = -\frac{1}{\sqrt{l(l+1) - m(m-1)}} \left(\frac{\partial P_{lm}}{\partial \theta} + \frac{m}{\tan \theta} P_{lm} \right). \quad (8.7.151)$$

Starting from $P_{ll}(\theta)$ which we have found, we can use equation this to recursively compute all of the P_{lm} for $m < l$. Thus, this fully determines all of the spherical harmonics. In particular, using an integrating factor we can write the right hand side as:

$$P_{l(m-1)}(\theta) = -\frac{1}{\sqrt{l(l+1) - m(m-1)}} \frac{1}{\sin^m \theta} \frac{\partial}{\partial \theta} (\sin^m \theta P_{lm}). \quad (8.7.152)$$

Then, defining $x = \cos \theta$ and $Q_{lm}(x) = \sin^m \theta P_{lm}(\theta)$ this becomes:

$$Q_{l(m-1)}(x) = \frac{1}{\sqrt{l(l+1) - m(m-1)}} \frac{\partial Q_{lm}}{\partial x} \quad (8.7.153)$$

$$\Rightarrow Q_{lm}(x) = \prod_{n=m}^{l-1} \left(\frac{1}{\sqrt{l(l+1) - n(n-1)}} \right) \left(\frac{\partial}{\partial x} \right)^{l-m} Q_{ll}(x). \quad (8.7.154)$$

This last formula is gotten by applying equation (8.7.153) $l-m$ times. Renaming the product variable to $k = l-n$, we have:

$$\prod_{n=m}^{l-1} \left(\frac{1}{\sqrt{l(l+1) - n(n-1)}} \right) = \prod_{k=1}^{l-m} \frac{1}{\sqrt{k(2l+1-k)}} \quad (8.7.155)$$

$$= \frac{1}{\sqrt{1 \cdot 2 \cdot \dots \cdot (l-m)}} \frac{1}{\sqrt{(l+m+1) \dots (2l)}} \quad (8.7.156)$$

$$= \frac{1}{\sqrt{(l-m)!}} \sqrt{\frac{(l+m)!}{(2l)!}}. \quad (8.7.157)$$

Then, recalling the definition of x , $Q_{lm}(x)$, and $P_{ll}(\theta)$:

$$Q_{lm}(x) = \sqrt{\frac{(l+m)!}{(l-m)!(2l)!}} \left(\frac{\partial}{\partial x} \right)^{l-m} \left(\frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} (1-x^2)^l \right) \quad (8.7.158)$$

$$\Rightarrow Y_{lm}(\theta, \varphi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!} \frac{e^{im\varphi}}{\sin^m(\theta)}} \left(\frac{\partial}{\partial \cos(\theta)} \right)^{l-m} \sin^{2l}(\theta). \quad (8.7.159)$$

Altogether, we have that a spatial wavefunction $\psi(t, \vec{x})$ may be expressed in spherical coordinates as:

$$\psi(t, \vec{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l R_{lm}(t, r) Y_{lm}(\theta, \varphi) \quad (8.7.160)$$

where $Y_{lm}(\theta, \varphi)$ are the spherical harmonics given explicitly by (8.7.159) and $R_{lm}(t, r)$ are the radial wavefunctions corresponding to each value of l, m . The spherical harmonics are the eigenfunctions of the orbital angular momentum operators in the sense that when they are expressed as states $|l, m\rangle$ in the Hilbert space of functions on the unit sphere, they are orthonormal and satisfy (8.7.130).

Exercises

Problem 8.38: Spin Precession. Consider a quantum system with a wavefunction of spin s and Hamiltonian operator:

$$\hat{H} = \omega \vec{n} \cdot \hat{\vec{S}}$$

for a constant unit vector $\vec{n}$ and constant ω .

(a) Show using Ehrenfest's theorem that the total spin angular momentum of the wavefunction satisfies:

$$\frac{d\vec{S}}{dt} = \omega \vec{n} \times \vec{S}.$$

(b) Solve this equation of motion to show that the spin evolves in time as:

$$\vec{S}(t) = \vec{S}(0) \cos \omega t + \vec{n} \vec{n} \cdot \vec{S}(0) (1 - \cos \omega t) + \vec{n} \times \vec{S}(0) \sin \omega t.$$

Interpret this result geometrically.

Problem 8.39: Spin-1/2 Rotations. For this question it is useful to remember the results of 8.4. By the logic leading to (8.7.111), for a wavefunction of spin s , a rotation by angle θ in the (unit vector) $\vec{n}$ direction is represented on the internal space by the operator:

$$\hat{U} = e^{-\frac{i}{\hbar} \theta \vec{n} \cdot \hat{\vec{S}}}.$$

In this question we will specialize our interest to wavefunctions of spin $s = 1/2$.

(a) Let $\hat{S}_n = \vec{n} \cdot \hat{\vec{S}}$. Show that the eigenstates of $\hat{S}_n$ are given by:

$$|+\rangle = \begin{pmatrix} e^{-\frac{i\varphi}{2}} \cos \frac{\theta}{2} \\ e^{\frac{i\varphi}{2}} \sin \frac{\theta}{2} \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} -e^{-\frac{i\varphi}{2}} \sin \frac{\theta}{2} \\ e^{\frac{i\varphi}{2}} \cos \frac{\theta}{2} \end{pmatrix}$$

$$\hat{S}_n |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle$$

where the angles θ and φ are defined in the usual way by the spherical coordinates representation of $\vec{n}$.

(b) Show that the general rotation operator $\hat{U}$ on the internal space can be written explicitly as:

$$\hat{U} = \cos \left(\frac{\theta}{2} \right) \mathbb{1} - i \sin \left(\frac{\theta}{2} \right) \vec{n} \cdot \hat{\vec{\sigma}}$$

where $\hat{\vec{\sigma}}$ is the vector of Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Problem 8.40: Spin-1 and electromagnetic polarization vectors. A three dimensional vector rotates irreducibly and carries 3 independent components, thus it must correspond in spin representation to spin-1, as it is the irreducible representation of dimension 3. Suppose we have a spin-1 (vectorial) wavefunction.

(a) Explicitly compute the spin matrices for spin-1 using Theorem 8.11 to show that:

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}} (|1, -1\rangle \langle 1, 0| + |1, 0\rangle \langle 1, -1| + |1, 1\rangle \langle 1, 0| + |1, 0\rangle \langle 1, 1|),$$

$$\hat{S}_y = \frac{i\hbar}{\sqrt{2}} (|1, -1\rangle \langle 1, 0| - |1, 0\rangle \langle 1, -1| + |1, 0\rangle \langle 1, 1| - |1, 1\rangle \langle 1, 0|),$$

$$\hat{S}_z = \hbar|1, 1\rangle\langle 1, 1| - \hbar|1, -1\rangle\langle 1, -1|.$$

- (b) Show that each of $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ have an eigenvector with eigenvalue of 0. Explain that consequently any rotation on the internal space leaves a particular direction vector unchanged. Define $|x\rangle$, $|y\rangle$, $|z\rangle$ as the unit vectors in the directions left unchanged by x, y, z rotations respectively. Explain why this means $|x\rangle$, $|y\rangle$, $|z\rangle$ must correspond geometrically to the x, y, z coordinate directions. Show that $|x\rangle$, $|y\rangle$, $|z\rangle$ are given explicitly by:

$$|x\rangle = \frac{1}{\sqrt{2}}(|1, 1\rangle - |1, -1\rangle), \quad |y\rangle = -\frac{i}{\sqrt{2}}(|1, 1\rangle + |1, -1\rangle), \quad |z\rangle = -|1, 0\rangle.$$

Show that these can be inverted to give:

$$|1, 1\rangle = \frac{|x\rangle + i|y\rangle}{\sqrt{2}}, \quad |1, 0\rangle = -|z\rangle, \quad |1, -1\rangle = \frac{-|x\rangle + i|y\rangle}{\sqrt{2}}.$$

Thus explain how the $|l, m\rangle$ states for spin-1 correspond exactly with the helicity basis vectors found previously in our studies of electromagnetism (such as in problems 4.40, 4.44).

- (c) Show that in terms of $|x\rangle$, $|y\rangle$, $|z\rangle$, the spin-1 matrices can be written as:

$$\hat{S}_x = i\hbar(|z\rangle\langle y| - |y\rangle\langle z|) \quad \hat{S}_y = i\hbar(|x\rangle\langle z| - |z\rangle\langle x|) \quad \hat{S}_z = i\hbar(|y\rangle\langle x| - |x\rangle\langle y|)$$

and show that using the $\hat{J}$ matrices originally defined in section 2.4 these are given simply by:

$$\hat{S}_a = i\hbar\hat{J}_a.$$

Show that the internal rotation matrix $\hat{U}$ then for spin-1 can be identified precisely with our previous definition of a 3x3 rotation matrix $\hat{R}$:

$$\hat{U} = e^{-\frac{i}{\hbar}\theta^a\hat{S}_a} = e^{\theta^a\hat{J}_a} = \hat{R}.$$

Problem 8.41: An Integral Identity. For this question it is useful to recall the definitions of the Gamma function $\Gamma(x)$ and the Beta function $B(x, y)$. Consider the integral:

$$I(l) = \int_0^\pi \sin^{2l+1} \theta d\theta$$

for nonnegative integer l .

- (a) Let $x = \cos^2 \theta$ to show that the integral becomes:

$$I(l) = \int_0^1 x^{-\frac{1}{2}} (1-x)^l dx.$$

- (b) Now use the definition of the Beta function to show that:

$$I(l) = B\left(\frac{1}{2}, l+1\right) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma(l+1)}{\Gamma\left(l+\frac{3}{2}\right)}.$$

- (c) Use that the Gamma function satisfies $\Gamma(x+1) = x\Gamma(x)$ to show:

$$\Gamma\left(l+\frac{3}{2}\right) = \frac{\Gamma\left(\frac{1}{2}\right)}{2^{l+1}} \prod_{k=0}^l (2k+1).$$

- (d) Use the definition of the factorial to show:

$$\prod_{k=0}^l (2k+1) = \frac{(2l+1)!}{2^l l!}.$$

- (e) Return these results to the integral and simplify to find:

$$I(l) = 2^{2l+1} \frac{l!^2}{(2l+1)!}.$$

Problem 8.42: The Schwinger Model. Consider a quantum system with Hilbert space spanned by the orthonormal states labeled $|n_a, n_b\rangle$ where n_a and n_b each run from 0, 1, 2, 3, 4, ... which represent the eigenstates of two independent quantum harmonic oscillators with annihilation operators $\hat{a}$ and $\hat{b}$. That is:

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= [\hat{b}, \hat{b}^\dagger] = 1, & [\hat{a}, \hat{b}] &= [\hat{a}^\dagger, \hat{b}] = 0, \\ \hat{a}|n_a, n_b\rangle &= \sqrt{n_a}|n_a-1, n_b\rangle, & \hat{b}|n_a, n_b\rangle &= \sqrt{n_b}|n_a, n_b-1\rangle. \end{aligned}$$

Define the operators:

$$\hat{J}_x = \frac{\hbar}{2}(\hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a}), \quad \hat{J}_y = \frac{\hbar}{2i}(\hat{a}^\dagger \hat{b} - \hat{b}^\dagger \hat{a}), \quad \hat{J}_z = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b}), \quad \hat{J} = \frac{\hbar}{2}(\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b}).$$

(a) Show that $\hat{J}_x, \hat{J}_y, \hat{J}_z$ satisfy the SU(2) algebra:

$$[\hat{J}_a, \hat{J}_b] = i\hbar \epsilon_{ab}^{c} \hat{J}_c$$

and that:

$$[\hat{J}_a, \hat{J}] = 0, \quad \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = \hat{J}(\hat{J} + \hbar \mathbb{1}).$$

(b) Show using knowledge about the quantum harmonic oscillator that the eigenvalues of $\hat{J}$ come in half-integers (0, 1/2, 1, 3/2, ...) and that the eigenspace of $\hat{J}$ with eigenvalue $\hbar j$ forms an irreducible representation of the space of angular momentum j . Show explicitly that the $|j, m\rangle_{\text{AM}}$ angular momentum states can be related to the $|n_a, n_b\rangle_{\text{HO}}$ harmonic oscillator states by:

$$|j, m\rangle_{\text{AM}} = |j + m, j - m\rangle_{\text{HO}}.$$

(c) Show that this two harmonic oscillator model of angular momentum, called the Schwinger model, contains precisely one representation of every possible angular momentum.

Problem 8.43: Central Potential Problem. Consider a nonrelativistic scalar Schrödinger wave in 3 spatial dimensions subject to a spherically symmetric potential $U(r)$ so that the Hamiltonian operator of the system is:

$$\hat{H} = \frac{|\hat{\vec{p}}|^2}{2M} + U(\hat{r}).$$

(a) Show that $|\hat{\vec{p}}|^2$ can be written in the form:

$$|\hat{\vec{p}}|^2 = \hat{p}_r^2 + \frac{\hat{L}^2}{\hat{r}^2}$$

where $\hat{p}_r$ is defined so that:

$$\langle \vec{x} | \hat{p}_r | \psi \rangle = -i\hbar \left(\frac{\partial \psi}{\partial r} + \frac{\psi}{r} \right).$$

Show that:

$$\hat{p}_r = \hat{p}_r^\dagger, \quad [\hat{r}, \hat{p}_r] = i\hbar \mathbb{1}.$$

(b) Show using the decomposition in (8.7.160) that the eigenfunctions of this Hamiltonian operator with eigenvalue E can be written in the form:

$$\psi_{Elm}(\vec{x}) = R_{El}(r) Y_{lm}(\theta, \varphi)$$

where Y_{lm} are the spherical harmonics and the radial functions R_{El} satisfy:

$$\frac{\partial^2 R_{El}}{\partial r^2} + \frac{2}{r} \frac{\partial R_{El}}{\partial r} - \frac{l(l+1)}{r^2} R_{El} - \frac{2M}{\hbar^2} (U(r) - E) R_{El} = 0.$$

Thus, the eigenvalue problem for spherically symmetric potentials can be reduced to this radial ordinary differential equation.

Problem 8.44: The Eccentricity Vector in Classical Mechanics. In this question we will study a purely classical mechanical system. The insights we learn we help us later study a corresponding quantum system. Consider a nonrelativistic point particle with mass m evolving according to the Hamiltonian:

$$\mathcal{H} = \frac{|\vec{p}|^2}{2m} - \frac{K}{r}$$

for a positive constant K . Define the eccentricity vector:

$$\vec{\varepsilon} = \frac{1}{mK} \vec{p} \times \vec{L} - \frac{\vec{x}}{r}.$$

(a) Show that:

$$\{\vec{\varepsilon}, \mathcal{H}\} = 0, \quad \{\varepsilon_a, L_b\} = \epsilon_{ab}^{c} \varepsilon_c, \quad \{\varepsilon_a, \varepsilon_b\} = -\frac{2\mathcal{H}}{mK^2} \epsilon_{ab}^{c} L_c.$$

- (b) Show that $\vec{\varepsilon}$ is conserved in time and that geometrically $|\vec{\varepsilon}|$ equals the eccentricity of the orbit, using knowledge of the Kepler problem. $\vec{\varepsilon}$ (up to a constant multiplier) has been discovered and rediscovered many times and is often called the Laplace-Runge-Lenz vector.
- (c) Define:

$$\vec{D} = K \sqrt{\frac{m}{2|\mathcal{H}|}} \vec{\varepsilon}.$$

Consider positive energy trajectories of the motion (unbound orbits, hyperbolas specifically by using Kepler's laws); show that:

$$\{D_a, D_b\} = -\epsilon_{ab}^c L_c, \quad \{D_a, L_b\} = \epsilon_{ab}^c D_c, \quad \{L_a, L_b\} = \epsilon_{ab}^c L_c$$

and that this closed algebra is precisely the Lie algebra of $\mathfrak{so}(3,1)$ (mathematically the same algebra as that of the connected Lorentz group).

- (d) Consider negative energy trajectories of the motion (bound orbits, ellipses specifically by using Kepler's laws); show that:

$$\{D_a, D_b\} = \epsilon_{ab}^c L_c, \quad \{D_a, L_b\} = \epsilon_{ab}^c D_c, \quad \{L_a, L_b\} = \epsilon_{ab}^c L_c$$

and that this closed algebra is precisely the Lie algebra of $\mathfrak{so}(4)$ (mathematically the same algebra as that of rotations in 4 spatial dimensions).

Problem 8.45: ★ Solving the Hydrogen Atom. A hydrogen atom consists of a positively charged proton of charge q_e and mass m_p and negatively charged electron of charge $-q_e$ and mass m_e . (In magnitude the proton charge is by all experiments equal in magnitude to the electron charge. This enormous “coincidence” will get a lot more attention in later chapters.) The separation between the electron and the proton is very large compared to the size of either and the mass of the proton is much larger than the mass of the electron. So, the electric field produced by the proton is approximately the electric field of a point charge of charge q_e in the neighborhood of the electron (using the exterior multipole expansion) and we can approximate the proton as not moving.

- (a) Explain based on the above physical properties why the approximate Hamiltonian operator of the electron as a Schrödinger wave can be taken to be:

$$\hat{H} = \frac{|\hat{p}|^2}{2m_e} - \frac{q_e^2}{4\pi\epsilon_0 \hat{r}}.$$

For the rest of this question we will let $M = m_e$ and $K = \frac{q_e^2}{4\pi\epsilon_0}$ and we will seek to determine all of the eigenstates of this Hamiltonian operator for bound states of the system (states in which the electron stays finitely close to the proton).

- (b) Using the radial equation from problem 8.43, show that bound orbits must have energy eigenvalue $E < 0$ as for $E > 0$ the solutions become asymptotically plane waves (and so are not spatially bounded; the electron extends arbitrarily far from the proton).
- (c) Define the eccentricity vector operator $\hat{\varepsilon}$ and $\hat{D}$ exactly analogously to the classical quantities:

$$\hat{\varepsilon} = \frac{1}{2MK} (\hat{p} \times \hat{L} - \hat{L} \times \hat{p}) - \frac{\hat{x}}{\hat{r}}, \quad \hat{D} = K \sqrt{\frac{M}{2|\hat{H}|}} \hat{\varepsilon}.$$

Show that these operators are self-adjoint and that:

$$|\hat{\varepsilon}|^2 = \mathbb{1} + \frac{2\hat{H}}{MK^2} (\hat{L}^2 + \hbar^2 \mathbb{1}).$$

Further, show that when acting on bound states:

$$\mathbb{1} + \frac{2\hat{H}}{MK^2} (\hbar^2 \mathbb{1} + \hat{L}^2 + \hat{D}^2) = 0.$$

- (d) Show that:

$$[\hat{D}, \hat{H}] = 0, \quad \hat{L} \cdot \hat{D} = \hat{D} \cdot \hat{L} = 0.$$

- (e) Let:

$$\hat{B}_{\pm} = \frac{\hat{L} \pm \hat{D}}{2}.$$

Show that:

$$[\hat{B}_{\pm}, \hat{H}] = 0, \quad [\hat{B}_{+a}, \hat{B}_{+b}] = i\hbar\epsilon_{ab}^c \hat{B}_{+c}, \quad [\hat{B}_{+a}, \hat{B}_{-b}] = 0, \quad [\hat{B}_{-a}, \hat{B}_{-b}] = i\hbar\epsilon_{ab}^c \hat{B}_{-c}.$$

(f) Let:

$$\hat{C}_+ = \hat{B}_+^2 + \hat{B}_-^2, \quad \hat{C}_- = \hat{B}_+^2 - \hat{B}_-^2.$$

Considering only acting on bound states, show that:

$$\hat{C}_- = 0, \quad [\hat{C}_+, \hat{H}] = [\hat{C}_+, \hat{L}_a] = 0, \quad \mathbb{1} + \frac{2\hat{H}}{MK^2}(\hbar^2 \mathbb{1} + 2\hat{C}_+) = 0, \quad \hat{C}_+|\psi\rangle = 2\hbar^2 b(b+1)|\psi\rangle$$

where $|\psi\rangle$ is a simultaneous eigenstate of $\hat{H}$, $\hat{C}_+$, $\hat{L}^2$, $\hat{L}_z$ (explain why such eigenstates exist) and b is an arbitrary half-integer (explain why it must be a half-integer).

(g) Let $n = 2b + 1$ be an arbitrary whole number. Show using the above results that the energy eigenvalues of the hydrogen atom are given by:

$$E_n = -\frac{MK^2}{2\hbar^2 n^2} = -\frac{m_e q_e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

and that the total orbital angular momentum eigenvalue l must satisfy $l < n$.

(h) Show that the radial part of the wavefunction R_{nl} for eigenstates of $\hat{H}$ satisfy:

$$\frac{\partial^2 R_{nl}}{\partial r^2} + \frac{2}{r} \frac{\partial R_{nl}}{\partial r} - \frac{l(l+1)}{r^2} R_{nl} + \frac{2MK}{\hbar^2 r} R_{nl} - \left(\frac{MK}{\hbar^2 n}\right)^2 R_{nl} = 0.$$

(i) The radial equation is still quite nasty. Change variables to $x = \frac{2MK}{n\hbar^2} r$ and define the function:

$$f_{nl}(x) = x^{-l} e^{\frac{x}{2}} R_{nl} \left(\frac{n\hbar^2}{2MK} x \right) \implies R_{nl}(r) = \left(\frac{2MK}{n\hbar^2} r \right)^l e^{-\frac{MKr}{n\hbar^2}} f_{nl} \left(\frac{2MK}{n\hbar^2} r \right).$$

Show that $f_{nl}(x)$ satisfies:

$$x f_{nl}''(x) + (2l + 2 - x) f_{nl}'(x) + (n - l - 1) f_{nl}(x) = 0.$$

(j) The differential equation satisfied by f_{nl} can be put in a more standard mathematical form by defining $\alpha = 2l + 1$ and $k = n - l - 1$. Then, let $g(x)$ be a generic function satisfying:

$$x g''(x) + (\alpha + 1 - x) g'(x) + k g(x) = 0.$$

This differential equation can be solved by the Frobenius method. Near $x = 0$ the solution will behave at worst like $x^{-\beta}$ for some nonnegative power β so that we can develop a Taylor series solution for $g(x)$ as:

$$g(x) = \sum_{j=0}^{\infty} c_j x^{j-\beta}.$$

Explain why, by returning our definitions to the original wavefunction, in order for $g(x)$ participate in a physically reasonable solution for the hydrogen atom (and so be square-integrable) we must have $\beta \leq l + 1$. Then, show by inserting the series solution for $g(x)$ into the differential equation that the two possible values of β are 0 and $2l + 1$ and thus conclude that $\beta = 0$. Further, show that the c_j coefficients satisfy:

$$c_{j+1} = -\frac{k-j}{(j+1)(j+\alpha+1)} c_j.$$

(k) Show that up to an arbitrary choice of c_0 , the c_j are solved by:

$$c_j = \frac{(-1)^j}{j!} \binom{k+\alpha}{k-j}$$

and consequently that $g(x)$ is a polynomial (known as the generalized Laguerre polynomial of $L_k^{(\alpha)}(x)$) given by:

$$g(x) = L_k^{(\alpha)}(x) = \sum_{j=0}^k \frac{(-1)^j}{j!} \binom{k+\alpha}{k-j} x^j = \frac{x^{-\alpha} e^x}{k!} \left(\frac{\partial}{\partial x} \right)^k (e^{-x} x^{\alpha+k}) = \frac{x^{-\alpha}}{k!} \left(\frac{\partial}{\partial x} - 1 \right)^k x^{\alpha+k}.$$

(l) Normalize the wavefunction to have norm 1 and show finally that the radial solution to the Hydrogen

atom is given by:

$$R_{nl}(r) = \left(\frac{2MK}{n\hbar^2}\right)^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{2n(n+l)!}} \left(\frac{2MK}{n\hbar^2}r\right)^l L_{n-l-1}^{(2l+1)}\left(\frac{2MK}{n\hbar^2}r\right) e^{-\frac{MKr}{n\hbar^2}}.$$

Note that the radial wavefunctions depend on a single overall length scale a_0 given by:

$$a_0 = \frac{\hbar^2}{MK} = \frac{4\pi\epsilon_0\hbar^2}{q_e^2 m_e}$$

known as the Bohr radius. Experimentally, its value is $a_0 = 5.29177210903(80) \times 10^{-11}\text{m}$ thus characterizing the size of the hydrogen atom. However, while we know the values of q_e , ϵ_0 , and m_e by previous experiments or choice of units, in order to determine a_0 we need to know the value of $\hbar$ in our unit system which we will determine in the next problem.

(m) Explain that any bound solution to the Hydrogen atom is given in the form:

$$\psi(t, \vec{x}) = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^l C_{nlm} e^{-\frac{i}{\hbar} E_n t} R_{nl}(r) Y_{lm}(\theta, \varphi)$$

for some initial conditions C_{nlm} and that each energy level (determined by n) has degeneracy n^2 .

Problem 8.46: ★ Atomic Spectral Lines and Measuring $\hbar$. This problem is based on chapter 9 of [66]. Consider an electron in an atom, modeled so that the electron has wavefunction $\psi(t, \vec{x})$ with Hamiltonian operator $\hat{H}_0$. This Hamiltonian operator will take the form:

$$\hat{H}_0 = \frac{|\hat{p}|^2}{2m} + \hat{U}(\hat{x})$$

where $U(\vec{x})$ is some potential which encodes the atomic structure. The particular details of this potential will be generally irrelevant for this question. We assume that we know the normalized eigenstates $|n\rangle$ of $\hat{H}_0$ and that they have eigenvalues E_n (such as for the hydrogen atom). Now consider this electron to be perturbed by an incoming electromagnetic plane wave. Choose the gauge of the plane wave so that it takes the form:

$$\phi = 0, \quad \vec{A} = \epsilon \text{Re} \left(\vec{\xi} e^{i(\vec{k} \cdot \vec{x} - \omega t)} \right)$$

where ϵ is a constant encoding the strength of the plane wave, $\vec{\xi}$ is a complex unit vector encoding the polarization of the plane wave with $\vec{k} \cdot \vec{\xi} = 0$, and $\omega = c|\vec{k}|$ due to the dispersion relation for Maxwell's equations in free space.

(a) Show that the perturbed electron now satisfies the Schrödinger equation with a new Hamiltonian operator $\hat{H}$ which can be put in the form:

$$\hat{H} = \hat{H}_0 + \epsilon \hat{H}_1 + \mathcal{O}(\epsilon^2)$$

where $\hat{H}_1$ is independent of ϵ and show in particular that:

$$\hat{H}_1 = -\frac{q}{2m} e^{i\vec{k} \cdot \vec{x} - i\omega t} \vec{\xi} \cdot \hat{\vec{p}} - \frac{q}{2m} e^{-i\vec{k} \cdot \vec{x} + i\omega t} \vec{\xi}^* \cdot \hat{\vec{p}}.$$

(b) Assume that the electromagnetic plane-wave has wavelength much longer than the atomic size. Show that this allows us to approximate $\hat{H}_1$ as:

$$\hat{H}_1 = -\frac{q}{m} \text{Re} \left(e^{-i\omega t} \vec{\xi} \right) \cdot \hat{\vec{p}}.$$

Show that for the hydrogen atom this approximation is valid for a plane-wave with frequency ω such that:

$$\omega \ll \frac{q_e^2 m_e c}{2\epsilon_0 \hbar^2}.$$

(c) While we have not yet discussed precisely how to apply thermodynamics and statistical mechanics to quantum mechanics, you should be unsurprised to learn that in thermodynamic equilibrium the distribution of states of a statistical sample of atoms will be proportional to $e^{-\frac{E}{T}}$ where E is the energy of that state and T is the temperature. If there is a significant gap between the ground state (the lowest energy state) energy eigenvalue of the atom and the energy eigenvalue of the next lowest state (called the first excited state) compared to the temperature of the system, the atoms will overwhelmingly be in the ground state. For now, we will simply assume this to be true (physically it is very accurate for

ordinary atoms at or below ordinary temperatures¹⁰). Let $|g\rangle$ be the ground state of the atom and let it have energy eigenvalue E_g . Assume that the atom is initially in the ground state before being perturbed by the electromagnetic field. Show that the solution to the Schrödinger equation has the form:

$$|\psi(t)\rangle = e^{-i\frac{E_g}{\hbar}t}|g\rangle + \epsilon|\delta\psi(t)\rangle + \mathcal{O}(\epsilon^2)$$

where $|\delta\psi(t)\rangle$ evolves according to:

$$i\hbar\frac{d|\delta\psi\rangle}{dt} = \hat{H}_0|\delta\psi\rangle - \frac{q}{m}e^{-i\frac{E_g}{\hbar}t}\text{Re}\left(e^{-i\omega t}\vec{\xi}\right) \cdot \hat{\vec{p}}|g\rangle.$$

Let $a_n(t)$ be defined by:

$$a_n(t) = e^{i\frac{E_n}{\hbar}t}\langle n|\delta\psi(t)\rangle$$

where $|n\rangle$ are orthonormal eigenstates of $\hat{H}_0$ and E_n are the corresponding eigenvalues. Show that:

$$\frac{da_n}{dt} = \frac{iq}{m\hbar}e^{i\frac{E_n}{\hbar}(E_n-E_g)t}\text{Re}\left(e^{-i\omega t}\vec{\xi}\right) \cdot \langle n|\hat{\vec{p}}|g\rangle.$$

Solve this differential equation to show that $|\delta\psi(t)\rangle$ is given explicitly by:

$$|\delta\psi(t)\rangle = \frac{q}{2m}e^{-i\frac{E_g}{\hbar}t}\sum_n\left(\frac{e^{-i\omega t}\vec{\xi}}{E_n-E_g-\hbar\omega} + \frac{e^{i\omega t}\vec{\xi}^*}{E_n-E_g+\hbar\omega}\right) \cdot \langle n|\hat{\vec{p}}|g\rangle|n\rangle.$$

(d) Using (8.6.130), compute the integral of the current density $\vec{J}$ over all space. Show that:

$$\begin{aligned}\int_{\mathbb{S}}\vec{J}(t,\vec{x})d^3\vec{x} &= \frac{q}{m}\langle\psi|(\hat{\vec{p}}-q\vec{A})|\psi\rangle \\ &= \frac{q}{m}\langle g|\hat{\vec{p}}|g\rangle + \frac{q^2\epsilon}{m^2}\text{Re}\left(\sum_n\left(\frac{e^{-i\omega t}\vec{\xi}}{E_n-E_g-\hbar\omega} + \frac{e^{i\omega t}\vec{\xi}^*}{E_n-E_g+\hbar\omega}\right) \cdot \langle n|\hat{\vec{p}}|g\rangle\langle g|\hat{\vec{p}}|n\rangle\right) \\ &\quad - \frac{q^2\epsilon}{m}\text{Re}\left(\vec{\xi}e^{-i\omega t}\right) + \mathcal{O}(\epsilon^2).\end{aligned}$$

Using the results of problems 4.55 and 4.56, show that (in the fully nonrelativistic limit), the electromagnetic radiation vector $\vec{\alpha}_*(t, \theta, \varphi)$ becomes:

$$\vec{\alpha}_* = \frac{q^2\omega\epsilon}{m^2}\text{Im}\left(\sum_n\left(\frac{e^{-i\omega t}\vec{\xi}}{E_n-E_g-\hbar\omega} - \frac{e^{i\omega t}\vec{\xi}^*}{E_n-E_g+\hbar\omega}\right) \cdot \langle n|\hat{\vec{p}}|g\rangle\langle g|\hat{\vec{p}}|n\rangle\right) - \frac{q^2\omega\epsilon}{m}\text{Im}\left(\vec{\xi}e^{-i\omega t}\right).$$

(e) Show using the result of problem 4.59 that the total electromagnetic scattering cross section of light off of the atom is given by:

$$\sigma = \frac{\mu_0^2 q^4}{12\pi m^2}\text{Tr}(\perp \hat{K}^2(\omega))$$

where $\perp$ is a 3x3 projection matrix that projects out components of a vector in the direction of the incoming wavenumber $\vec{k}$:

$$\perp = \mathbb{1} - \frac{\vec{k}\vec{k}}{|\vec{k}|^2}$$

and $\hat{K}$ is the 3x3 matrix with components:

$$K_{ab}(\omega) = \delta_{ab} - \frac{1}{m}\sum_n\left(\frac{\langle g|\hat{p}_a|n\rangle\langle n|\hat{p}_b|g\rangle}{E_n-E_g-\hbar\omega} + \frac{\langle g|\hat{p}_b|n\rangle\langle n|\hat{p}_a|g\rangle}{E_n-E_g+\hbar\omega}\right).$$

Notice that the cross section becomes very large whenever $E_g + \hbar\omega$ approaches an eigenvalue of $\hat{H}_0$ (due to the denominator $E_n - E_g - \hbar\omega$ in the definition of $\hat{K}$). Notice further that because E_g is the lowest eigenvalue of $\hat{H}_0$ and $\omega > 0$ by definition, the denominator $E_n - E_g + \hbar\omega$ never gets near 0 and so never contributes the same peak behavior that the $E_n - E_g - \hbar\omega$ denominator does. Because of this, when the incoming beam of light on the atom is tuned to have appropriate frequency, a stimulated emission of

¹⁰Those who do know how to treat this with statistical mechanics may object that the partition function of the hydrogen atom is divergent. This divergence is due to the very slow fall off of the Coulomb interaction and can be removed as a problem by cutting off the involved integrals at a finite volume, computing physical quantities from the cutoff results, and then taking the cutoff to infinity at the end. See [8]

light from the atom will occur, which is confirmed by experiment. That significantly increased response of the atom thus occurs at $\hbar\omega = E_n - E_g$ for some n and gives a direct probe of the atomic energy eigenvalues and a way to measure the value of $\hbar$. These peaks in the emitted light of stimulated atoms are called the atomic spectral lines. They provide a direct access point to the (relative to the ground state) energy eigenvalues of an atomic system.

- (f) Suppose we target hydrogen atoms with our light. Let ω_n be the angular frequency at which peak emission occurs for transitions from the hydrogen ground state with energy eigenvalue $E_g = E_1$ to a state of hydrogen energy eigenvalue E_n . Show that the value of $\hbar$ is given by:

$$\hbar = \left(\frac{m_e q_e^4}{32\pi^2 \epsilon_0^2} \frac{1 - \frac{1}{n^2}}{\omega_n} \right)^{\frac{1}{3}}$$

and that by scanning over a range of such n allows the accurate measurement of the value of $\hbar$. In SI units the value of $\hbar$ is exactly:

$$\hbar = \frac{6.62607015}{2\pi} \times 10^{-34} \frac{\text{kg m}^2}{\text{s}}$$

(The value of $\hbar$ is exact because as of 2019 SI units defines the unit of the kilogram so that $\hbar$ takes this value. Historical SI units chose a particular arbitrary object as having a mass of a kilogram, in terms of which the value of $\hbar$ could be measured.) Explain how alternatively using natural units in which $\hbar = \epsilon_0 = 1$, this same experiment provides a measurement of the electron mass in natural units.

- (g) Use the given value of $\hbar$ to check the value of the Bohr radius given in problem 8.45.
 (h) Show using the formula for the hydrogen spectrum that the hydrogen ground state energy is:

$$E_1 = -13.605693122994(26) \text{ eV}.$$

Compute the energy of the first excited state of hydrogen and show that at any reasonable temperature our assumption that the hydrogen is in the ground state is valid.

Problem 8.47: ★ The Photoelectric Effect. This problem is based on [59]. When we solved the hydrogen atom previously, we only considered states in which the electron was bound to the proton. Consequently, the electron wavefunction decayed quickly at large distances. It is also possible to consider unbound states in which the electron becomes arbitrarily far away from the proton.

- (a) Suppose that the electron is able to get arbitrarily far away from the proton. Show that when it does so the asymptotic behavior of the electron wavefunction can be expanded in terms of plane waves and that the energy of the electron is greater than 0. Suppose instead that the electron is bound. Show that its energy is less than 0. (Use the Hamiltonian operator from the hydrogen atom question; the choice of gauge that the potential from the proton should go to 0 at spatial infinity determines the 0 point of the energy which is in general gauge dependent.) Note that the bound eigenstates of the hydrogen atom are square-integrable and have discretely separated energy eigenvalues while the unbounded “eigenstates” are actually generalized eigenstates in the rigged Hilbert space, in the sense that they are not square-integrable (they are asymptotically plane-waves) and also they have take any positive energy as an eigenvalue. The magnitude of the energy of a bound state is called the binding energy Φ of that state.
- (b) Consider the setup of the the previous problem with the electron in the atom beginning in its ground state $|g\rangle$ with energy $E_g = -\Phi$ subject to an incoming electromagnetic plane wave as described in that problem but also subject to a uniform voltage V . Generalize the result of Fermi’s Golden Rule by considering the time dependent perturbation found in the previous problem to show that to lowest order in perturbation theory the transition rate for the electron from $|g\rangle$ to a different atomic eigenstate $|n\rangle$ from an unpolarized light beam is:

$$\Gamma_n = \frac{\pi q^2 \epsilon^2}{4\hbar m^2} \delta(E_n + \Phi - \hbar\omega) \langle n | \hat{p} | g \rangle \perp \langle g | \hat{p} | n \rangle.$$

- (c) Let Γ be the total transition rate for electrons to go from the ground state to an unbound state and suppose that in the unbound region the uniform potential has dropped off to zero. Let $T(E, V) = |t|^2$ where t is the transmission coefficient for an unbound electron in the region of voltage V to escape to the region of voltage 0 so that its final energy is E . Show that Γ is given by:

$$\Gamma = \int_{\mathbb{R}^3} \frac{\pi q^2 \epsilon^2}{4\hbar m^2} T(E(\vec{p}), V) \delta(E(\vec{p}) + \Phi - qV - \hbar\omega) \langle \psi_{\vec{p}} | \hat{p} | g \rangle \perp \langle g | \hat{p} | \psi_{\vec{p}} \rangle d^3 \vec{p}$$

where $E(\vec{p}) = \frac{|\vec{p}|^2}{2m}$ and $|\psi(\vec{p})\rangle$ is the unbound atomic eigenstate which asymptotically at large distances becomes a conventionally normalized eigenvector of the momentum operator $\hat{p}$.

- (d) Suppose that the unpolarized beam of light is shone on a material so that effectively N electrons in a material are subject to the perturbation and suppose that the electrons which escape due to the light (called photoelectrons) travel toward a conducting wire so that they produce an electrical current I which can be measured. Show that the electrical current is given by:

$$I = qN\Gamma.$$

Notice that the current is proportional to the intensity of the incoming light and that there is a critical frequency $\omega_{\min} = \frac{\Phi}{\hbar}$ below which no current is produced at $V = 0$. Now suppose we adjust the voltage V until the electrical current drops to 0. The voltage at which this occurs is called the stopping voltage V_{stop} . Recall that q_e is used for the magnitude of the electron charge, so that $q = -q_e$ and $q_e > 0$. Show that the stopping voltage is given by:

$$V_{\text{stop}} = \frac{\hbar\omega - \Phi}{q_e}.$$

Explain that given that we know the electron charge from previous experiments, by measuring the stopping voltage across many different frequencies of incoming light we can measure the values of $\hbar$ and the binding energy Φ of our material by plotting V_{stop} versus ω . Notice that the stopping voltage depends only on the frequency of the light and not at all on its intensity¹¹.

Problem 8.48: ★ The Fine-Structure Constant. Let $E_e = m_e c^2$ be the electron rest energy (using the relativistic energy zero-point).

- (a) Using the previously established value of the electron mass, show that E_e is given by:

$$E_e = 510.99895000(15) \text{ keV}$$

(keV = kiloelectronvolts = 10^3 eV). In natural units then the above is the value of the electron mass.

- (b) Show that the energy eigenvalues of the hydrogen atom can be expressed as:

$$E_n = -\frac{\alpha^2 E_e}{2n^2}$$

where α , known as the **fine-structure constant**, is a dimensionless physical constant defined by:

$$\alpha = \frac{q_e^2}{4\pi\epsilon_0\hbar c}.$$

- (c) Explain from all three perspectives of historical SI units in which $q_e, \epsilon_0, \hbar, c$ are measured, modern SI in which ϵ_0 is measured and $q_e, \hbar, c$ are defined by exact values, and natural units in which q_e is measured and $\epsilon_0 = \hbar = c = 1$ that by combining the results of previously described experiments we can measure the value of α . Show using the established values of $q_e, \epsilon_0, \hbar, c$ that α takes the value:

$$\alpha = 0.0072973525693(11).$$

From this show that the magnitude of the electron charge in natural units, more generally called the **elementary charge e** is:

$$e = \sqrt{4\pi\alpha} = 0.302822120872(22).$$

α or equivalently **e** is a fundamental parameter of our universe which cannot be gotten rid of by any choice of unit system. It is determined only by experiment. If you found a theory that could derive the value of α mathematically, you would have an instant Nobel prize. The elementary charge (also called the electromagnetic coupling constant) **e** is always unitless. It is related to the magnitude of the electron charge q_e in SI units by:

$$q_e = e\sqrt{\epsilon_0\hbar c}.$$

Because the proton has exactly charge q_e , the neutron has exactly charge 0, and the electron has exactly charge $-q_e$ and all atomic matter is comprised of these constituents, the electric charge q of any object

¹¹Readers who have heard introductory explanations of the photoelectric effect before are likely surprised to see an explanation of the effect without any reference to the concept of a photon. This is because the photon concept has nothing to do with the photoelectric effect; the common confusion to the contrary is a historical accident.

consisting of these particles is of the form:

$$q = Qq_e = Q\mathbf{e}\sqrt{\epsilon_0\hbar c}$$

where Q is an **integer** known as the “charge number” of the object (we will see in the next chapter that because other particles exist than protons, neutrons, and electrons the Q for those particles is a rational number instead). Essentially, Q is the charge of the object “in units of q_e ”. Unfortunately, myself and other physicists will lazily call q , $\mathbf{e}$, or Q simply “charge” from time to time, and one has to understand which is intended from context.

8.8 Spinor Theory - The Pauli Equation

The first theory to study after the scalar (spin-0) theory with $D = 2s + 1 = 1$ is the spinor (spin-1/2) theory with $D = 2s + 1 = 2$. While the spin-0 theory is pretty good for describing the behavior of electrons in some experiments, it turns out that electrons are spin-1/2 particles (we will study how this is demonstrated in the homework). Because the wavefunction of a spin-1/2 particle has 2 components, we write $\psi(t, \vec{x})$ as:

$$\psi(t, \vec{x}) = \psi_+(t, \vec{x}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_-(t, \vec{x}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \quad (8.8.1)$$

where the vector with the upper component 1 corresponds to $|\frac{1}{2}, \frac{1}{2}\rangle$, the vector in the spin space with $\hat{S}_z$ eigenvalue of $\hbar/2$ and the vector with lower component 1 corresponds to $|\frac{1}{2}, -\frac{1}{2}\rangle$, the vector in the spin space with $\hat{S}_z$ eigenvalue of $-\hbar/2$ and $\psi_{\pm}$ correspond to the components of ψ in each of these two directions in the spin space. From Theorem 8.11, immediately in this notation the spin matrices for spin-1/2 are given by:

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.8.2)$$

It is useful to define the Pauli matrices σ_a as the matrices appearing here without the factors of $\frac{\hbar}{2}$:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.8.3)$$

We will make repeated use of these matrices, so remember them! By direct calculation, they satisfy several very nice properties. In particular:

$$\sigma_a \sigma_b - \sigma_b \sigma_a = 2i\epsilon_{ab}^c \sigma_c \quad \sigma_a \sigma_b + \sigma_b \sigma_a = 2\delta_{ab} \mathbb{1}. \quad (8.8.4)$$

The first of these had to be true by definition of the spin operators but the second is non-trivial and highly convenient. Now let us go through the commutators again to find the Hamiltonian:

$$[\hat{x}, \hat{G}] = 0 \implies \hat{G} = \hat{G}(t, \hat{x}, \hat{S}). \quad (8.8.5)$$

Because $\hat{G}$ commutes with $\hat{x}$ it still cannot be a function of $\hat{p}$. However, now that we have spin degrees of freedom, each of the vector components of $\hat{G}$ is a 2x2 matrix on the spin space. Now commuting with the momentum:

$$[\hat{p}, \hat{G}] = im\mathbb{1} = m[\hat{x}, \hat{p}] \implies [\hat{p}, \hat{G} + m\hat{x}] = 0 \implies \hat{G} = -m\hat{x} + \hat{F}(t). \quad (8.8.6)$$

Now let us use parity symmetry. Parity by definition inverts space and so a Dirac delta at $\vec{x}$ becomes a Dirac delta at $-\vec{x}$:

$$\hat{\mathcal{P}}|\vec{x}\rangle \stackrel{\text{def}}{=} |-\vec{x}\rangle \quad (8.8.7)$$

$$\implies \hat{\mathcal{P}} \int_{\mathbb{S}} |\vec{x}\rangle \langle \vec{x}| d\mathbb{S} = \int_{\mathbb{S}} |-\vec{x}\rangle \langle \vec{x}| d\mathbb{S} \quad (8.8.8)$$

$$\implies \hat{\mathcal{P}} = \int_{\mathbb{S}} |-\vec{x}\rangle \langle \vec{x}| d\mathbb{S}. \quad (8.8.9)$$

Because this is supposed to be a symmetry transformation (and time is not reversed), this better be unitary by Wigner's Theorem. It is and in fact parity is its own inverse (this should not be surprising as inverting space twice brings everything back to its original orientation):

$$\hat{\mathcal{P}}^\dagger = \left(\int_{\mathbb{S}} |-\vec{x}\rangle \langle \vec{x}| d\mathbb{S} \right)^\dagger = \int_{\mathbb{S}} |\vec{x}\rangle \langle -\vec{x}| d\mathbb{S} = \int_{\mathbb{S}} |-\vec{x}\rangle \langle \vec{x}| d\mathbb{S} = \hat{\mathcal{P}} \quad (8.8.10)$$

$$\implies \hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} |\vec{x}\rangle = \hat{\mathcal{P}}^2 |\vec{x}\rangle = \hat{\mathcal{P}} |-\vec{x}\rangle = |\vec{x}\rangle \implies \hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} = \mathbb{1}. \quad (8.8.11)$$

This tells us how parity acts on the Hilbert space. It is also possible to act parity on the operators. Consider an orthonormal basis $|n\rangle$ and act an operator $\hat{\mathcal{O}}$ on it. By definition, $\hat{\mathcal{O}}|n\rangle$ must be in the Hilbert space and so can be written as a linear combination of the $|n\rangle$. Therefore, there exist coefficients $\mathcal{O}_{mn}$ so that:

$$\hat{\mathcal{O}}|n\rangle = \sum_{mn} \mathcal{O}_{mn} |m\rangle \quad (8.8.12)$$

$$\implies \hat{\mathcal{O}} \sum_n |n\rangle \langle n| = \sum_{mn} \mathcal{O}_{mn} |m\rangle \langle n| \quad (8.8.13)$$

$$\implies \hat{\mathcal{O}} = \sum_{mn} \mathcal{O}_{mn} |m\rangle \langle n|. \quad (8.8.14)$$

Now because we know how the vectors transform under parity, we can consider how the operators transform under parity as:

$$\hat{\mathcal{O}}' = \sum_{mn} \mathcal{O}_{mn} |m'\rangle \langle n'| = \sum_{mn} \mathcal{O}_{mn} \hat{\mathcal{P}} |m\rangle \langle n| \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} \sum_{mn} \mathcal{O}_{mn} |m\rangle \langle n| \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} \hat{\mathcal{O}} \hat{\mathcal{P}}^\dagger. \quad (8.8.15)$$

From this we can see that the $\hat{\vec{x}}$ and $\hat{\vec{p}}$ operators are inverted by parity:

$$\hat{\mathcal{P}} \hat{\vec{x}} \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} \int_{\mathbb{S}} \vec{x} |\vec{x}\rangle \langle \vec{x}| d\mathbb{S} \hat{\mathcal{P}}^\dagger = \int_{\mathbb{S}} \vec{x} |-\vec{x}\rangle \langle -\vec{x}| d\mathbb{S} = - \int_{\mathbb{S}} \vec{x} |\vec{x}\rangle \langle \vec{x}| d\mathbb{S} = -\hat{\vec{x}} \quad (8.8.16)$$

$$\hat{\mathcal{P}} \hat{\vec{p}} \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} \int_{\mathbb{S}} (-i\hbar \nabla) |\vec{x}\rangle \langle \vec{x}| d\mathbb{S} \hat{\mathcal{P}}^\dagger = \int_{\mathbb{S}} (-i\hbar \nabla) |-\vec{x}\rangle \langle -\vec{x}| d\mathbb{S} = \int_{\mathbb{S}} i\hbar \nabla |\vec{x}\rangle \langle \vec{x}| d\mathbb{S} = -\hat{\vec{p}}. \quad (8.8.17)$$

This exactly matches the classical transformation property of $\vec{x}$ and $\vec{p}$ under parity. Because $\hat{\vec{x}}$ and $\hat{\vec{p}}$ are inverted under parity, they are called parity odd. Anything which rotates by a rotation matrix when a rotation is applied and is parity odd is called a proper vector, so $\hat{\vec{x}}$ and $\hat{\vec{p}}$ are proper vectors. We can see how the orbital angular momentum changes:

$$\hat{\mathcal{P}} \hat{L}_a \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} \epsilon_{ab}^c \hat{x}^b \hat{p}_c \hat{\mathcal{P}}^\dagger = \epsilon_{ab}^c \hat{\mathcal{P}} \hat{x}^b \hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} \hat{p}_c \hat{\mathcal{P}}^\dagger = \epsilon_{ab}^c (-\hat{x}^b) (-\hat{p}_c) = \hat{L}_a. \quad (8.8.18)$$

So while the angular momentum does rotate by a rotation matrix, it is actually parity even (it is not inverted by parity). Such an object is called a pseudovector. Because angular momentum is a pseudovector, spin angular momentum is also parity even (angular momentum conservation conserves the total of $\vec{S} + \vec{L}$ and parity leaves $\vec{L}$ unchanged; therefore for the transformed angular momentum conservation to hold we need $\vec{S}$ to also stay $\vec{S}$ as angular momentum can flow between the two of them). Because $\vec{x}$ is inverted by parity and t is not, the velocity $\vec{v} = \frac{d\vec{x}}{dt}$ is also inverted under parity. Therefore, under parity a velocity boost goes to a boost by the same amount in the opposite direction which means that the generator of velocity boosts is also parity odd (in a theory with parity symmetry). So:

$$\hat{\mathcal{P}} \hat{\vec{S}} \hat{\mathcal{P}}^\dagger = \hat{\vec{S}}, \quad \hat{\mathcal{P}} \hat{\vec{v}} \hat{\mathcal{P}}^\dagger = -\hat{\vec{v}}, \quad \hat{\mathcal{P}} \hat{\vec{G}} \hat{\mathcal{P}}^\dagger = -\hat{\vec{G}}. \quad (8.8.19)$$

Now applying this to (8.8.6):

$$\hat{\mathcal{P}} \hat{\vec{G}} \hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}} (-m\hat{\vec{x}} + \hat{\vec{F}}(t, \hat{\vec{S}})) \hat{\mathcal{P}}^\dagger \quad (8.8.20)$$

$$\implies -\hat{\vec{G}} = m\hat{\vec{x}} + \hat{\vec{F}}(t, \hat{\vec{S}}). \quad (8.8.21)$$

By matching (8.8.21) to (8.8.6) we see that $\hat{\vec{F}} = 0$. Continuing with the final commutator:

$$[\hat{\vec{v}}, \hat{\vec{G}}] = i\hbar \mathbb{1} \quad (8.8.22)$$

$$\implies [\hat{\vec{v}}, -m\hat{\vec{x}}] = [\hat{\vec{x}}, \hat{\vec{p}}] \quad (8.8.23)$$

$$\implies [\hat{\vec{x}}, \hat{\vec{p}} - m\hat{\vec{v}}] = 0 \quad (8.8.24)$$

$$\implies \hat{\vec{p}} - m\hat{\vec{v}} = \hat{\vec{f}}(t, \hat{\vec{x}}) \quad (8.8.25)$$

for some $\hat{\vec{f}}(t, \hat{\vec{x}})$ which is again a 2x2 matrix on the spin space. To this point we haven't actually used that we are working with spin-1/2 (and so the results to this point apply to any spin) but here spin-1/2 will be critical. Consider an arbitrary self-adjoint operator $\hat{\mathcal{O}}$ on the spin space. Then, for some real coefficients a, b, c, d, e, f, g, h :

$$\hat{\mathcal{O}} = \begin{pmatrix} a + ib & c + id \\ e + if & g + ih \end{pmatrix} \quad (8.8.26)$$

$$\hat{\mathcal{O}}^\dagger = \begin{pmatrix} a - ib & e - if \\ c - id & g - ih \end{pmatrix} \stackrel{!}{=} \hat{\mathcal{O}} = \begin{pmatrix} a + ib & c + id \\ e + if & g + ih \end{pmatrix} \quad (8.8.27)$$

$$\implies b = 0, \quad e = c, \quad f = -d, \quad h = 0 \quad (8.8.28)$$

$$\implies \hat{\mathcal{O}} = \begin{pmatrix} a & c + id \\ c - id & g \end{pmatrix} = \frac{a+g}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + c \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - d \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{a-g}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8.8.29)$$

$$\implies \hat{\mathcal{O}} = \frac{a+g}{2} \mathbb{1} + c\sigma_1 - d\sigma_2 + \frac{a-g}{2} \sigma_3. \quad (8.8.30)$$

Hence any self-adjoint operator on the spin-1/2 space can be written as a linear combination of the identity on that space and the Pauli matrices (and correspondingly the spin matrices). Hence, for spin-1/2 we don't have to consider arbitrary functions of the spin and can instead take without loss of generality:

$$\hat{f}(t, \hat{x}) = \hat{K}(t, \hat{x}) \mathbb{1} + \hat{g}(t, \hat{x}) \cdot \hat{S} \quad (8.8.31)$$

here $\hat{K}$ is a vector of operators and $\hat{g}$ is a matrix of operators neither of which act on the spin space. Then we have:

$$\hat{p} - m\hat{v} = \hat{K}(t, \hat{x}) + \hat{g}(t, \hat{x}) \cdot \hat{S} \quad (8.8.32)$$

$$\implies \frac{\hat{p} - \hat{K} - \hat{g} \cdot \hat{S}}{m} = \hat{v} = \frac{1}{i\hbar} [\hat{x}, \hat{H}]. \quad (8.8.33)$$

Equation (8.8.33) is a pretty complicated restraint on $\hat{H}$ but we can solve it in steps. We know how to produce the first term from the spin-0 theory:

$$\frac{1}{i\hbar} [\hat{x}, \frac{|\hat{p} - \hat{K}|^2}{2m}] = \frac{\hat{p} - \hat{K}}{m}. \quad (8.8.34)$$

Therefore, define $\hat{H}_0$ as this term. We then have:

$$\hat{H}_0 = \frac{|\hat{p} - \hat{K}|^2}{2m} \quad (8.8.35)$$

$$\implies \frac{1}{i\hbar} [\hat{x}, \hat{H}_0] - \frac{\hat{g} \cdot \hat{S}}{m} = \frac{1}{i\hbar} [\hat{x}, \hat{H}] \quad (8.8.36)$$

$$\implies -\frac{\hat{g} \cdot \hat{S}}{m} = \frac{1}{i\hbar} [\hat{x}, \hat{H} - \hat{H}_0]. \quad (8.8.37)$$

Next we need to find a term with produces the left hand side of (8.8.37). It has no dependence on $\hat{p}$ and is the result of commuting with $\hat{x}$. Commuting with $\hat{x}$ kills one power of $\hat{p}$ and so the term will be some linear function of $\hat{p}$. Consider:

$$\hat{H}_1 = \frac{1}{2} \hat{p}^a \hat{O}_{ab}(t, \hat{x}) \hat{S}^b + \frac{1}{2} \hat{S}^b \hat{O}_{ab}^\dagger(t, \hat{x}) \hat{p}^a \quad (8.8.38)$$

$$\implies \frac{1}{i\hbar} [\hat{x}_c, \hat{H}_1] = \frac{1}{i\hbar} [\hat{x}_c, \frac{1}{2} \hat{p}^a \hat{O}_{ab} \hat{S}^b + \frac{1}{2} \hat{S}^b \hat{O}_{ab}^\dagger \hat{p}^a] \quad (8.8.39)$$

$$\implies \frac{1}{i\hbar} [\hat{x}_a, \hat{H}_1] = \frac{1}{2} \hat{O}_{ab} \hat{S}^b + \frac{1}{2} \hat{O}_{ab}^\dagger \hat{S}^b. \quad (8.8.40)$$

Hence by identifying:

$$\hat{g}_{ab} = -m \frac{\hat{O}_{ab} + \hat{O}_{ab}^\dagger}{2} \quad (8.8.41)$$

$$\implies -\frac{\hat{g} \cdot \hat{S}}{m} = \frac{1}{i\hbar} [\hat{x}, \hat{H}_1] \quad (8.8.42)$$

$$\implies 0 = \frac{1}{i\hbar} [\hat{x}, \hat{H} - \hat{H}_0 - \hat{H}_1] \quad (8.8.43)$$

$$\implies \hat{H} - \hat{H}_0 - \hat{H}_1 = \hat{H}_2(t, \hat{x}, \hat{S}) \quad (8.8.44)$$

for some $\hat{H}_2(t, \hat{x}, \hat{S})$. We can use our spin-1/2 trick from before to expand $\hat{H}_2$ as:

$$\hat{H}_2(t, \hat{x}, \hat{S}) = \hat{U}(t, \hat{x}) + \hat{v}(t, \hat{x}) \cdot \hat{S}. \quad (8.8.45)$$

Hence we can finally put together the most general Galilean symmetric Hamiltonian operator as:

$$\hat{H} = \frac{|\hat{p} - \hat{K}(t, \hat{x})|^2}{2m} + \hat{U}(t, \hat{x}) + \frac{1}{2} \hat{p}^a \hat{O}_{ab}(t, \hat{x}) \hat{S}^b + \frac{1}{2} \hat{O}_{ab}^\dagger(t, \hat{x}) \hat{p}^a \hat{S}^b + \hat{v}(t, \hat{x}) \cdot \hat{S}. \quad (8.8.46)$$

Now taking the parity of the Hamiltonian operator:

$$\hat{P} \hat{H} \hat{P}^\dagger = \hat{P} \frac{|\hat{p} - \hat{K}|^2}{2m} \hat{P}^\dagger + \hat{P} \hat{U} \hat{P}^\dagger + \hat{P} \frac{1}{2} \hat{p}^a \hat{O}_{ab} \hat{S}^b \hat{P}^\dagger + \hat{P} \frac{1}{2} \hat{O}_{ab}^\dagger \hat{p}^a \hat{S}^b \hat{P}^\dagger + \hat{P} \hat{v} \cdot \hat{S} \hat{P}^\dagger \quad (8.8.47)$$

$$= \frac{|\hat{p}\hat{p}^\dagger - \hat{p}\hat{K}\hat{p}^\dagger|^2}{2m} + \hat{p}\hat{U}\hat{p}^\dagger + \frac{1}{2}\hat{p}\hat{p}^a\hat{p}^\dagger\hat{p}\hat{O}_{ab}\hat{p}^\dagger\hat{p}\hat{S}^b\hat{p}^\dagger + \frac{1}{2}\hat{p}\hat{O}_{ab}^\dagger\hat{p}^\dagger\hat{p}\hat{p}^a\hat{p}^\dagger\hat{p}\hat{S}^b\hat{p}^\dagger + \hat{p}\hat{v}\hat{p}^\dagger \cdot \hat{p}\hat{S}\hat{p}^\dagger \quad (8.8.48)$$

$$= \frac{|\hat{p} + \hat{p}\hat{K}\hat{p}^\dagger|^2}{2m} + \hat{p}\hat{U}\hat{p}^\dagger - \frac{1}{2}\hat{p}^a\hat{p}\hat{O}_{ab}\hat{p}^\dagger\hat{S}^b - \frac{1}{2}\hat{p}\hat{O}_{ab}^\dagger\hat{p}^\dagger\hat{p}^a\hat{S}^b + \hat{p}\hat{v}\hat{p}^\dagger \cdot \hat{S} \quad (8.8.49)$$

$$\stackrel{!}{=} \hat{H} = \frac{|\hat{p} - \hat{K}|^2}{2m} + \hat{U} + \frac{1}{2}\hat{p}^a\hat{O}_{ab}\hat{S}^b + \frac{1}{2}\hat{O}_{ab}^\dagger\hat{p}^a\hat{S}^b + \hat{v} \cdot \hat{S} \quad (8.8.50)$$

$$\implies \hat{p}\hat{K}\hat{p}^\dagger = -\hat{K}, \quad \hat{p}\hat{U}\hat{p}^\dagger = \hat{U}, \quad \hat{p}\hat{O}_{ab}\hat{p}^\dagger = -\hat{O}_{ab}, \quad \hat{p}\hat{v}\hat{p}^\dagger = \hat{v}. \quad (8.8.51)$$

Hence these are the required parity transformation of each these unknown quantities for the Hamiltonian operator to have parity symmetry. If the spin-1/2 particle is free (so that the Hamiltonian should have translational and rotational symmetry as well), then all of the appearing quantities must be independent of $\hat{x}$ and t (and so $\hat{U}$ becomes a constant removable by a gauge transformation), the vectors $\hat{K}$ and $\hat{v}$ become 0, and $\hat{O}_{ab}$ becomes proportional to δ_{ab} and then must be 0 due to its parity transformation property. So, for a free spin-1/2 particle we recover $\hat{H} = \frac{|\hat{p}|^2}{2m}$, just as for a scalar particle.

Now let us consider our spin-1/2 theory interacting with the electromagnetic potentials. Just as before, it is possible for us to make local U(1) transformations by the same phase transformation done in (8.6.61) and doing so again reproduces the same replacement $\hat{p} \rightarrow \hat{p} - q\hat{A}$ and $\hat{H} \rightarrow \hat{H} + q\hat{\phi}$ which produces the correct electromagnetic coupling in the classical limit. So again we have the covariant derivative with the same definition and have to have each derivative (momentum operator) pick up a connection term to have the gauge symmetry. This allows us to make the correspondence again that $\hat{K} = q\hat{A}$ and $\hat{U} = q\hat{\phi}$. So:

$$\hat{H} = \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} + \frac{1}{2}\hat{p}^a\hat{O}_{ab}\hat{S}^b + \frac{1}{2}\hat{O}_{ab}^\dagger\hat{p}^a\hat{S}^b + \hat{v} \cdot \hat{S}. \quad (8.8.52)$$

We can split up $\hat{O}$ in terms of its self-adjoint and anti-self-adjoint parts. Define:

$$\hat{Y}_{ab} = \frac{\hat{O}_{ab} + \hat{O}_{ab}^\dagger}{2}, \quad \hat{Z}_{ab} = \frac{\hat{O}_{ab} - \hat{O}_{ab}^\dagger}{2i} \quad (8.8.53)$$

$$\implies \hat{O}_{ab} = \hat{Y}_{ab} + i\hat{Z}_{ab}, \quad \hat{O}_{ab}^\dagger = \hat{Y}_{ab} - i\hat{Z}_{ab}. \quad (8.8.54)$$

Here both $\hat{Y}_{ab}(t, \hat{x})$ and $\hat{Z}_{ab}(t, \hat{x})$ are self-adjoint operators. Returning these to the Hamiltonian operator:

$$\hat{H} = \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} + \frac{1}{2}(\hat{p}^a\hat{Y}_{ab} + \hat{Y}_{ab}\hat{p}^a)\hat{S}^b + \frac{i}{2}(\hat{p}^a\hat{Z}_{ab} - \hat{Z}_{ab}\hat{p}^a)\hat{S}^b + \hat{v} \cdot \hat{S}. \quad (8.8.55)$$

Consider how the $\hat{Z}_{ab}$ part of the Hamiltonian operator acts on an arbitrary wavefunction:

$$\langle \hat{x} | \frac{i}{2}(\hat{p}^a\hat{Z}_{ab} - \hat{Z}_{ab}\hat{p}^a)\hat{S}^b | \psi \rangle = \frac{i}{2}[-i\hbar\nabla_a, Z^{ab}(t, \vec{x})]\hat{S}_b\psi(t, \vec{x}) = \frac{\hbar}{2}(\nabla_a Z^{ab})\hat{S}^b\psi. \quad (8.8.56)$$

Thus, we can equivalently write the Hamiltonian operator as:

$$\hat{H} = \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} + \frac{1}{2}(\hat{p}^a\hat{Y}_{ab} + \hat{Y}_{ab}\hat{p}^a)\hat{S}^b + \left(\hat{v}^b + \frac{\hbar}{2}(\nabla_a \hat{Z}^{ab})(t, \vec{x}) \right) \hat{S}_b. \quad (8.8.57)$$

This is precisely of the same form as (8.8.52) but with $\hat{v}$ shifted by this $\hat{Z}$ piece and with $\hat{O}$ replaced only by its self-adjoint part $\hat{Y}$. Consequently, we can take without loss of generality $\hat{O}$ to be self-adjoint and use the appropriately shift $\hat{v}$ so that now:

$$\hat{H} = \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} + \frac{1}{2}\hat{p}^a\hat{O}_{ab}\hat{S}^b + \frac{1}{2}\hat{O}_{ab}\hat{p}^a\hat{S}^b + \hat{v} \cdot \hat{S}. \quad (8.8.58)$$

Next we would like to understand what form $\hat{O}_{ab}$ and $\hat{v}$ take specifically. By our parity analysis, $\hat{O}$ has to be parity odd and because it is in a dot product with a vector (momentum) and a pseudovector (spin), in order for it to not break rotational invariance it has to transform under rotations like a matrix as $\hat{O}' = \hat{R}\hat{O}\hat{R}^T$. Because out of the electromagnetic potentials and fields we only have $\phi, \vec{A}, \vec{E}, \vec{B}$ dependence, we can restrict the possibilities for $\hat{O}$ greatly. We have already established in problem 4.79 that under rotations ϕ is a scalar and $\vec{A}$ is a vector and that consequently $\vec{E}$ is a vector and $\vec{B}$ is a pseudovector. If the only other fields for ψ to interact with are the electromagnetic ones, then $\hat{O}$ must be some linear combination of all of

the outer products we can make from $\vec{A}, \vec{B}, \vec{E}$ with coefficients that may depend on the fields and potentials as well as a term corresponding to the identity matrix (the only rotationally invariant matrix):

$$\begin{aligned}\hat{O}_{ab} = & \alpha\delta_{ab} + \mathfrak{b}\epsilon_{abc}A^c + \mathfrak{c}\epsilon_{abc}E^c + \mathfrak{d}\epsilon_{abc}B^c + eA_aB_b + \mathfrak{f}A_aE_b + \mathfrak{g}A_aB_b + \mathfrak{h}E_aA_b \\ & + iE_aE_b + jE_aB_b + \mathfrak{k}B_aA_a + \ell B_aE_b + mB_aB_b\end{aligned}\quad (8.8.59)$$

All of the terms with a factor of $\vec{A}$ are not gauge invariant and no combination of them restores gauge invariance. Therefore, to maintain the gauge invariance of the theory, $\hat{O}$ is reduced to:

$$\hat{O}_{ab} = \alpha\delta_{ab} + \mathfrak{c}\epsilon_{abc}E^c + \mathfrak{d}\epsilon_{abc}B^c + iE_aE_b + jE_aB_b + \ell B_aE_b + mB_aB_b. \quad (8.8.60)$$

To maintain the Galilean boost symmetry of the Hamiltonian, $\hat{O}$ must be unchanged by a boost. Because $\vec{E}$ is changed by a Galilean boost (by (3.3.77)) but $\vec{B}$ is not, we are left with:

$$\hat{O}_{ab} = \alpha\delta_{ab} + \mathfrak{d}\epsilon_{abc}B^c + mB_aB_b. \quad (8.8.61)$$

Now under parity we have:

$$\hat{O}'_{ab} = \alpha'\delta_{ab} + \mathfrak{d}'\epsilon_{abc}B'^c + m'B'_aB'_b = \alpha'\delta_{ab} - \mathfrak{d}'\epsilon_{abc}B^c + mB_aB_b \stackrel{!}{=} -\hat{O}_{ab} \quad (8.8.62)$$

$$\implies \alpha' = -\alpha, \quad \mathfrak{d}' = \mathfrak{d}, \quad m' = -m. \quad (8.8.63)$$

Hence the coefficient functions $\alpha, \mathfrak{d}, m$ must be gauge, Galilean, and rotation invariant while $\mathfrak{d}$ is parity even and α and m are parity odd. We know that there are only two gauge, Galilean, and rotation invariant quantities we can make of out the fields, $|\vec{B}|^2$ and $\vec{E} \cdot \vec{B}$. Further, $\vec{E} \cdot \vec{B}$ is actually odd under parity. Hence, for some functions D_1, D_2, D_3 we have that:

$$\alpha = \vec{E} \cdot \vec{B} D_1(|\vec{B}|^2, (\vec{E} \cdot \vec{B})^2), \quad \mathfrak{d} = D_2(|\vec{B}|^2, (\vec{E} \cdot \vec{B})^2), \quad m = \vec{E} \cdot \vec{B} D_3(|\vec{B}|^2, (\vec{E} \cdot \vec{B})^2) \quad (8.8.64)$$

$$\implies \hat{O}_{ab} = \vec{E} \cdot \vec{B} (D_1\delta_{ab} + D_3B_aB_b) + D_2\epsilon_{abc}B^c. \quad (8.8.65)$$

This is the most general form for $\hat{O}$.

For $\hat{\vec{v}}$, it has to be parity even, rotate like a vector, be gauge invariant, and be Galilean invariant to not break the symmetries of the Hamiltonian. The only such vector we have which satisfies these properties is $\vec{B}$ and so for some function D_4 :

$$\vec{v} = D_4(|\vec{B}|^2, (\vec{E} \cdot \vec{B})^2)\vec{B}. \quad (8.8.66)$$

Together then, the most general Galilean symmetric Hamiltonian operator for a spin-1/2 charged particles interacting with electromagnetism is:

$$\begin{aligned}\hat{H} = & \frac{|\hat{\vec{p}} - q\hat{\vec{A}}|^2}{2m} + q\hat{\phi} + \frac{1}{2}((\hat{\vec{p}} \cdot \hat{\vec{S}}\hat{D}_1 + \hat{\vec{p}} \cdot \hat{\vec{B}}\hat{S} \cdot \hat{\vec{B}}\hat{D}_3)\hat{\vec{E}} \cdot \hat{\vec{B}} + \hat{\vec{E}} \cdot \hat{\vec{B}}(\hat{D}_1\hat{\vec{p}} \cdot \hat{\vec{S}} + \hat{D}_3\hat{\vec{S}} \cdot \hat{\vec{B}}\hat{\vec{B}} \cdot \hat{\vec{p}})) \\ & + \frac{1}{2}\epsilon_{abc}\hat{p}^a\hat{S}^b\hat{B}^c\hat{D}_2 + \frac{1}{2}\epsilon_{abc}\hat{D}_2\hat{B}^c\hat{S}^b\hat{p}^a + \hat{D}_4\hat{\vec{B}} \cdot \hat{\vec{S}}.\end{aligned}\quad (8.8.67)$$

The functions D_1, D_2, D_3, D_4 may depend only on $|\vec{B}|^2$ and $(\vec{E} \cdot \vec{B})^2$. As usual, we are most interested in the lowest order behavior of this Hamiltonian operator as that is what is most relevant for typical experiment. The D_1 and D_3 functions are attached to terms which are already quadratic in the electromagnetic field and so they are suppressed relative to the D_2 and D_4 terms which are only linear in the electromagnetic field and so to lowest order, we drop D_1 and D_3 (the quadratic $|\vec{A}|^2$ term in the $|\hat{\vec{p}} - q\hat{\vec{A}}|^2$ is necessary for gauge invariance so it cannot be excluded). Similarly, at lowest order D_2 and D_4 are just constants given by their value at 0 field. So, at lowest order then we have:

$$D_1 = D_3 = 0, \quad D_2 = \beta, \quad D_4 = -\gamma \quad (8.8.68)$$

for some constants β and γ . The constant γ is known as the gyromagnetic ratio of the particle. Hence, to lowest order our Hamiltonian operator is:

$$\hat{H} = \frac{|\hat{\vec{p}} - q\hat{\vec{A}}|^2}{2m} + q\hat{\phi} + \frac{\beta}{2}\epsilon_{abc}\hat{p}^a\hat{S}^b\hat{B}^c + \frac{\beta}{2}\epsilon_{abc}\hat{B}^c\hat{S}^b\hat{p}^a - \gamma\hat{\vec{B}} \cdot \hat{\vec{S}}. \quad (8.8.69)$$

There is another symmetry of interest for our Hamiltonian operator. Although we did not explicitly require it, all of our theories in Part I were automatically time reversal symmetric. The Hamiltonian operator in (8.8.69) is not automatically time reversal symmetry. It is a genuine experimental question whether we should expect time reversal symmetry. Experimentally, nonrelativistic quantum mechanics is consistent with time reversal symmetry. Therefore, we take:

Assumption :: GQMV: Time Reversal Symmetry

Isolated systems have time reversal symmetry.

Let us now see explicitly what this requires of our Hamiltonian operator. Let $\hat{\mathcal{T}}$ be the time reversal pseudo-operator. That is, we write:

$$|\psi'\rangle = \hat{\mathcal{T}}|\psi\rangle \quad (8.8.70)$$

to indicate the time reversed wavefunction. By problem 9.23, the position and momentum operators satisfy:

$$\hat{\mathcal{T}}\hat{x}\hat{\mathcal{T}}^{-1} = \hat{x}, \quad \hat{\mathcal{T}}\hat{p}\hat{\mathcal{T}}^{-1} = -\hat{p}. \quad (8.8.71)$$

Automatically, the orbital angular momentum operator is time reversal odd:

$$\hat{\mathcal{T}}\hat{L}_a\hat{\mathcal{T}}^{-1} = \epsilon_{abc}\hat{\mathcal{T}}\hat{x}^b\hat{\mathcal{T}}^{-1}\hat{\mathcal{T}}\hat{p}^c\hat{\mathcal{T}}^{-1} = -\hat{L}_a. \quad (8.8.72)$$

Spin angular momentum must have the same time reversal property because of the combined conservation law of total angular momentum and lack of individual conservation law for either spin or orbital. Therefore, however $\hat{\mathcal{T}}$ acts on the internal degrees of freedom, it must perform:

$$\hat{\mathcal{T}}\hat{S}\hat{\mathcal{T}}^{-1} = -\hat{S}. \quad (8.8.73)$$

As well, the vector potential is time reversal odd and so the magnetic field is as well. Thus, under time reversal, $\hat{H}$ transforms as:

$$\hat{H}' = \frac{|\hat{p}' - q\hat{A}'|^2}{2m} + q\hat{\phi}' + \frac{\beta}{2}\epsilon_{abc}\hat{p}'^a\hat{S}'^b\hat{B}'^c + \frac{\beta}{2}\epsilon_{abc}\hat{B}'^c\hat{S}'^b\hat{p}'^a - \gamma\hat{B}' \cdot \hat{S}' \quad (8.8.74)$$

$$= \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} - \frac{\beta}{2}\epsilon_{abc}\hat{p}^a\hat{S}^b\hat{B}^c - \frac{\beta}{2}\epsilon_{abc}\hat{B}^c\hat{S}^b\hat{p}^a - \gamma\hat{B} \cdot \hat{S} \stackrel{!}{=} \hat{H}_0. \quad (8.8.75)$$

Thus, in order to have time reversal symmetry we must have $\beta = 0$. Altogether then:

Theorem 8.12: The Galilean Spinor Schrödinger Equation

To leading order in the electromagnetic fields, the general parity and time reversal symmetric Hamiltonian operator for a Spin-1/2 Galilean quantum wave interacting with electromagnetism is:

$$\hat{H} = \frac{|\hat{p} - q\hat{A}|^2}{2m} + q\hat{\phi} - \gamma\hat{B} \cdot \hat{S}. \quad (8.8.76)$$

The corresponding equation of motion is then:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\nabla - i\frac{q}{\hbar}\vec{A}\right)^2\psi + q\phi\psi - \gamma\vec{B} \cdot \hat{S}\psi \quad (8.8.77)$$

$$\implies i\hbar\mathcal{D}_t\psi = -\frac{\hbar^2}{2m}\mathcal{D}^2\psi - \gamma\vec{B} \cdot \hat{S}\psi. \quad (8.8.78)$$

And so the spin-1/2 theory is not all that different from the spin-0 theory; there is simply one extra term. This theory automatically has the exact same local U(1) gauge symmetry as the spin-0 theory which now that we have a geometric interpretation of what local gauge symmetry actually means this should not be surprising. We can compute the equations of motion for $\vec{x}_{cl}$ to see what the modification of this extra term is:

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{x}, \hat{H}]\rangle = \left\langle\frac{\hat{p} - q\hat{A}}{m}\right\rangle = \frac{\langle\hat{p}\rangle - q\langle\hat{A}\rangle}{m} \quad (8.8.79)$$

$$\frac{d^2\langle\hat{x}\rangle}{dt^2} = \frac{1}{m}\frac{d\langle\hat{p}\rangle}{dt} - \frac{q}{m}\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{mi\hbar}\langle[\hat{p}, \hat{H}]\rangle - \frac{q}{m}\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle - \frac{q}{mi\hbar}\langle[\hat{A}, \hat{H}]\rangle \quad (8.8.80)$$

$$\frac{d^2\langle\hat{x}\rangle}{dt^2} = \frac{1}{mi\hbar}\langle[\hat{p}, \hat{H}_0 - \gamma\hat{B} \cdot \hat{S}]\rangle - \frac{q}{m}\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle - \frac{q}{mi\hbar}\langle[\hat{A}, \hat{H}_0 - \gamma\hat{B} \cdot \hat{S}]\rangle \quad (8.8.81)$$

$$m\frac{d^2\langle\hat{x}\rangle}{dt^2} = q\left\langle-\frac{\partial\hat{A}}{\partial t} - \nabla\phi\right\rangle - \frac{q}{2}\left\langle(\nabla \times \hat{A}) \times \hat{v}\right\rangle + \frac{q}{2}\left\langle\hat{v} \times (\nabla \times \hat{A})\right\rangle + \gamma\langle\nabla(\hat{B} \cdot \hat{S})\rangle \quad (8.8.82)$$

$$\implies m \frac{d^2 \langle \hat{x} \rangle}{dt^2} = q \langle \vec{E}(t, \hat{x}) \rangle + \frac{q}{2} \langle (\hat{v} \times \vec{B}(t, \hat{x}) - \vec{B}(t, \hat{x}) \times \hat{v}) \rangle + \gamma \langle \nabla (\vec{B}(t, \hat{x}) \cdot \hat{S}) \rangle. \quad (8.8.83)$$

Hence we can see that only one term is added. As long as this new term is small in approximately classical situations we will still get approximately classical behavior. This new term will be small as long as the magnetic field does not vary too much over the scale of the size of the wave (size meaning the width of the region in which it is mainly localized). Because the two eigenvectors of $\vec{B} \cdot \hat{S}$ have opposite eigenvalues, the new term will have equal and opposite effects on the two components of ψ projected into the directions aligned and anti-aligned with $\vec{B}$. So the presence of a magnetic field gradient causes these two components to be pulled away from each other (which is known as the Stern-Gerlach effect). If $\vec{B}$ is persistently in approximately the same direction, this will cause an initial wave-packet to separate into two separate wave-packets each with spin polarized according to being either aligned or anti-aligned with $\vec{B}$, which leads immediately to interesting experimental consequences. In particular, because it rips the wave-packet apart, it often breaks the validity of the classical limit.

The Spin-1/2 Theory unsurprisingly gives currents which satisfy the continuity equation by a quick calculation. The Lagrangian with the new term is:

$$\mathcal{L} = \int_{\mathbb{S}} \left(i\hbar \psi^\dagger \mathcal{D}_t \psi - \frac{\hbar^2}{2m} |\vec{\mathcal{D}}\psi|^2 + \gamma \psi^\dagger \vec{B} \cdot \hat{S} \psi \right) d\mathbb{S}. \quad (8.8.84)$$

Therefore the charge density is unchanged but the current density picks up a new term:

$$\rho = -\frac{\delta \mathcal{L}_{\text{int}}}{\delta \phi} = q|\psi|^2, \quad \vec{J} = \frac{\delta \mathcal{L}_{\text{int}}}{\delta \vec{A}} = \frac{q\hbar}{m} \text{Im}(\psi^\dagger \vec{\mathcal{D}}\psi) + \gamma \nabla \times (\psi^\dagger \hat{S} \psi). \quad (8.8.85)$$

This new current density is again automatically gauge invariant as the phase added by gauge transformation cancels between the ψ and the $\psi^\dagger$. The continuity equation follows easily from our prior calculation because the divergence of any curl is 0:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = \frac{\partial}{\partial t} q|\psi|^2 + \nabla \cdot \left(\frac{\hbar q}{m} \text{Im}(\psi^\dagger \vec{\mathcal{D}}\psi) + \gamma \nabla \times (\psi^\dagger \hat{S} \psi) \right) \quad (8.8.86)$$

$$= \frac{q}{i\hbar} \psi^* \left(i\hbar \mathcal{D}_t \psi + \frac{\hbar^2}{2m} \mathcal{D}^2 \psi \right) - \frac{q}{i\hbar} \left(-i\hbar \mathcal{D}_t \psi^* + \frac{\hbar^2}{2m} \mathcal{D}^2 \psi^* \right) \psi + 0 \quad (8.8.87)$$

$$= \frac{q}{i\hbar} \psi^* \left(-\gamma \vec{B} \cdot \hat{S} \right) \psi - \frac{q}{i\hbar} \psi^* (-\gamma \vec{B} \cdot \hat{S}) \psi \quad (8.8.88)$$

$$= 0. \quad (8.8.89)$$

And so, the continuity equation is indeed preserved as expected. Because the charge density is the same as in the scalar theory, equation (8.6.137) still holds for the electric dipole moment. For the magnetic dipole moment, we have a new contribution:

$$\vec{\mu} = \frac{1}{2} \int_{\mathbb{S}} \vec{x} \times \vec{J} d\mathbb{S} = \frac{1}{2} \int_{\mathbb{S}} \vec{x} \times \left(\frac{q\hbar}{2m} \text{Im}(\psi^\dagger \vec{\mathcal{D}}\psi) + \gamma \nabla \times (\psi^\dagger \hat{S} \psi) \right) d\mathbb{S} \quad (8.8.90)$$

$$= \frac{q}{2m} \langle \hat{x} \times (-i\hbar \vec{\mathcal{D}}) \rangle + \frac{\gamma}{2} \int_{\mathbb{S}} \left(\nabla (\psi^\dagger \hat{S} \psi) \cdot \vec{x} - (\vec{x} \cdot \nabla) (\psi^\dagger \hat{S} \psi) \right) d\mathbb{S} \quad (8.8.91)$$

$$= \frac{q}{2m} \langle \hat{x} \times (-i\hbar \vec{\mathcal{D}}) \rangle + \frac{\gamma}{2} \int_{\mathbb{S}} \left(-(\psi^\dagger \hat{S} \psi) \cdot \nabla \vec{x} + \psi^\dagger \hat{S} \psi (\nabla \cdot \vec{x}) \right) d\mathbb{S} \quad (8.8.92)$$

$$= \frac{q}{2m} \langle \hat{x} \times (-i\hbar \vec{\mathcal{D}}) \rangle + \frac{\gamma}{2} \int_{\mathbb{S}} \left(-\psi^\dagger \hat{S} \psi + 3\psi^\dagger \hat{S} \psi \right) d\mathbb{S} \quad (8.8.93)$$

$$= \frac{q}{2m} \vec{L} + \gamma \langle \hat{S} \rangle = \frac{q}{2m} \vec{L} + \gamma \vec{S}. \quad (8.8.94)$$

Thus, the new contribution of the angular momentum to the magnetic dipole moment is proportional to the spin. If the gyromagnetic ratio $\gamma = \frac{q}{2m}$ then we would have that μ is simply proportional to the total angular momentum of the wavefunction $\vec{L} + \vec{S}$. So, it is typical to define g , called the g-factor, by:

$$g = \frac{2m\gamma}{q} \implies \gamma = \frac{gq}{2m}. \quad (8.8.95)$$

Then:

$$\vec{\mu} = \frac{q}{2m} (\vec{L} + g\vec{S}). \quad (8.8.96)$$

When $g = 1$, $\vec{\mu}$ is simply proportional to $\vec{J}$. However, for different species of spin-1/2 particles g or equivalently γ can take any value and is unrestricted by symmetries.

In terms of the g factor, the Hamiltonian operator can also be written nicely using the the Pauli-matrices. Using (8.8.4):

$$(\sigma^a(\hat{p}_a - q\hat{A}_a))^2 = \sigma^a\sigma^b(\hat{p}_a - q\hat{A}_a)(\hat{p}_b - q\hat{A}_b) \quad (8.8.97)$$

$$= \left(\frac{\sigma^a\sigma^b + \sigma^b\sigma^a}{2} + \frac{\sigma^a\sigma^b - \sigma^b\sigma^a}{2} \right) (\hat{p}_a - q\hat{A}_a)(\hat{p}_b - q\hat{A}_b) \quad (8.8.98)$$

$$= (\delta^{ab}\mathbb{1} + i\epsilon^{abc}\sigma_c)(\hat{p}_a - q\hat{A}_a)(\hat{p}_b - q\hat{A}_b) \quad (8.8.99)$$

$$= |\hat{\vec{p}} - q\hat{\vec{A}}|^2 + \frac{i}{2}\epsilon^{abc}\sigma_c[\hat{p}_a - q\hat{A}_a, \hat{p}_b - q\hat{A}_b] \quad (8.8.100)$$

$$= |\hat{\vec{p}} - q\hat{\vec{A}}|^2 + \frac{i}{2}\epsilon^{abc}\sigma_c i\hbar q(\partial_a A_b - \partial_b A_a) \quad (8.8.101)$$

$$= |\hat{\vec{p}} - q\hat{\vec{A}}|^2 - 2q\vec{B} \cdot \hat{\vec{S}}. \quad (8.8.102)$$

Returning this to our Hamiltonian operator, we have that it can be written in the Pauli form as:

$$\hat{H} = \frac{(\hat{\vec{\sigma}} \cdot (\hat{\vec{p}} - q\hat{\vec{A}}))^2}{2m} + q\hat{\phi} - \frac{q(g-2)}{2m}\hat{\vec{B}} \cdot \hat{\vec{S}}. \quad (8.8.103)$$

This form is particularly nice if the particle of interest has $g = 2$ or very close to it. Historically, for reasons we will partly understand in a few sections, the electron was originally believed to have a value of $g = 2$ exactly, motivating this form. It turns out due to effects we haven't yet studied, the value of g for an electron is not exactly 2, however it is quite close. The experimentally measured g factor for the electron is:

$$g_e = 2.00231930436118(27). \quad (8.8.104)$$

Exercises

Problem 8.49: Rabi Flopping. Consider a spin-1/2 particle which is approximately localized in an approximately uniform but time-dependent magnetic field $\vec{B}(t)$.

- (a) Show that the relevant Hamiltonian operator for describing the evolution of the spin degrees of freedom of the system is:

$$\hat{H} = -\gamma\hat{\vec{B}} \cdot \hat{\vec{S}}.$$

Show that due to the approximate localization of the particle, we can describe the evolution of the wavefunction's spin degrees of freedom by components $\psi_+(t)$ and $\psi_-(t)$ which represent the total wavefunction of the particle at the localized location in each of the two spin polarization directions.

- (b) Consider the magnetic field to have a constant component along the z axis and a rotating piece in the xy plane so that for some constants B_0, B_1, ω :

$$\vec{B}(t) = (B_1 \cos \omega t, -B_1 \sin \omega t, B_0).$$

Show using the Schrödinger equation that the equations of motion for the components of the wavefunction become:

$$\begin{aligned} \dot{\psi}_+ &= \frac{i\gamma B_0}{2}\psi_+ + \frac{i\gamma B_1}{2}e^{i\omega t}\psi_- \\ \dot{\psi}_- &= \frac{i\gamma B_1}{2}e^{-i\omega t}\psi_+ - \frac{i\gamma B_0}{2}\psi_-. \end{aligned}$$

- (c) Define a new wavefunction $|\phi\rangle$ by rotating the system about the z axis at angular velocity ω . That is, define:

$$|\phi\rangle = \hat{U}(\omega t)|\psi\rangle$$

where $\hat{U}(\theta)$ is the representation of a rotation about the z axis by an angle θ on the spin-1/2 Hilbert space. Show that the equations of motion for ϕ_+ and ϕ_- become:

$$\begin{aligned} \dot{\phi}_+ &= \frac{i}{2}(\gamma B_0 - \omega)\phi_+ + \frac{i\gamma B_1}{2}\phi_- \\ \dot{\phi}_- &= \frac{i\gamma B_1}{2}\phi_+ - \frac{i}{2}(\gamma B_0 - \omega)\phi_-. \end{aligned}$$

- (d) Solve the equations of motion for $|\phi\rangle$ and return them to the definition of $|\psi\rangle$ to show that:

$$\begin{aligned}\psi_+(t) &= e^{\frac{i}{2}\omega t} \left(\left(\cos\left(\frac{\Omega t}{2}\right) - i \sin \delta \sin\left(\frac{\Omega t}{2}\right) \right) \psi_+(0) + i \cos \delta \sin\left(\frac{\Omega t}{2}\right) \psi_-(0) \right) \\ \psi_-(t) &= e^{-\frac{i}{2}\omega t} \left(i \cos \delta \sin\left(\frac{\Omega t}{2}\right) \psi_+(0) + \left(\cos\left(\frac{\Omega t}{2}\right) + i \sin \delta \sin\left(\frac{\Omega t}{2}\right) \right) \psi_-(0) \right)\end{aligned}$$

where:

$$\omega - \gamma B_0 = \Omega \sin \delta, \quad \gamma B_1 = \Omega \cos \delta.$$

- (e) Suppose the particle begins initially in the “spin-down” state ($|\psi_-(0)| = 1$). Let $I(t)$ be the projection intensity of $|\psi(t)\rangle$ onto the “spin-up” state. That is, define:

$$I(t) = |\psi_+(t)|^2.$$

Show that $I(t)$ is given by:

$$I(t) = \frac{\gamma^2 B_1^2}{\gamma^2 B_1^2 + (\omega - \gamma B_0)^2} \sin^2 \left(\frac{t}{2} \sqrt{\gamma^2 B_1^2 + (\omega - \gamma B_0)^2} \right).$$

Information can be stored in the spin state of the spin-1/2 particle. By keeping a spin-1/2 particle in a background uniform magnetic field (that given by B_0), it stably precesses about the direction of that field “saving” its state. By then turning on an oscillatory field (that given by B_1) we see that we can change the spin state of the particle. Show that by choosing the frequency ω of the oscillatory field correctly, for an arbitrarily weak applied field B_1 , we can fully flip the spin state of the particle (change spin-down to spin-up or vice versa). Find the characteristic time τ necessary to completely flip the spin.

Problem 8.50: ★ The Stern-Gerlach Experiment. Consider a spin-1/2 particle experiencing the interior quadrupole magnetic field:

$$\vec{B} = (0, -My, Mz)$$

for a constant M . (This magnetic field is just an interior quadrupole field and so may be produced in the interior region of two appropriate spaced current carrying coils which are oppositely oriented.) Assume further that the particle is charge neutral ($q = 0$) but has a gyromagnetic ratio ($\gamma \neq 0$).

- (a) For the moment, assume the particle is localized as a wave packet and that it remains localized as it evolves. Show that the center of the particle $\vec{x}(t)$ and the spin angular momentum $\vec{S}(t)$ of the particle satisfy the equations of motion:

$$\begin{aligned}m\ddot{\vec{x}} &= \gamma \nabla(\vec{B}(t, \vec{x}) \cdot \vec{S}(t)) \\ \frac{d\vec{S}}{dt} &= \gamma \vec{S}(t) \times \vec{B}(t, \vec{x}(t)).\end{aligned}$$

Suppose further the particle is initially moving in the x direction with velocity v beginning from an emitter at the origin and travels from where it is emitted to a screen a distance ℓ away at which it is detected (through some interaction with the screen). Show that to leading order in M , the particle hits the screen at z coordinate:

$$z = \frac{\gamma M \ell^2}{2mv^2} S_z(0) + \mathcal{O}(M^2).$$

- (b) Suppose we now have a beam of particles of the same mechanical properties (m, q, γ) emitted as above with different initial spin directions but the same initial velocity. Show that if all initial spin directions are present in the beam, then the beam of particles will produce collisions on the detector in an interval of z coordinates which has length d given to leading order in M by:

$$d \approx \frac{\gamma M \hbar \ell^2}{2mv^2}.$$

Show that for a single particle the projective intensity per unit length in the z direction on the screen is given by:

$$I(z) = \delta \left(z - \frac{\gamma M \hbar \ell^2}{4mv^2} \cos \theta \right)$$

where $S_z(0) = \frac{\hbar}{2} \cos \theta$. Show that if the initial spins in the beam are uniformly distributed the resulting

average intensity per unit length on the screen is given by a uniform distribution from $-\frac{d}{2}$ to $\frac{d}{2}$.

- (c) There is a critical flaw in the preceding analysis. It is the result for classical spinning particles as derived from the classical limit of the Schrödinger equation, assuming the particles actually remain as well-packed little wave-packets during their evolution. However, due to the $\langle \nabla(\hat{S} \cdot \vec{B}) \rangle$ term in (8.8.83) the different spin polarizations are dynamically separated during the actual evolution of the wave. Let $\vec{x}_+$ and $\vec{x}_-$ be the summary positions gotten from using the components ψ_+ and ψ_- as wavefunctions respectively (and normalizing them appropriately). Show that to leading order in M , $\vec{x}_+$ and $\vec{x}_-$ separate in the z direction so that by the time they have reached the screen they have a separation of d as given above. Therefore, if that separation is large enough to be experimentally meaningful to us, the full wavefunction cannot be said to be in the classical limit. Using this, show that instead the classical limit can be valid for each of the two polarizations separately and that the resulting more accurate estimate of the projective intensity per unit length on the screen for a beam of N particles with the same spin is given by:

$$I(z) = N \cos^2\left(\frac{\theta}{2}\right) \delta\left(z - \frac{\gamma M \hbar \ell^2}{4mv^2}\right) + N \sin^2\left(\frac{\theta}{2}\right) \delta\left(z + \frac{\gamma M \hbar \ell^2}{4mv^2}\right).$$

Using this show that if the initial spins in the beam are uniformly distributed the resulting average intensity per unit length on the screen is given by:

$$\mathbb{E}(I) = \frac{N}{2} \delta\left(z - \frac{d}{2}\right) + \frac{N}{2} \delta\left(z + \frac{d}{2}\right).$$

Thus rather than a uniformly dense line segment of collisions on the screen (which would be expected from pure classical mechanics), a better approximation of the Schrödinger equation suggests one should expect two bright spots with clear separation between them on the screen. The two bright spots in reality will certainly not be point-like Dirac deltas and there will be some intensity of signal inbetween them if one uses the full Schrödinger equation (which can be confirmed with numerical simulations or more detailed analytical calculations). But, the prediction of two brighter regions near $\pm \frac{d}{2}$ with a reduced signal between them is correct.

Historically, this experiment was first done with silver atoms for several reasons. By being an atom, the silver atom is charge neutral. Silver atoms have 47 protons, 47 electrons, and stable forms have either 60 or 62 neutrons. The lowest energy configuration of the silver atom involves 46 of the electrons coming in pairs of oppositely oriented spins and forming a spherically symmetric charge density around the atomic nucleus. As well, protons and neutrons have much smaller magnetic moments than the electron. Together these cause the total magnetic moment of a silver atom to be very nearly the magnetic moment of the single unpaired electron and so to act as spin-1/2 with the electron's value of γ (protons and neutrons are also spin-1/2 and do have nonzero magnetic moments, but they are much smaller than the electron magnetic moment). The fact that such a beam splits into two bright spots acts as a confirmation that in fact the electron is spin-1/2. (The number of spots formed on the screen is $2s+1$, think about why.)

Problem 8.51: The Stern-Gerlach Polarizer. The Stern-Gerlach experimental setup from the previous question can be used like a “spin polarizer”, in the sense that it separates the beam of incoming atoms of various spin directions into two beams, each of which has a specific spin-direction. By keeping only one of the separated beams, we then have ideally a fully (or in reality a mostly) polarized output beam. When we use a Stern-Gerlach magnet setup as in the previous question with the beam separation occurring in the direction $\vec{n}$ and keep for future use only the separated beam which has its spin aligned in the $\vec{n}$ direction, we call it a Stern-Gerlach polarizer in the direction $\vec{n}$. The mathematical structure of this polarizer is nearly identical to the mathematical structure of polarizers of light.

- (a) Suppose that $|\psi_{\text{in}}\rangle$ is the (spatially localized, and so given simply by two complex numbers) wavefunction of a spin-1/2 particle entering a Stern-Gerlach polarizer in the direction $\vec{n}$. Show that the wavefunction of the polarizer output $|\psi_{\text{out}}\rangle$ is given by:

$$|\psi_{\text{out}}\rangle = e^{i\alpha} \hat{J} |\psi_{\text{in}}\rangle$$

where α is some phase accumulated while traveling through the polarizer and $\hat{J}$, called the Jones matrix of the polarizer, is given by:

$$\hat{J} = \frac{\mathbb{1} + \vec{n} \cdot \hat{\vec{\sigma}}}{2}.$$

- (b) Suppose there is an angle θ between the spin directions of $|\psi_{\text{in}}\rangle$ and $|\psi_{\text{out}}\rangle$ as above. Let $\mathcal{I}_{\text{in}} = \|\psi_{\text{in}}\|^2$ and $\mathcal{I}_{\text{out}} = \|\psi_{\text{out}}\|^2$ be the projective intensities of the two beams. Show that:

$$\mathcal{I}_{\text{out}} = \mathcal{I}_{\text{in}} \cos^2 \frac{\theta}{2}.$$

Compare this result to Malus' law from electromagnetism.

- (c) Suppose we pass the incoming beam through a sequence of three Stern-Gerlach polarizers with Jones matrices $\hat{J}_1, \hat{J}_2, \hat{J}_3$ in the order 1,2,3. Show that the resulting wavefunction of the final beam is:

$$|\psi_{\text{out}}\rangle = \hat{J}_3 \hat{J}_2 \hat{J}_1 |\psi_{\text{in}}\rangle.$$

Problem 8.52: Partially Polarized Particle Beams and Density Matrices.

- (a) Let G be a quantity of interest that depends on the spin of the beam particle so that it takes the form $G = \langle \psi | \hat{G} | \psi \rangle$ where $\hat{G}$ is a self-adjoint operator on the spin space of the wavefunction. Show that alternatively, G may be written as:

$$G = \text{Tr}(\hat{G}\hat{\rho})$$

where:

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

is a non-negative self-adjoint operator called the density matrix corresponding to $|\psi\rangle$. Show as well that:

$$\mathcal{I} = \text{Tr}(\hat{\rho}).$$

- (b) Now consider a particle beam source which does not produce particles with exactly predictable spins. Instead, due to our incomplete knowledge we model the source as producing wavefunctions $|\psi_1\rangle, |\psi_2\rangle, \dots$ each with probabilities $p_1, p_2, \dots$. Each particle emitted from the source will have some independently selected $|\psi_1\rangle$ from this distribution. Explain then that as is typical in experiment by sampling many waves from the source one can measure the expected value of the previous mentioned quantity G by:

$$\mathbb{E}(G) = \sum_n p_n \langle \psi_n | \hat{G} | \psi_n \rangle.$$

As well, show that one can **NOT** in general identify a wavefunction $|\psi_0\rangle$ so that:

$$\mathbb{E}(G) \stackrel{!}{=} \langle \psi_0 | \hat{G} | \psi_0 \rangle$$

and thus that there is no way to define an effective wavefunction for a probabilistic source. However, show that one can in general define the density matrix $\hat{\rho}$ so that:

$$\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

$$\mathbb{E}(G) = \text{Tr}(\hat{G}\hat{\rho}).$$

As well, show that in addition to reducing to the original expression given for the density matrix in the case that only one value of $|\psi\rangle$ is possible, this general density matrix is also self-adjoint, has nonnegative eigenvalues, and has trace given by the expected intensity of the beam. Thus, while the wavefunction description cannot be generalized to the case of a probabilistic source, the density matrix description can. Many sources are probabilistic due to them having very complicated internal dynamics and little if any bias toward any particular directions of polarizations. Thus, for modeling real equipment the density matrix formalism is often a necessity.

- (c) Show that if the beam from such a source passes through a linear component with Jones matrix $\hat{J}$ the density matrix afterward is given by:

$$\hat{\rho}' = \hat{J}\hat{\rho}\hat{J}^\dagger.$$

As well, show that if a sequence of multiple (say 3) components of Jones matrices $\hat{J}_1, \hat{J}_2, \hat{J}_3$ are passed through in that order the resulting density matrix is:

$$\hat{\rho}' = \hat{J}_3 \hat{J}_2 \hat{J}_1 \hat{\rho} \hat{J}_1^\dagger \hat{J}_2^\dagger \hat{J}_3^\dagger.$$

- (d) Show that there exists an effective wavefunction $|\psi_0\rangle$ for a given density matrix (meaning $\hat{\rho} = |\psi_0\rangle\langle\psi_0|$) if and only if $\text{Tr}(\hat{\rho}^2) = (\text{Tr}(\hat{\rho}))^2$ or if the beam is of spin-1/2 particles equivalently if and only if $\det(\hat{\rho}) = 0$ (because $\hat{\rho}$ is a 2x2 matrix). Such a source is called completely polarized.
- (e) Consider a spin-1/2 beam source which produces all polarizations uniformly. That is, the spin direction

of the wavefunction is uniformly distributed. Show that the corresponding density matrix is proportional to the identity matrix. Such a source is called “unpolarized”. Show that an unpolarized beam produces the same expected values as a source which takes spin-up and spin-down along any particular axis each with probability $1/2$.

- (f) For a spin-1/2 beam, using that $\hat{\rho}$ is a 2x2 Hermitian matrix, show that for real parameters S_0, S_1, S_2, S_3 (called Stokes’ parameters) the density matrix can be written:

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} S_0 + S_3 & S_1 - iS_2 \\ S_1 + iS_2 & S_0 - S_3 \end{pmatrix}.$$

Show that S_0 is the intensity of the beam and that the vector $\frac{\hbar}{2}(S_1, S_2, S_3)$ gives the total expected spin angular momentum of the beam. Let d , the “degree of polarization” be defined by:

$$d = \frac{\sqrt{S_1^2 + S_2^2 + S_3^2}}{S_0}.$$

Show that $0 \leq d \leq 1$ with $d = 0$ if and only if the source is unpolarized and $d = 1$ if and only if the source is completely polarized. Show that the density matrix can be written as the sum of a completely unpolarized part of intensity $\mathcal{I}_u$ and a completely polarized part of intensity $\mathcal{I}_p$ and polarization (normalized wavefunction) $|\psi\rangle$ as:

$$\hat{\rho} = \mathcal{I}_u \frac{\mathbb{1}}{2} + \mathcal{I}_p |\psi\rangle\langle\psi|$$

and find the relationship between $\mathcal{I}_u, \mathcal{I}_p$, the explicit component expression for $|\psi\rangle$, and the four Stokes parameters. As well, show that the total expected intensity $\mathcal{I}$ is given by $\mathcal{I} = \mathcal{I}_u + \mathcal{I}_p$ and that the degree of polarization can be reexpressed as:

$$d = \frac{\mathcal{I}_p}{\mathcal{I}_p + \mathcal{I}_u}$$

and thus can be understood as the fraction of the total intensity which is due to the polarized beam.

Problem 8.53: Stokes Vectors and Mueller Calculus for Spin-1/2 Particles. Consider a beam of spin-1/2 particles with polarization state represented by the density matrix $\hat{\rho}$ as in the previous problem. For this question, let $\sigma^0 = \mathbb{1}$ so that we can make a 4-dimensional vector of matrices with components σ^μ and μ going 0, 1, 2, 3. In this question we raise and lower that index using the identity metric $\delta^{\mu\nu}$, so that there is no difference between upper indices and lower indices.

- (a) Show that any 2x2 self-adjoint matrix $\hat{G}$ can be written for some real coefficients G_0, G_1, G_2, G_3 as:

$$\hat{G} = G_0 \sigma^0 + G_1 \sigma^1 + G_2 \sigma^2 + G_3 \sigma^3 = G_\mu \sigma^\mu$$

where the index μ is used for implicit summation and ranges from 0 to 3.

- (b) Show that:

$$\text{Tr}(\sigma^\mu \sigma^\nu) = 2\delta^{\mu\nu}.$$

- (c) Define for a Hermitian matrix $\hat{G}$ the 4 dimensional vector $\vec{G} = (G_0, G_1, G_2, G_3)$ and define the Stokes vector $\vec{S} = (S_0, S_1, S_2, S_3)$ so that $S_\mu = \mathbb{E}(\sigma_\mu)$. Show then that:

$$\mathbb{E}(G) = \text{Tr}(\hat{\rho} \hat{G}) = S^\mu G_\mu = \vec{G} \cdot \vec{S}, \quad S^\mu = \text{Tr}(\sigma^\mu \hat{\rho}), \quad G_\mu = \frac{1}{2} \text{Tr}(\sigma_\mu \hat{G}).$$

- (d) Show that if a beam source of Stokes vector $\vec{S}$ passes through a linear component with Jones matrix $\hat{J}$ the resultant Stokes vector satisfies:

$$\vec{S}' = \hat{M} \vec{S}$$

where the real 4x4 matrix $\hat{M}$, called the Mueller matrix, has components given by:

$$M_{\mu\nu} = \frac{1}{2} \text{Tr}(\sigma_\mu \hat{J} \sigma_\nu \hat{J}^\dagger).$$

- (e) Find the Mueller matrix for a Stern-Gerlach polarizer of direction $\vec{n}$.
- (f) Sometimes, even the components of a system will be probabilistic in their macroscopic behavior due to their complicated internal dynamics. As such, it is sometimes appropriate to model a linear component as having Jones matrix $\hat{J}_1$ with probability p_1 , $\hat{J}_2$ with probability p_2 , and so on. Let $\hat{\rho}'_n$ be the density matrix of a source with incoming density matrix $\hat{\rho}$ after passing through such a component when it had

Jones matrix $\hat{J}_n$. Because the component has probabilistic behavior, it is necessary to now sample many times results and use statistical averages to make experimental measurements. So, for a quantity of interest G (with associated $\hat{G}$) for the beam after passing through the component, define the expected value $\mathbb{E}(G)$ by averaging over the possible results of the component:

$$\mathbb{E}(G) = \sum_n p_n \text{Tr}(\hat{G}\hat{\rho}'_n).$$

Show that equivalently one may write:

$$\mathbb{E}(G) = \text{Tr}(\hat{G}\hat{\rho}')$$

where the effective density matrix $\hat{\rho}'$ is given by:

$$\hat{\rho}' = \sum_n p_n \hat{\rho}'_n.$$

As well, show that $\hat{\rho}'$ is Hermitian, has nonnegative eigenvalues, and has trace:

$$\text{Tr}(\hat{\rho}') = \mathbb{E}(\mathcal{I}).$$

Thus, even in the case of a probabilistic Jones matrix, one can identify an effective density matrix.

(g) Show that the $\hat{\rho}'$ of the previous part is related to $\hat{\rho}$ by:

$$\hat{\rho}' = \sum_n p_n \hat{J}_n \hat{\rho} \hat{J}_n^\dagger$$

and thus explain that it is **NOT** in general possible to define an effective Jones matrix $\hat{J}_0$ for a probabilistic component so that:

$$\hat{\rho}' = \hat{J}_0 \hat{\rho} \hat{J}_0^\dagger.$$

However, show that the Stokes vector $\vec{S}'$ corresponding to $\hat{\rho}'$ is related to the Stokes vector $\vec{S}$ corresponding to $\hat{\rho}$ by:

$$\vec{S}' = \hat{M} \vec{S}$$

where $\hat{M}$ has components given by:

$$M_{\mu\nu} = \sum_n \frac{1}{2} p_n \text{Tr}(\sigma_\mu \hat{J}_n \sigma_\nu \hat{J}_n^\dagger).$$

Thus, in the case of probabilistic components, while it is typically not possible to define an effective Jones matrix it is possible to define an effective Mueller matrix. So, probabilistic sources demand the density matrix formalism and probabilistic components demand the Stokes vector and Mueller matrix formalism.

8.9 Scattering Theory

Just as in classical mechanics and electromagnetism, scattering experiments are immensely important in quantum mechanics (and truly even more so than in our previous theories). In scattering we are ultimately interested in answering the question: given an incoming state from the distant past, what will the outgoing state be in the distant future? This may seem bizarre as certainly all experiments take place over finite time. But, if we wait for a time much longer than the time it takes our system to stabilize it is effectively like waiting forever. More rigorously, we could treat scattering as the lowest order approximation in a series expansion in powers of $t_{\text{evolve}}/t_{\text{wait}}$ where t_{evolve} is a typical characteristic timescale of the Hamiltonian of our system and t_{wait} is how long we let it evolve before making measurements. For many quantum systems, t_{evolve} is millionths of a second (or potentially much much less) and t_{wait} will be a macroscopic human relevant time scale so their ratio will be extremely small and we can effectively treat it as 0. The scattering formalism is gotten by taking the formal limit $t_{\text{wait}} \rightarrow \infty$. Consequently, often we can treat a quantum system as being essentially “free” initially, interacting for a while, and then being free again in the end.

More formally, for scattering we consider a Hamiltonian operator $\hat{H} = \hat{H}_0 + \hat{H}_1$ where $\hat{H}_0$ is called the “free-part” of the Hamiltonian operator and $\hat{H}_1$ is called the “interacting-part” of the Hamiltonian operator. The free-part $\hat{H}_0$ will be chosen to be the Hamiltonian operator when the quantum system of interest is isolated and has all symmetries of interest. For example, for a scalar Galilean particle, we have already found that $\hat{H}_0 = \frac{\hat{p}^2}{2m}$. $\hat{H}_1$ will be the rest of the total Hamiltonian operator not contained in $\hat{H}_0$. In scattering, we consider initial states which are approximately free. This is made precise by requiring that at very early times (as $t \rightarrow -\infty$), $\hat{H}_1$ should approximately annihilate the incoming states:

$$\lim_{t \rightarrow -\infty} \|\hat{H}_1|\psi(t)\rangle\|^2 = 0. \quad (8.9.1)$$

Similarly, in scattering we consider final states which are approximately free so that:

$$\lim_{t \rightarrow \infty} \|\hat{H}_1|\psi(t)\rangle\|^2 = 0. \quad (8.9.2)$$

In practice the way that these equalities tend to work is that $\hat{H}_1$ will depend on functions or external fields (like electromagnetic fields or atomic potentials) which are only nonzero in a finite region of space and the incoming/outgoing states will be wavepackets coming in from far away or going out to far away, so there is very little (asymptotically 0) overlap between the regions in which $\hat{H}_1$ and $|\psi\rangle$ are nonvanishing at very early or very late times.

One may worry that the assumption that we can treat our system as asymptotically not interacting in some appropriate sense will miss important physics. It can! Scattering theory is valid in physical circumstances where your system decomposes into asymptotically not interacting parts, and cannot just be blindly assumed to have told you everything about the system outside of that regime. If λ is some parameter that controls the strength of the interaction, scattering theory is excellent at giving an approximation to the full theory as a power series in λ (perturbation theory). However, sometimes the physical properties of a system may have some behavior in some parameter region that cannot be captured by a power series, such as the behavior of $e^{-\frac{1}{\lambda}}$ as $\lambda \rightarrow 0$ (a nonperturbative effect). Scattering theory is essentially intrinsically perturbative in that it treats the interacting theory as a perturbation of a simpler noninteracting theory and it is just a mathematical fact that perturbation theory cannot tell you everything. There may be genuine interacting states of your system no matter how long you wait that need some effective description as a composite object, and such things are missed by perturbation theory, which essentially presupposes that the qualitative behavior of the system at long times is captured by the free theory. While scattering theory can tell you a great deal about a physical system it often cannot always tell you everything. There are many advanced tools for how to treat these naively missed pieces within scattering theory and try to develop something more complete, but we will not dwell on them here.

Because of (8.9.1) and (8.9.2), scattering essentially separates time into three sections, the very distant past of the experiment in which the incoming state is approximately free (like a freely propagating wavepacket), the present middle in which there are significant interactions between the parts of the system and any relevant external fields, and the very distant future in which the outgoing state is approximately free. In the experiment, the distant past is represented by whatever beam of incoming free particles is present, the present is represented by the time interval when that beam is close to whatever target it is fired at and all the interest interactions happen, and the distant future is represented by what is seen on the detector once the particle spray coming out of the target region results again in approximately free particles.

As a technical point, note that when we do scattering we are not interested in the whole Hilbert space or

rigged Hilbert space. We are only interested in states which have support very far away, and so are necessarily not square-integrable. Consequently, generally the asymptotic incoming and outgoing states will look like plane waves.

8.9.1 The Interaction Picture

Because we consider incoming states which asymptotically evolve according to $\hat{H}_0$, it is useful to decompose those states into eigenstates of $\hat{H}_0$. Under the time evolution generated by $\hat{H}_0$ in the Schrödinger equation, an eigenstate of $\hat{H}_0$ will remain that same eigenstate, up to a phase, for all time. Consequently, it is useful to define a way of “dividing out” this phase, so that in an appropriate sense it is possible to identify a static decomposition of the incoming state in eigenstates of $\hat{H}_0$. Similarly so the for outgoing states. We do this by introducing the interaction picture. Consider a system with state $|\psi(t)\rangle$ evolving under the time independent Hamiltonian operator $\hat{H}$:

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle. \quad (8.9.3)$$

Then, the time evolved state is given by:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle. \quad (8.9.4)$$

As well, any operator summary can be computed in time as:

$$\mathcal{O}(t) = \langle\psi(t)|\hat{\mathcal{O}}|\psi(t)\rangle = \langle\psi(0)|e^{\frac{i}{\hbar}\hat{H}t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle. \quad (8.9.5)$$

We define the interaction picture state $|\psi_I(t)\rangle$ by:

$$|\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle. \quad (8.9.6)$$

Using the decomposition $\hat{H} = \hat{H}_0 + \hat{H}_1$, the interaction picture state then evolves according to:

$$i\hbar \frac{d|\psi_I\rangle}{dt} = i\hbar \frac{d}{dt} \left(e^{\frac{i}{\hbar}\hat{H}_0t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle \right) \quad (8.9.7)$$

$$= i\hbar \left(\frac{i}{\hbar}\hat{H}_0e^{\frac{i}{\hbar}\hat{H}_0t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle + e^{\frac{i}{\hbar}\hat{H}_0t} \left(-\frac{i}{\hbar}\hat{H} \right) e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle \right) \quad (8.9.8)$$

$$= -\hat{H}_0|\psi_I(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0t} \left(\hat{H}_0 + \hat{H}_1 \right) e^{-\frac{i}{\hbar}\hat{H}_0t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle \quad (8.9.9)$$

$$= -\hat{H}_0|\psi_I(t)\rangle + \hat{H}_0|\psi_I(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0t}\hat{H}_1e^{-\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle \quad (8.9.10)$$

$$= e^{\frac{i}{\hbar}\hat{H}_0t}\hat{H}_1e^{-\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle. \quad (8.9.11)$$

So, we define the interaction picture Hamiltonian operator by:

$$\hat{H}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0t}\hat{H}_1e^{-\frac{i}{\hbar}\hat{H}_0t} \quad (8.9.12)$$

and from this we have the interaction picture Schrodinger equation:

$$i\hbar \frac{d|\psi_I\rangle}{dt} = \hat{H}_I(t)|\psi_I\rangle. \quad (8.9.13)$$

We can see that the interaction picture has the advantage that the state only evolves “due to the interaction”. That is, if $\hat{H}_1 = 0$ then the state does not evolve at all. Because we consider past and future states on which $\hat{H}_1$ asymptotically vanishes, this means that as $t \rightarrow \pm\infty$, $|\psi_I(t)\rangle$ becomes asymptotically constant.

Inverting (8.9.6) and returning it to (8.9.5)

$$|\psi(0)\rangle = e^{\frac{i}{\hbar}\hat{H}t}e^{-\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle \quad (8.9.14)$$

$$\mathcal{O}(t) = \langle\psi_I(t)|e^{\frac{i}{\hbar}\hat{H}_0t}e^{-\frac{i}{\hbar}\hat{H}t}e^{\frac{i}{\hbar}\hat{H}t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}t}e^{\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle \quad (8.9.15)$$

$$= \langle\psi_I(t)|e^{\frac{i}{\hbar}\hat{H}_0t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle. \quad (8.9.16)$$

Thus, we define the interaction picture operators by:

$$\hat{\mathcal{O}}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0t}\hat{\mathcal{O}}e^{-\frac{i}{\hbar}\hat{H}_0t} \quad (8.9.17)$$

$$\implies \mathcal{O}(t) = \langle\psi_I(t)|\hat{\mathcal{O}}_I(t)|\psi_I(t)\rangle. \quad (8.9.18)$$

So, in the interaction picture the operators evolve in time according to the free Hamiltonian operator $\hat{H}_0$ only while the state evolves in time according to the interaction part. The interaction picture essentially divides the time evolution among the state and operators according to whether that part of the time evolution is due to the interaction or is free.

In scattering, by definition we always consider systems for which the interaction's effect goes to 0 in the distant past or future and so the interaction state $|\psi_I(t)\rangle$ asymptotically becomes constant. The value that $|\psi_I\rangle$ takes in the distant past is called $|\psi_{\text{in}}\rangle$ and the value it takes in the distant future is called $|\psi_{\text{out}}\rangle$. Precisely:

$$|\psi_{\text{in}}\rangle = \lim_{t \rightarrow -\infty} |\psi_I(t)\rangle = \left(\lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \right) |\psi(0)\rangle. \quad (8.9.19)$$

Importantly, note that the system is free in the limit $t \rightarrow \pm\infty$. At finite times, (for example in $|\psi(0)\rangle$) the system is in the middle interacting region. We define the “Backward” operator $\hat{\Omega}_-$ by:

$$\hat{\Omega}_- = \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \quad (8.9.20)$$

as it takes a state in the interacting present at time $t = 0$ and pulls it all the way back into the free past:

$$|\psi_{\text{in}}\rangle = \hat{\Omega}_- |\psi(0)\rangle. \quad (8.9.21)$$

We can see automatically from the definition of the backward operator that it is unitary¹²:

$$\hat{\Omega}_-^{-1} = \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} = \left(\lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \right)^\dagger = \hat{\Omega}_-^\dagger. \quad (8.9.22)$$

Similarly:

$$|\psi_{\text{out}}\rangle = \lim_{t \rightarrow \infty} |\psi_I(t)\rangle = \left(\lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \right) |\psi(0)\rangle. \quad (8.9.23)$$

So, we define the “Forward” operator $\hat{\Omega}_+$ by:

$$\hat{\Omega}_+ = \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \quad (8.9.24)$$

as it takes a state in the interacting present at time $t = 0$ and pushes it all the way forward into the free future:

$$|\psi_{\text{out}}\rangle = \hat{\Omega}_+ |\psi(0)\rangle. \quad (8.9.25)$$

The forward operator that it is also unitary:

$$\hat{\Omega}_+^{-1} = \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} = \left(\lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} \right)^\dagger = \hat{\Omega}_+^\dagger. \quad (8.9.26)$$

Combining (8.9.21) and (8.9.25), we can see that the outgoing state is related to the incoming state as:

$$|\psi_{\text{out}}\rangle = \hat{\Omega}_+ \hat{\Omega}_-^\dagger |\psi_{\text{in}}\rangle. \quad (8.9.27)$$

Thus, all of scattering is encoded in the Scattering Operator $\hat{S}$ or “S Matrix” defined by:

$$\hat{S} = \hat{\Omega}_+ \hat{\Omega}_-^\dagger \implies \boxed{|\psi_{\text{out}}\rangle = \hat{S} |\psi_{\text{in}}\rangle}. \quad (8.9.28)$$

Automatically, it follows that the S Matrix is unitary:

$$\hat{S}^{-1} = \left(\hat{\Omega}_-^\dagger \right)^{-1} \hat{\Omega}_+^{-1} = \hat{\Omega}_- \hat{\Omega}_+^\dagger = \left(\hat{\Omega}_+ \hat{\Omega}_-^\dagger \right)^\dagger = \hat{S}^\dagger. \quad (8.9.29)$$

The unitarity of the S matrix is very important in proving several other important results. As was its intent, the S Matrix pulls a state from the free past and pushes it into the free future. In quantum mechanics, the whole theoretical side of the business of scattering amounts to computing the S matrix.

8.9.2 The Dyson Series

The most direct way to compute the S Matrix is to simply solve the interaction picture Schrodinger equation perturbatively. Because equation (8.9.13) is linear, we know that $|\psi_I(t)\rangle$ is related to $|\psi_I(t_0)\rangle$ by

¹²Permitting some lack of care on the commutation of limits. This issue is actually extremely technically subtle, but the details are not necessary for any of our analysis.

some linear operator $\hat{U}(t, t_0)$ as:

$$|\psi_I(t)\rangle = \hat{U}(t, t_0)|\psi_I(t_0)\rangle. \quad (8.9.30)$$

This operator $\hat{U}(t, t_0)$ is the interaction picture time evolution operator. Taking the limits that $t \rightarrow \infty$ and $t_0 \rightarrow -\infty$ we have:

$$|\psi_{\text{out}}\rangle = \lim_{\substack{t \rightarrow \infty \\ t_0 \rightarrow -\infty}} \hat{U}(t, t_0)|\psi_{\text{in}}\rangle \quad (8.9.31)$$

and so we can identify that the S matrix is given in terms of the time evolution operator by:

$$\hat{S} = \lim_{\substack{t \rightarrow \infty \\ t_0 \rightarrow -\infty}} \hat{U}(t, t_0). \quad (8.9.32)$$

It follows from (8.9.30) that $\hat{U}(t_0, t_0) = \mathbb{1}$. Further, by inserting (8.9.30) into (8.9.13) we find:

$$i\hbar \frac{d\hat{U}(t, t_0)}{dt} = \hat{H}_I(t)\hat{U}(t, t_0). \quad (8.9.33)$$

Integrating both sides with respect to t from t_0 to t :

$$i\hbar(\hat{U}(t, t_0) - \hat{U}(t_0, t_0)) = \int_{t_0}^t \hat{H}_I(t')\hat{U}(t', t_0)dt' \quad (8.9.34)$$

$$\implies \hat{U}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t')\hat{U}(t', t_0)dt'. \quad (8.9.35)$$

Equation (8.9.35) is not obviously helpful as $\hat{U}$ is expressed in terms of itself. But, by inserting another copy of (8.9.35) back into itself on the right hand side we see:

$$\hat{U}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t')dt' - \frac{1}{\hbar^2} \int_{t_0}^t \int_{t_0}^{t'} \hat{H}_I(t')\hat{H}_I(t'')\hat{U}(t'', t_0)dt''dt'. \quad (8.9.36)$$

We could again circuitously insert equation (8.9.35) back into this again and again and after several iterations we would arrive at:

$$\hat{U}(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t')dt' + \dots + \left(\frac{-i}{\hbar}\right)^N \int_{t_0}^t \dots \int_{t_0}^{t_2} \hat{H}_I(t_N)\dots\hat{H}_I(t_1)\hat{U}(t_1, t_0)dt_1\dots dt_N. \quad (8.9.37)$$

As N gets larger, t_N spends an increasing portion of its integral close to t_0 and so as $N \rightarrow \infty$ we have $\hat{U}(t_1, t_0) \rightarrow \hat{U}(t_0, t_0) = \mathbb{1}$. Thus, in the $N \rightarrow \infty$ limit we have:

$$\boxed{\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^t \dots \int_{t_0}^{t_2} \hat{H}_I(t_n)\dots\hat{H}_I(t_1)dt_1\dots dt_n.} \quad (8.9.38)$$

This series expansion is called the Dyson series. Cutting off the series after a finite number of terms at least gives an approximation for $\hat{U}(t, t_0)$ and thus can be used then to obtain an approximation for $\hat{S}$. Equation (8.9.38) is the most useful equation for perturbatively computing the time evolution operator $\hat{U}$. However, it can be simplified in terms of notation (though made less useful for calculation), by introducing the time ordering transformation $\mathcal{T}$: which is **NOT** an operator. It is a transformation which acts on a product of operators which are functions of time and is defined by reordering all of the operators into order from last to first time. That is, for 2 operators $\hat{A}(t_1)$ and $\hat{B}(t_2)$:

$$\mathcal{T} : \hat{A}(t_1)\hat{B}(t_2) = \begin{cases} \hat{A}(t_1)\hat{B}(t_2), & t_1 > t_2 \\ \frac{\hat{A}(t_1)\hat{B}(t_2) + \hat{B}(t_2)\hat{A}(t_1)}{2}, & t_1 = t_2 \\ \hat{B}(t_2)\hat{A}(t_1), & t_1 < t_2 \end{cases} \quad (8.9.39)$$

and similarly so for products of 3 or more operators. Then, because $t_1 < \dots < t_n < t$ in (8.9.38), it is already time ordered and so we can trivially apply the time ordering transformation to it:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \mathcal{T} : \int_{t_0}^t \dots \int_{t_0}^{t_2} \hat{H}_I(t_n)\dots\hat{H}_I(t_1)dt_1\dots dt_n. \quad (8.9.40)$$

Because of the time ordering, we can reorder the factors of $\hat{H}_I$ arbitrarily as the time ordering will just return them back to their original order anyway. There are $n!$ ways to order n factors and so we can sum over all $n!$ orderings and divide by $n!$ because under the time ordering all of the terms in such a sum are equal. Let σ

be a list containing each of the numbers 1 to n once each in some order (this is called a permutation of n). Then, let σ_k be the k^{th} entry in that list. Then:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n \mathcal{T} : \int_{t_0}^t \dots \int_{t_0}^{t_2} \sum_{\text{All } \sigma} \hat{H}_I(t_{\sigma_n}) \dots \hat{H}_I(t_{\sigma_1}) dt_1 \dots dt_n. \quad (8.9.41)$$

In each term of the sum over all σ , rename t_{σ_k} to t_k . Then, the resulting integration region will be the set of all values of $t_1, \dots, t_n$ from t_0 to t with the t_k ordered so that the k^{th} highest element is t_{σ_k} . The region of values of $t_1, \dots, t_n$ each from t_0 to t can be divided into $n!$ regions in which the t_k take a particular ordering on each region. Then, the sum over all such orderings of these integrals is equivalent to simply integrating each t_k from t_0 to t without having to sum over orderings:

$$\sum_{\text{All } \sigma} \int_{t_0}^t \dots \int_{t_0}^{t_2} \hat{H}_I(t_{\sigma_n}) \dots \hat{H}_I(t_{\sigma_1}) dt_1 \dots dt_n = \int_{t_0}^t \dots \int_{t_0}^t \hat{H}_I(t_n) \dots \hat{H}_I(t_1) dt_1 \dots dt_n. \quad (8.9.42)$$

Then, $\hat{U}(t, t_0)$ becomes:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n \mathcal{T} : \int_{t_0}^t \dots \int_{t_0}^t \hat{H}_I(t_n) \dots \hat{H}_I(t_1) dt_1 \dots dt_n \quad (8.9.43)$$

$$= \mathcal{T} : \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n \left(\int_{t_0}^t \hat{H}_I(t') dt' \right)^n \quad (8.9.44)$$

$$= \mathcal{T} : e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}_I(t') dt'}. \quad (8.9.45)$$

Finally then, the S Matrix is given by (8.9.32) as:

$$\boxed{\hat{S} = \mathcal{T} : e^{-\frac{i}{\hbar} \int_{-\infty}^{\infty} \hat{H}_I(t) dt}}. \quad (8.9.46)$$

This formula is true but usually not very useful, at least in ordinary quantum mechanics. However, we will find uses for it much later on.

8.9.3 The Lippmann-Schwinger Equation

There is another other way of computing the S matrix which has the advantage of taking the $t \rightarrow \pm\infty$ limits early rather than at the end. Let $\{|\alpha_0\rangle\}$ be an orthonormal basis of eigenvectors of the scattering states of the free Hamiltonian operator $\hat{H}_0$. That is:

$$\hat{H}_0|\alpha_0\rangle = E_{\alpha}|\alpha_0\rangle \quad (8.9.47)$$

$$\int |\alpha_0\rangle\langle\alpha_0| d\alpha = \mathbb{1} \quad (8.9.48)$$

$$\langle\alpha_0|\beta_0\rangle = \delta(\alpha - \beta) \quad (8.9.49)$$

where the $\mathbb{1}$ operator is understood as the identity operator on the scattering subspace of the rigged Hilbert space (meaning we exclude all the “bound states” which decay too quickly to reach a far away detector). Here we will use α, β, γ as labels on these states. Because often these labels will be continuous (such as labeling the outgoing wavenumbers of plane waves), we write “sums” over them as integrals. Because we assume we know how to diagonalize $\hat{H}_0$, the scattering operator $\hat{S}$ can be written as:

$$\hat{S} = \int |\beta_0\rangle\langle\beta_0| d\beta \hat{S} \int |\alpha_0\rangle\langle\alpha_0| d\alpha = \int |\beta_0\rangle\langle\beta_0| \hat{S} |\alpha_0\rangle\langle\alpha_0| d\alpha d\beta. \quad (8.9.50)$$

Here the $|\alpha_0\rangle$ and $|\beta_0\rangle$ states are known and so all we need to fully specify the S matrix are the “S matrix elements”:

$$S_{\beta\alpha} = \langle\beta_0|\hat{S}|\alpha_0\rangle. \quad (8.9.51)$$

Suppose we begin our system with the incoming state as an eigenstate of $\hat{H}_0$:

$$|\psi_{\text{in}}\rangle = |\alpha_0\rangle. \quad (8.9.52)$$

Then, the present state is given by:

$$|\psi(0)\rangle = \hat{\Omega}_-^\dagger |\alpha_0\rangle. \quad (8.9.53)$$

If we now act the full Hamiltonian operator $\hat{H}$ on this state:

$$\hat{H}|\psi(0)\rangle = \hat{H} \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle = \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.54)$$

$$= \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} (\hat{H}_0 + \hat{H}_1) e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.55)$$

$$= \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} \hat{H}_0 |\alpha_0\rangle + \lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H} t} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.56)$$

$$= E_\alpha |\psi(0)\rangle + \left(\lim_{t \rightarrow -\infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H} t} \right) |\psi(0)\rangle. \quad (8.9.57)$$

This second term is the expression for the interaction term of the Hamiltonian operator in the “active picture” going into the distant past. Because we require for scattering that the interaction in the distant past and future vanishes on our states, this term is required for scattering states to go to 0. Thus:

$$\hat{H}|\psi(0)\rangle = E_\alpha |\psi(0)\rangle. \quad (8.9.58)$$

The requirement that the second term in equation (8.9.57) vanishes puts a significant restriction on what $\hat{H}_0$ and $\hat{H}_1$ can be for the scattering formalism to be valid. We see that automatically from this condition $|\psi(0)\rangle$ is now an eigenstate of the total Hamiltonian operator $\hat{H}$ and that it has the same eigenvalue as $|\alpha_0\rangle$. Thus, one aspect at the very least of requiring the interaction to asymptotically vanish is that $\hat{H}$ and $\hat{H}_0$ have the same spectrum of scattering states. We see that if the incoming state is an eigenstate $|\alpha_0\rangle$ of $\hat{H}_0$ with eigenvalue E_α then the present state is an eigenstate of $\hat{H}$ with the same eigenvalue. Because we have pushed this incoming state forward into the present, we call this eigenstate $|\alpha_+\rangle$:

$$\boxed{|\alpha_+\rangle = \hat{\Omega}_+^\dagger |\alpha_0\rangle.} \quad (8.9.59)$$

Similarly, suppose instead that our system had ended up as an outgoing state which is an eigenstate of $\hat{H}_0$:

$$|\psi_{\text{out}}\rangle = |\alpha_0\rangle. \quad (8.9.60)$$

Then, the present state would be given by:

$$|\psi(0)\rangle = \hat{\Omega}_+^\dagger |\alpha_0\rangle. \quad (8.9.61)$$

And, if we now act the full Hamiltonian operator on this state:

$$\hat{H}|\psi(0)\rangle = \hat{H} \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle = \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.62)$$

$$= \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} (\hat{H}_0 + \hat{H}_1) e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.63)$$

$$= \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} \hat{H}_0 |\alpha_0\rangle + \lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H} t} e^{\frac{i}{\hbar} \hat{H} t} e^{-\frac{i}{\hbar} \hat{H}_0 t} |\alpha_0\rangle \quad (8.9.64)$$

$$= E_\alpha |\psi(0)\rangle + \left(\lim_{t \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H} t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H} t} \right) |\psi(0)\rangle. \quad (8.9.65)$$

Again, we require that asymptotically in the future the interaction piece of Hamiltonian operator acting on our states vanishes and so the second term in (8.9.65) is required in the scattering formalism to be 0. Then, we again have:

$$\hat{H}|\psi(0)\rangle = E_\alpha |\psi(0)\rangle. \quad (8.9.66)$$

So, if we take an outgoing eigenstate of $\hat{H}_0$ and pull it back into the present we also will recover an eigenstate of the full Hamiltonian operator $\hat{H}$. Because we have pulled the outgoing state back into the present, we call this eigenstate $|\alpha_-\rangle$:

$$\boxed{|\alpha_-\rangle = \hat{\Omega}_+^\dagger |\alpha_0\rangle} \quad (8.9.67)$$

Together then, we have that the plus and minus states are the results of pushing forward or pulling back eigenstates of the unperturbed Hamiltonian operator into the present and that doing so gives eigenstates of the full Hamiltonian operator:

$$\boxed{\hat{H}|\alpha_\pm\rangle = E_\alpha |\alpha_\pm\rangle.} \quad (8.9.68)$$

The plus and minus states give a nice way of expressing the S matrix elements:

$$S_{\beta\alpha} = \langle \beta_0 | \hat{S} | \alpha_0 \rangle = \langle \beta_0 | \hat{\Omega}_+ \hat{\Omega}_+^\dagger | \alpha_0 \rangle \implies \boxed{S_{\beta\alpha} = \langle \beta_- | \alpha_+ \rangle.} \quad (8.9.69)$$

So, if we can find expressions for the plus and minus states, we can directly compute the $\hat{S}$ matrix elements. Doing so will be our next goal.

Using equation (8.9.68),

$$(\hat{H}_0 + \hat{H}_1)|\alpha_{\pm}\rangle = E_{\alpha}|\alpha_{\pm}\rangle \implies (E_{\alpha} - \hat{H}_0)|\alpha_{\pm}\rangle = \hat{H}_1|\alpha_{\pm}\rangle. \quad (8.9.70)$$

The combination $E_{\alpha} - \hat{H}_0$ is short for $E_{\alpha}\mathbb{1} - \hat{H}_0$ where $\mathbb{1}$ is the identity operator. The operator $E_{\alpha} - \hat{H}_0$ is not invertible because it annihilates any eigenstate of $\hat{H}_0$ with eigenvalue E_{α} (and we know at least one such state, $|\alpha_0\rangle$, exists). However, because $\hat{H}_0$ is self-adjoint and so has real eigenvalues only, the operator $E_{\alpha} - \hat{H}_0 + i\varepsilon$ annihilates no state for any real $\varepsilon \neq 0$. Thus, it is invertible. So, letting ε be a positive real number:

$$(E_{\alpha} - \hat{H}_0 \pm i\varepsilon)|\alpha_{\pm}\rangle = \hat{H}_1|\alpha_{\pm}\rangle \pm i\varepsilon|\alpha_{\pm}\rangle \quad (8.9.71)$$

$$\implies |\alpha_{\pm}\rangle = (E_{\alpha} - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{H}_1|\alpha_{\pm}\rangle \pm i\varepsilon(E_{\alpha} - \hat{H}_0 \pm i\varepsilon)^{-1}|\alpha_{\pm}\rangle. \quad (8.9.72)$$

Now recall the integral fact that for a complex number z with positive real part:

$$\int_0^{\infty} e^{-zx} dx = \frac{-1}{z} e^{-zx} \Big|_0^{\infty} = \frac{1}{z}. \quad (8.9.73)$$

The operator $\varepsilon \mp i(E_{\alpha} - \hat{H}_0)$ has complex eigenvalues with positive real part only and so (recalling how an operator exponential is defined):

$$\int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} dx |\beta_0\rangle = \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - E_{\beta}))x} dx |\beta_0\rangle = \frac{1}{\varepsilon \mp i(E_{\alpha} - E_{\beta})} |\beta_0\rangle = \frac{\pm i}{E_{\alpha} - \hat{H}_0 \pm i\varepsilon} |\beta_0\rangle. \quad (8.9.74)$$

Here the operator reciprocal is just notation for the inverse of that operator. Then, because this operator equation holds for the whole basis $|\beta_0\rangle$, it holds in general:

$$\int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} dx = \frac{\pm i}{E_{\alpha} - \hat{H}_0 \pm i\varepsilon}. \quad (8.9.75)$$

Then, equation (8.9.72) becomes:

$$|\alpha_{\pm}\rangle = \frac{1}{E_{\alpha} - \hat{H}_0 \pm i\varepsilon} \hat{H}_1|\alpha_{\pm}\rangle + \varepsilon \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} dx |\alpha_{\pm}\rangle. \quad (8.9.76)$$

This is true for all positive ε . Let us consider it in the limit $\varepsilon \rightarrow 0^+$:

$$|\alpha_{\pm}\rangle = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_{\alpha} - \hat{H}_0 \pm i\varepsilon} \hat{H}_1|\alpha_{\pm}\rangle + \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} dx |\alpha_{\pm}\rangle. \quad (8.9.77)$$

One needs to be careful handling the limit on the first term because at $\varepsilon = 0$, the operator $E_{\alpha} - \hat{H}_0 \pm i\varepsilon$ loses invertibility. The second term is more straightforward using another integral fact. Consider a function $f(x)$ which has a finite limit as $x \rightarrow \infty$:

$$\lim_{\varepsilon \rightarrow 0^+} \int_0^{\infty} \varepsilon e^{-\varepsilon x} f(x) dx \stackrel{(u=\varepsilon x)}{=} \lim_{\varepsilon \rightarrow 0^+} \int_0^{\infty} e^{-u} f\left(\frac{u}{\varepsilon}\right) du \quad (8.9.78)$$

$$= \int_0^{\infty} e^{-u} \lim_{\varepsilon \rightarrow 0^+} f\left(\frac{u}{\varepsilon}\right) du \quad (8.9.79)$$

$$= \int_0^{\infty} e^{-u} \lim_{x \rightarrow \infty} f(x) du = \lim_{x \rightarrow \infty} f(x) \int_0^{\infty} e^{-u} du \quad (8.9.80)$$

$$= \lim_{x \rightarrow \infty} f(x). \quad (8.9.81)$$

Then:

$$\lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} |\alpha_{\pm}\rangle dx = \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - \hat{H}_0))x} \int |\beta_0\rangle \langle \beta_0| d\beta |\alpha_{\pm}\rangle dx \quad (8.9.82)$$

$$= \int \lim_{\varepsilon \rightarrow 0^+} \varepsilon \int_0^{\infty} e^{-(\varepsilon \mp i(E_{\alpha} - E_{\beta}))x} dx |\beta_0\rangle \langle \beta_0| \alpha_{\pm}\rangle d\beta \quad (8.9.83)$$

$$= \lim_{x \rightarrow \infty} \int e^{\pm i(E_{\alpha} - E_{\beta})x} |\beta_0\rangle \langle \beta_0| \alpha_{\pm}\rangle d\beta \quad (8.9.84)$$

$$= \lim_{x \rightarrow \infty} e^{\pm i(E_{\alpha} - \hat{H}_0)x} \int |\beta_0\rangle \langle \beta_0| d\beta |\alpha_{\pm}\rangle \quad (8.9.85)$$

$$= \lim_{t \rightarrow \pm\infty} e^{-\frac{i}{\hbar} \hat{H}_0 t} e^{\frac{i}{\hbar} E_\alpha t} |\alpha_\pm\rangle \quad (8.9.86)$$

$$= \lim_{t \rightarrow \pm\infty} e^{-\frac{i}{\hbar} \hat{H}_0 t} e^{\frac{i}{\hbar} \hat{H} t} |\alpha_\pm\rangle \quad (8.9.87)$$

$$= \hat{\Omega}_\mp |\alpha_\pm\rangle = \hat{\Omega}_\mp \hat{\Omega}_\mp^\dagger |\alpha_0\rangle \quad (8.9.88)$$

$$= |\alpha_0\rangle. \quad (8.9.89)$$

Returning this to (8.9.77) gives us the Lippmann-Schwinger equation:

$$|\alpha_\pm\rangle = |\alpha_0\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H}_0 \pm i\varepsilon} \hat{H}_1 |\alpha_\pm\rangle. \quad (8.9.90)$$

Unfortunately, $|\alpha_\pm\rangle$ appears on both sides of the Lippmann-Schwinger equation. Because it is implicit, it isn't immediately able to be used to compute $|\alpha_\pm\rangle$. But, it is well-designed for perturbation theory, which in this context is often called the **Born Approximation**. Consider a perturbative expansion of $|\alpha_\pm\rangle$ in powers of its dependence on $\hat{H}_1$:

$$|\alpha_\pm\rangle = \sum_{n=0}^{\infty} |\alpha_\pm^{(n)}\rangle. \quad (8.9.91)$$

That is, the term $|\alpha_\pm^{(n)}\rangle$ should involve n factors of $\hat{H}_1$ when actually solved for. Inserting this series into the Lippmann-Schwinger equation gives:

$$\sum_{n=0}^{\infty} |\alpha_\pm^{(n)}\rangle = |\alpha_0\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H}_0 \pm i\varepsilon} \hat{H}_1 \left(\sum_{n=0}^{\infty} |\alpha_\pm^{(n)}\rangle \right) \quad (8.9.92)$$

$$\Rightarrow |\alpha_\pm^{(0)}\rangle = |\alpha_0\rangle, \quad |\alpha_\pm^{(n+1)}\rangle = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H}_0 \pm i\varepsilon} \hat{H}_1 |\alpha_\pm^{(n)}\rangle. \quad (8.9.93)$$

Hence the perturbation series can be computed iteratively using (8.9.93) to give approximate solutions for $|\alpha_\pm\rangle$.

There is another useful (and equivalent) way to solve the Lippmann-Schwinger equation by using a Green's Operator (which is just the operator way of writing a Green's function, also called a resolvent operator). Define, for a complex number z :

$$\hat{G}(z) = (z - \hat{H}_0)^{-1}, \quad \hat{R}(z) = (z - \hat{H})^{-1}. \quad (8.9.94)$$

$\hat{G}$ is the Green's operator of the unperturbed Hamiltonian operator $\hat{H}_0$ and $\hat{R}$ is the Green's operator of the full Hamiltonian operator $\hat{H}$. As long as z has non-zero imaginary part these inverses exist because the eigenvalues of $\hat{H}_0$ and $\hat{H}$ are purely real. We will often be interested in the behavior of these operators as the complex number z limits toward being real (surprisingly perhaps, they have sensible limiting behavior). Consequently, we define for a real number E :

$$\hat{G}_\pm(E) = \lim_{\varepsilon \rightarrow 0^+} \hat{G}(E \pm i\varepsilon), \quad \hat{R}_\pm(E) = \lim_{\varepsilon \rightarrow 0^+} \hat{R}(E \pm i\varepsilon). \quad (8.9.95)$$

Soon we will understand precisely why $\hat{G}_+$ cannot possibly equal $\hat{G}_-$ (and identically so for $\hat{R}_\pm$). From the definition of $\hat{R}(z)$:

$$(z - \hat{H}_0 - \hat{H}_1) \hat{R}(z) = \mathbb{1} \quad (8.9.96)$$

$$\Rightarrow \hat{G}^{-1}(z) \hat{R}(z) - \hat{H}_1 \hat{R}(z) = \mathbb{1} \quad (8.9.97)$$

$$\Rightarrow \hat{R}(z) = \hat{G}(z) + \hat{G}(z) \hat{H}_1 \hat{R}(z) \quad (8.9.98)$$

Thus:

$$(\mathbb{1} - \hat{G}(z) \hat{H}_1)(\mathbb{1} + \hat{R}(z) \hat{H}_1) = \mathbb{1} - \hat{G}(z) \hat{H}_1 + \hat{R}(z) \hat{H}_1 - \hat{G}(z) \hat{H}_1 \hat{R}(z) \hat{H}_1 \quad (8.9.99)$$

$$= \mathbb{1} - \hat{G}(z) \hat{H}_1 + (\hat{G}(z) + \hat{G}(z) \hat{H}_1 \hat{R}(z)) \hat{H}_1 - \hat{G}(z) \hat{H}_1 \hat{R}(z) \hat{H}_1 \quad (8.9.100)$$

$$= \mathbb{1} - \hat{G}(z) \hat{H}_1 + \hat{G}(z) \hat{H}_1 + \hat{G}(z) \hat{H}_1 \hat{R}(z) \hat{H}_1 - \hat{G}(z) \hat{H}_1 \hat{R}(z) \hat{H}_1 \quad (8.9.101)$$

$$= \mathbb{1}. \quad (8.9.102)$$

By solving for $|\alpha_0\rangle$, the Lippmann-Schwinger equation can be rewritten as:

$$|\alpha_0\rangle = (\mathbb{1} - \hat{G}_\pm(E_\alpha)) \hat{H}_1 |\alpha_\pm\rangle. \quad (8.9.103)$$

By (8.9.102), this can be inverted to give:

$$|\alpha_0\rangle = \left(\mathbb{1} + \hat{R}_\pm(E_\alpha) \hat{H}_1 \right)^{-1} |\alpha_\pm\rangle \quad (8.9.104)$$

$$\implies |\alpha_\pm\rangle = \left(\mathbb{1} + \hat{R}_\pm(E_\alpha) \hat{H}_1 \right) |\alpha_0\rangle \quad (8.9.105)$$

$$\implies |\alpha_\pm\rangle = |\alpha_0\rangle + \hat{R}_\pm(E_\alpha) \hat{H}_1 |\alpha_0\rangle \quad (8.9.106)$$

$$\implies |\alpha_\pm\rangle = |\alpha_0\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H} \pm i\varepsilon} \hat{H}_1 |\alpha_0\rangle. \quad (8.9.107)$$

Hence, if $R(z)$ can be computed, it provides the solution to the Lippmann-Schwinger equation. Fortunately, the Green's operator can also be handled nicely by perturbation theory. Taking a perturbative expansion in the same way as we did the $|\alpha_\pm\rangle$:

$$\hat{R}(z) = \sum_{n=0}^{\infty} \hat{R}^{(n)}(z) \quad (8.9.108)$$

and using (8.9.98):

$$\sum_{n=0}^{\infty} \hat{R}^{(n)}(z) = \hat{G}(z) + \hat{G}(z) \hat{H}_1 \sum_{n=0}^{\infty} \hat{R}^{(n)}(z) \quad (8.9.109)$$

$$\implies \hat{R}^{(0)}(z) = \hat{G}(z), \quad \hat{R}^{(n+1)}(z) = \hat{G}(z) \hat{H}_1 \hat{R}^{(n)}(z). \quad (8.9.110)$$

Hence, if $\hat{G}(z)$ can be computed, then $\hat{R}(z)$ can be computed perturbatively. Because $\hat{G}$ is defined in terms of $\hat{H}_0$ which we are generally able to understand fully, typically $\hat{G}$ is known completely. Formally, the perturbative solution for $\hat{R}$ gives the series:

$$\hat{R} = \hat{G} + \hat{G} \hat{H}_1 \hat{G} + \hat{G} \hat{H}_1 \hat{G} \hat{H}_1 \hat{G} + \hat{G} \hat{H}_1 \hat{G} \hat{H}_1 \hat{G} \hat{H}_1 \hat{G} + \dots \quad (8.9.111)$$

Truncating this series after a finite number of terms gives an approximation of the full Green's operator.

8.9.4 The Transition Matrix

Both the S matrix and the Lippmann-Schwinger equation can be nicely understood in terms of the transition matrix. The transition operator $\hat{T}$ is defined to satisfy:

$$\hat{T}|\alpha_0\rangle = \hat{H}_1|\alpha_+\rangle \quad (8.9.112)$$

and the transition matrix $T_{\beta\alpha}$ is defined by:

$$T_{\beta\alpha} = \langle\beta_0|\hat{T}|\alpha_0\rangle = \langle\beta_0|\hat{H}_1|\alpha_+\rangle. \quad (8.9.113)$$

The matrix elements $T_{\beta\alpha}$ of the transition operator are also called **Transition Amplitudes** (one might say $T_{\beta\alpha}$ is the amplitude for transitioning from $|\alpha_0\rangle$ to $|\beta_0\rangle$ under the interaction). In terms of the transition operator, the plus Lippmann-Schwinger becomes:

$$|\alpha_+\rangle = |\alpha_0\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H}_0 + i\varepsilon} \hat{T}|\alpha_0\rangle. \quad (8.9.114)$$

With this, we can find a nice formula for the S matrix. From (8.9.107):

$$\langle\alpha_-| = \langle\alpha_0| + \langle\alpha_0|\hat{H}_1 \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H} + i\varepsilon}. \quad (8.9.115)$$

Then, using that $|\alpha_+\rangle$ is an eigenstate of $\hat{H}$:

$$S_{\beta\alpha} = \langle\beta_-|\alpha_+\rangle = \left(\langle\beta_0| + \langle\beta_0|\hat{H}_1 \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\beta - \hat{H} + i\varepsilon} \right) |\alpha_+\rangle \quad (8.9.116)$$

$$= \langle\beta_0|\alpha_+\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\beta - E_\alpha + i\varepsilon} \langle\beta_0|\hat{H}_1|\alpha_+\rangle \quad (8.9.117)$$

$$= \langle\beta_0|\alpha_+\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\beta - E_\alpha + i\varepsilon} \langle\beta_0|\hat{T}|\alpha_0\rangle \quad (8.9.118)$$

$$= \langle\beta_0| \left(|\alpha_0\rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - \hat{H}_0 + i\varepsilon} \hat{T}|\alpha_0\rangle \right) + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\beta - E_\alpha + i\varepsilon} T_{\beta\alpha} \quad (8.9.119)$$

$$= \langle \beta_0 | \alpha_0 \rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\alpha - E_\beta + i\varepsilon} \langle \beta_0 | \hat{T} | \alpha_0 \rangle + \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E_\beta - E_\alpha + i\varepsilon} T_{\beta\alpha} \quad (8.9.120)$$

$$= \delta(\alpha - \beta) + T_{\beta\alpha} \lim_{\varepsilon \rightarrow 0^+} \left(\frac{1}{E_\alpha - E_\beta + i\varepsilon} - \frac{1}{E_\alpha - E_\beta - i\varepsilon} \right) \quad (8.9.121)$$

This limit is a little tricky. Let:

$$f(E) = \lim_{\varepsilon \rightarrow 0^+} \left(\frac{1}{E + i\varepsilon} - \frac{1}{E - i\varepsilon} \right) = \lim_{\varepsilon \rightarrow 0^+} \frac{-2i\varepsilon}{E^2 + \varepsilon^2} \quad (8.9.122)$$

and consider a smooth function $g(E)$. Then:

$$\int_{-\infty}^{\infty} f(E) g(E) dE = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{-2i\varepsilon}{E^2 + \varepsilon^2} g(E) dE \quad (8.9.123)$$

$$\stackrel{E=\varepsilon u}{=} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{-2i}{u^2 + 1} g(\varepsilon u) du \quad (8.9.124)$$

$$= \int_{-\infty}^{\infty} \frac{-2i}{u^2 + 1} g(0) du = -2\pi i g(0) \quad (8.9.125)$$

$$= \int_{-\infty}^{\infty} (-2\pi i \delta(E)) g(E) dE. \quad (8.9.126)$$

Because this holds for all smooth $g(E)$, we have $f(E) = -2\pi i \delta(E)$. Consequently:

$$\lim_{\varepsilon \rightarrow 0^+} \left(\frac{1}{E_\alpha - E_\beta + i\varepsilon} - \frac{1}{E_\alpha - E_\beta - i\varepsilon} \right) = -2\pi i \delta(E_\alpha - E_\beta) \quad (8.9.127)$$

Together then, the S matrix can be written in terms of the transition matrix as:

$$\boxed{S_{\beta\alpha} = \delta(\alpha - \beta) - 2\pi i T_{\beta\alpha} \delta(E_\alpha - E_\beta).} \quad (8.9.128)$$

One can see that the S matrix can be thought of as decomposing into a part in which nothing happens (the $\delta(\alpha - \beta)$ term) and a term which contains the scattering (the transition matrix term). Further, the scattering term conserves energy due to the $\delta(E_\alpha - E_\beta)$. One can see immediately that if $\hat{H}_1 = 0$, then $T_{\beta\alpha} = 0$ and $S_{\beta\alpha} = \delta(\alpha - \beta)$ and so all scattering is due to the interaction part $\hat{H}_1$, as it must have been. Because the S matrix can be written in terms of the transition matrix and the transition matrix elements can be written as in (8.9.113) involving only the $|\alpha_+\rangle$ and not $|\alpha_-\rangle$, we only ever really need to study the $+$ solutions to the Lippmann-Schwinger equation.

Like the Lippmann-Schwinger equation or the Green's operator, the transition matrix can be computed perturbatively. Using (8.9.112) and (8.9.113):

$$\hat{T}|\alpha_0\rangle = \hat{H}_1|\alpha_0\rangle + \hat{H}_1\hat{G}_+(E_\alpha)\hat{T}|\alpha_0\rangle. \quad (8.9.129)$$

Reinserting this formula into the expression for $\hat{T}$ on the right hand side repeatedly gives:

$$\hat{T}|\alpha_0\rangle = (\hat{H}_1 + \hat{H}_1\hat{G}_+\hat{H}_1 + \hat{H}_1\hat{G}_+\hat{H}_1\hat{G}_+\hat{H}_1 + \dots)|\alpha_0\rangle \quad (8.9.130)$$

where each copy of $\hat{G}_+$ is evaluated at E_α . Because the argument of $\hat{G}_+$ depends on α , it is not possible to simply equate the term in parentheses with $\hat{T}$. However, we can define the operator function $\hat{V}(E)$ by:

$$\hat{V}(E) = \hat{H}_1 + \hat{H}_1\hat{G}_+(E)\hat{V}(E) \quad (8.9.131)$$

$$= \hat{H}_1 + \hat{H}_1\hat{G}_+(E)\hat{H}_1 + \hat{H}_1\hat{G}_+(E)\hat{H}_1\hat{G}_+(E)\hat{H}_1 + \hat{H}_1\hat{G}_+(E)\hat{H}_1\hat{G}_+(E)\hat{H}_1\hat{G}_+(E)\hat{H}_1 + \dots \quad (8.9.132)$$

Doing so, we have that the transition matrix elements are given by:

$$T_{\beta\alpha} = \langle \beta_0 | \hat{V}(E_\alpha) | \alpha_0 \rangle. \quad (8.9.133)$$

Using (8.9.127) we can identify the precise nature of the difference between $\hat{G}_+$ and $\hat{G}_-$:

$$\hat{G}_+(E) - \hat{G}_-(E) = \lim_{\varepsilon \rightarrow 0^+} \left(\frac{1}{E + i\varepsilon - \hat{H}_0} - \frac{1}{E - i\varepsilon - \hat{H}_0} \right) = -2\pi i \delta(E - \hat{H}_0) \quad (8.9.134)$$

(with an analogous identity for $R_\pm$ and $\hat{H}$). So $\hat{G}_+$ and $\hat{G}_-$ differ by an operator which annihilates any eigenstate of $\hat{H}_0$ that does not have eigenvalue E . As well, neither of $\hat{G}_\pm$ are self-adjoint, instead they are each other's adjoint:

$$\hat{G}_+^\dagger(E) = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - \hat{H}_0 - i\varepsilon} = \hat{G}_-(E). \quad (8.9.135)$$

8.9.5 Transition Rates and Fermi's Master Equation

The transition matrix is essential in characterizing the time averaged rate at which physical processes happen. Suppose at time t_0 our system begins in an eigenstate $|\iota\rangle$ of $\hat{H}_0$ (when represented in the interaction picture) and is subject to the perturbation $\hat{H}_1$ until a final time t . Let $P_{\iota \rightarrow f}$ be the transition intensity for transitions to a different eigenstate $|f\rangle$ of $\hat{H}_0$ at the time t . That is:

$$P_{\iota \rightarrow f} = |\langle f | \psi(t) \rangle|^2. \quad (8.9.136)$$

Using the interaction picture and that $|f\rangle$ is an eigenstate of $\hat{H}_0$:

$$P_{\iota \rightarrow f} = |\langle f | e^{\frac{i}{\hbar} \hat{H}_0 t} |\psi_I(t)\rangle|^2 = |\langle f | \psi_I(t) \rangle|^2 = |\langle f | \hat{U}(t, t_0) |\iota\rangle|^2 \quad (8.9.137)$$

The finite time transition rate is defined as the present rate at which transitions occur (and so the t derivative of the transition intensity). Using the interaction picture Schrödinger equation, we can simplify it significantly:

$$\frac{dP_{\iota \rightarrow f}}{dt} = \frac{d}{dt} (\langle f | \hat{U} |\iota\rangle \langle \iota | \hat{U}^\dagger | f \rangle) = \langle f | \frac{d\hat{U}}{dt} |\iota\rangle \langle \iota | \hat{U}^\dagger | f \rangle + \langle f | \hat{U} |\iota\rangle \langle \iota | \frac{d\hat{U}^\dagger}{dt} | f \rangle \quad (8.9.138)$$

$$= -\frac{i}{\hbar} \langle f | \hat{H}_I \hat{U} |\iota\rangle \langle \iota | \hat{U}^\dagger | f \rangle + \frac{i}{\hbar} \langle f | \hat{U} |\iota\rangle \langle \iota | \hat{U}^\dagger \hat{H}_I | f \rangle \quad (8.9.139)$$

$$= \frac{2}{\hbar} \text{Im} \left(\langle f | \hat{H}_I(t) \hat{U}(t, t_0) |\iota\rangle \langle \iota | \hat{U}^\dagger(t, t_0) | f \rangle \right). \quad (8.9.140)$$

The long time transition rate, also simply called the transition rate $\Gamma_{\iota \rightarrow f}$ is defined as the limit of $\frac{dP_{\iota \rightarrow f}}{dt}$ after we have allowed the process to go on for arbitrarily long. (The transition rate is the answer to the question, "At what rate will the process be happening now, if we started it a very long time ago?") Let $\tau = t - t_0$ be the duration for which the interaction has occurred. Keeping t to be in the finite present while taking $\tau \rightarrow \infty$, requires that t_0 is changed in the limit. Thus:

$$\Gamma_{\iota \rightarrow f} = \lim_{\tau \rightarrow \infty} \frac{dP_{\iota \rightarrow f}}{dt} = \lim_{\tau \rightarrow \infty} \frac{2}{\hbar} \text{Im} \left(\langle f | \hat{H}_I(t) \hat{U}(t, t - \tau) |\iota\rangle \langle \iota | \hat{U}^\dagger(t, t - \tau) | f \rangle \right). \quad (8.9.141)$$

The only τ dependence is in the time evolution operator. By using the definition of the interaction picture wavefunction:

$$|\psi_I(t)\rangle = e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} |\psi(0)\rangle = e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} t} e^{\frac{i}{\hbar} \hat{H} t_0} e^{-\frac{i}{\hbar} \hat{H}_0 t_0} |\psi_I(t_0)\rangle \quad (8.9.142)$$

and the definition of the time evolution operator $\hat{U}(t, t_0)$ in (8.9.30), we can identify:

$$\hat{U}(t, t_0) = e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} e^{-\frac{i}{\hbar} \hat{H}_0 t_0}. \quad (8.9.143)$$

Then, the τ limit is actually quite simple:

$$\lim_{\tau \rightarrow \infty} \hat{U}(t, t - \tau) = \lim_{\tau \rightarrow \infty} e^{\frac{i}{\hbar} \hat{H}_0 t} e^{-\frac{i}{\hbar} \hat{H} \tau} e^{\frac{i}{\hbar} \hat{H}_0 \tau} e^{-\frac{i}{\hbar} \hat{H}_0 t} = e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{\Omega}_-^\dagger e^{-\frac{i}{\hbar} \hat{H}_0 t}. \quad (8.9.144)$$

Returning this to the transition rate and using the definition of the interaction Hamiltonian:

$$\Gamma_{\iota \rightarrow f} = \frac{2}{\hbar} \text{Im} \left(\langle f | e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{H}_1 e^{-\frac{i}{\hbar} \hat{H}_0 t} e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{\Omega}_-^\dagger e^{-\frac{i}{\hbar} \hat{H}_0 t} |\iota\rangle \langle \iota | e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{\Omega}_- e^{-\frac{i}{\hbar} \hat{H}_0 t} | f \rangle \right) \quad (8.9.145)$$

$$= \frac{2}{\hbar} \text{Im} \left(e^{\frac{i}{\hbar} (E_f - E_\iota + E_\iota - E_f) t} \langle f | \hat{H}_1 \hat{\Omega}_-^\dagger |\iota\rangle \langle \iota | \hat{\Omega}_- | f \rangle \right) \quad (8.9.146)$$

$$= \frac{2}{\hbar} \text{Im} \left(\langle f | \hat{H}_1 \hat{\Omega}_-^\dagger |\iota\rangle \langle \iota | \hat{\Omega}_- | f \rangle \right) \quad (8.9.147)$$

By using the definition of the plus states, (8.9.113), and (8.9.114):

$$\langle f | \hat{H}_1 \hat{\Omega}_-^\dagger |\iota\rangle = \langle f | \hat{H}_1 |\iota_+\rangle = \langle f | \hat{T} |\iota\rangle = T_{f\iota} \quad (8.9.148)$$

$$\langle f | \hat{\Omega}_-^\dagger |\iota\rangle = \langle f | \iota_+\rangle = \langle f | \iota\rangle + \lim_{\varepsilon \rightarrow 0^+} \langle f | \frac{1}{E_\iota - \hat{H}_0 + i\varepsilon} \hat{T} |\iota\rangle \quad (8.9.149)$$

$$= \delta(f - \iota) + \lim_{\varepsilon \rightarrow 0^+} \frac{\langle f | \hat{T} |\iota\rangle}{E_\iota - E_f + i\varepsilon} = \lim_{\varepsilon \rightarrow 0^+} \frac{T_{f\iota}}{E_\iota - E_f + i\varepsilon} \quad (8.9.150)$$

where in the last step we used that we are considering a final eigenstate $|f\rangle \neq |\iota\rangle$. Using these, we can simplify the transition rate:

$$\Gamma_{\iota \rightarrow f} = \frac{2}{\hbar} \lim_{\varepsilon \rightarrow 0^+} \text{Im} \left(T_{f\iota} \frac{T_{f\iota}^*}{E_\iota - E_f - i\varepsilon} \right) \quad (8.9.151)$$

$$= \frac{2}{\hbar} \lim_{\varepsilon \rightarrow 0^+} \frac{|T_{f\iota}|^2}{2i} \left(\frac{1}{E_\iota - E_f - i\varepsilon} - \frac{1}{E_\iota - E_f + i\varepsilon} \right). \quad (8.9.152)$$

Finally using (8.9.127), we have:

$$\boxed{\Gamma_{\iota \rightarrow f} = \frac{2\pi}{\hbar} |T_{f\iota}|^2 \delta(E_f - E_\iota).} \quad (8.9.153)$$

This is the all-orders form of **Fermi's Golden Rule**. It may seem experimentally irrelevant to worry about the transition rate after a “very long time”, but because experimental timescales are typically many orders of magnitude larger than the microscopic evolution timescales of quantum systems, the “short term” behavior of the system (as considered relative to macroscopic timescales) is generally completely unnoticeable.

The total decay rate Γ_ι for the state $|\iota\rangle$ is defined as the long term value of the rate of change of $|\langle \iota | \psi(t) \rangle|^2$. That is:

$$\Gamma_\iota = \lim_{\tau \rightarrow \infty} \frac{dP_{\iota \rightarrow \iota}}{dt}. \quad (8.9.154)$$

Due to the unitarity of time evolution (and inserting a complete set of eigenstates $|n\rangle$ of $\hat{H}_0$, where a sum versus an integral is used as appropriate for the system of interest):

$$0 = \frac{d}{dt} \langle \psi_I | \psi_I \rangle = \frac{d}{dt} \sum_n \langle \psi_I | n \rangle \langle n | \psi_I \rangle = \frac{d}{dt} \left(P_{\iota \rightarrow \iota} + \sum_{f \neq \iota} P_{\iota \rightarrow f} \right) \quad (8.9.155)$$

$$\Rightarrow \boxed{\Gamma_\iota = - \sum_{f \neq \iota} \Gamma_{\iota \rightarrow f}} \quad (8.9.156)$$

where in the last line we have taken the $\tau \rightarrow \infty$ limit.

It is often useful to consider separately the magnitude and phase of each component of the interaction wavefunction (in the basis of free eigenstates). So, define ρ_n and φ_n as real quantities so that:

$$\langle n | \psi_I(t) \rangle = \sqrt{\rho_n(t)} e^{i\varphi_n(t)} \Rightarrow \rho_n = |\langle n | \psi_I(t) \rangle|^2. \quad (8.9.157)$$

We found in section 8.2 that the ρ_n are adiabatic invariants and so evolve much more slowly in time than the phases φ_n . As well, the operator summary of the free Hamiltonian and anything that commutes with it only depends on the wavefunction through the ρ_n . Therefore, often the ρ_n are all that is accessible in a direct way experimentally as the phases are generally much more temperamental (in some experiments, phase differences may be quite well-behaved, so this argument is only one which is often useful but not always). Using the definition of the time evolution operator, we can compute an exact formula for the time evolution of ρ_n , valid for all t and t_0 :

$$\rho_n(t) = |\langle n | \hat{U}(t, t_0) | \psi_I(t_0) \rangle|^2 = \sum_{ml} \langle \psi_I(t_0) | m \rangle \langle m | \hat{U}^\dagger | n \rangle \langle n | \hat{U} | l \rangle \langle l | \psi_I(t_0) \rangle \quad (8.9.158)$$

$$= \sum_{ml} \langle m | \hat{U}^\dagger | n \rangle \langle n | \hat{U} | l \rangle \sqrt{\rho_m(t_0) \rho_l(t_0)} e^{i(\varphi_l(t_0) - \varphi_m(t_0))}. \quad (8.9.159)$$

Every experiment is performed in a background of weakly coupled junk throughout the universe (for example, the electromagnetic field is everywhere and has infinitely many harmonic oscillator modes because it can oscillate with any frequency; those modes interact weakly with basically everything). Consequently, it is typically accurate to assume that the experiment is prepared in such a way that the initial phases of the system are completely random with respect to our preparation and to use that the phases evolve very quickly in time, effectively randomly so due to their weak bombardment from an inescapable background of degrees of freedom. The ρ_n are saved from this fate specifically due to their adiabatic invariance. Using this, we can define a sensible notion of a phase-averaged behavior of this equation. If $\varphi_n(t_0)$ is uniformly randomly distributed and each phase is independent, then averaging over such phases immediately gives:

$$\mathbb{E} \left(e^{i(\varphi_l(t_0) - \varphi_m(t_0))} \right) = \delta_{lm}. \quad (8.9.160)$$

When it is reasonable in regard to experimental knowledge to treat the phases of a quantum system as effectively random (essentially due to them oscillating extremely rapidly and subject to uncontrolled interactions with the environment), the system is said to be **decoherent**. Macroscopically large systems are essentially guaranteed to be decoherent because of the number of background degrees of freedom necessarily affecting them. Under

the decoherence approximation then, (8.9.159) becomes:

$$\rho_n(t) \approx \sum_{ml} \langle m | \hat{U}^\dagger | n \rangle \langle n | \hat{U} | l \rangle \sqrt{\rho_m(t_0) \rho_l(t_0)} \delta_{ml} \quad (8.9.161)$$

$$= \sum_m |\langle n | \hat{U} | m \rangle|^2 \rho_m(t_0) = \sum_m P_{m \rightarrow n} \rho_m(t_0). \quad (8.9.162)$$

Differentiating with respect to time gives:

$$\frac{d\rho_n}{dt} \approx \sum_m \frac{dP_{m \rightarrow n}}{dt}(t, t_0) \rho_m(t_0) = \sum_{m \neq n} \frac{dP_{m \rightarrow n}}{dt}(t, t_0) (\rho_m(t_0) - \rho_n(t_0)). \quad (8.9.163)$$

We now use the adiabatic invariance of ρ_n to further approximate this. The explicit duration dependence of $\frac{dP_{m \rightarrow n}}{dt}(t, t_0)$ is determined by the microscopic physics and so by the microscopic timescale τ_{micro} of the quantum system. That timescale is very small compared to the experimental resolution timescale τ_{exp} on which we will apply this equation, and so by taking $t - t_0$ to be of order τ_{exp} , we can approximately replace $\frac{dP_{m \rightarrow n}}{dt}(t, t_0)$ by its long duration value of $\Gamma_{m \rightarrow n}$. However, due to the adiabatic invariance theorem, the timescale $\tau_{\text{adiabatic}}$ on which the ρ_n change significantly is of order $\frac{\tau_{\text{exp}}^2}{\tau_{\text{micro}}}$, and so if $t - t_0$ is of order τ_{exp} then $\rho_n(t_0)$ is approximately $\rho_n(t)$ as there is not a significant enough time difference between t and t_0 for ρ_n to have changed appreciably. This hierarchy of timescales is valid precisely only because the ρ_n are the adiabatic invariants of $\hat{H}_0$. Under this approximation, (8.9.163) produces a closed differential equation for the $\rho_n(t)$:

$$\boxed{\frac{d\rho_n(t)}{dt} = \sum_{m \neq n} \Gamma_{m \rightarrow n} (\rho_m(t) - \rho_n(t))}. \quad (8.9.164)$$

This “equation” (which is only truly an often very good approximation valid for a decoherent system on long time scales) is called the **Fermi Master Equation**. It is very important to note that the Fermi master equation is only valid because there is a systematic information loss in treating the phases as decoherent. In general in a quantum system an enormity of the information in the system state is stored in the phases, and phase information is necessary for the existence of unitary, invertible time evolution. Decoherence occurs due to the assumption of a weak coupling to a large number of background degrees of freedom and a time averaging, with essentially identical thinking to how the canonical ensemble is achieved in statistical mechanics from those same factors.

8.9.6 Analytic Properties of the S Matrix

By using (8.9.107), we can find an explicit formula for $\hat{V}(E)$ in terms of the Green’s operator of the full system $\hat{R}_+(E)$:

$$\hat{T}|\alpha_0\rangle = \hat{H}_1|\alpha_0\rangle + \hat{H}_1\hat{R}_+(E_\alpha)\hat{H}_1|\alpha_0\rangle \quad (8.9.165)$$

$$\implies \hat{V}(E) = \hat{H}_1 + \hat{H}_1\hat{R}_+(E)\hat{H}_1. \quad (8.9.166)$$

Because of this formula, the behavior of the matrix elements of $\hat{V}(E)$ can reveal information about the bound states of the full Hamiltonian operator $\hat{H}$. The matrix elements of $\hat{R}_+$ corresponding to any square-integrable eigenstate $|\psi\rangle$ of $\hat{H}$ with energy eigenvalue E_ψ develop poles at that energy. One can see this by considering the operator summary of $\hat{R}_+$ in such a state:

$$\langle\psi|\hat{R}_+(E)|\psi\rangle = \lim_{\varepsilon \rightarrow 0^+} \langle\psi|\frac{1}{E - \hat{H} + i\varepsilon}|\psi\rangle = \lim_{\varepsilon \rightarrow 0^+} \frac{\langle\psi|\psi\rangle}{E - E_\psi + i\varepsilon} = \frac{1}{E - E_\psi}. \quad (8.9.167)$$

Consequently, through its dependence on $\hat{R}_+(E)$, the matrix elements of $\hat{V}(E)$ develop poles at values of E corresponding to the eigenvalues of normalizable eigenstates of the full Hamiltonian. The normalizable eigenstates are precisely states which decay sufficiently quickly at large distances to be square-integrable which is precisely what we mean by bound states. Therefore, bound states of $\hat{H}$ appear as poles in the transition amplitudes (even though we originally set out when doing scattering to study unbound states!) Moreover, the only place in (8.9.166) that poles may appear is in $\hat{R}_+$, and so **each bound state of the full theory manifests as a real energy pole in the transition amplitudes, and each real energy pole in the transition amplitudes indicates a bound state in the full theory.**

I was careful to indicate that bound states correspond specially to poles of the matrix elements of $\hat{V}(E)$ which occur at real values of E . It is also insightful to study the behavior of $\hat{V}(E)$ as a function of E treated

as a complex number. Because the Hamiltonian operator $\hat{H}$ is self-adjoint, all of its eigenvalues corresponding to normalizable eigenstates are guaranteed to be real. However, it may be possible (and often is) to construct “states”, called virtual states, which are not actually in the Hilbert space (but are in an appropriately larger set containing the Hilbert space) which have complex eigenvalues under $\hat{H}$. For example, if $\hat{H}$ were the simple free particle Hamiltonian $\frac{\hat{p}^2}{2m}$ in one spatial dimension, the function $\psi(x) = e^{i\kappa x}$ is an “eigenstate” of this operator for every complex value of κ , however if κ has any nonzero imaginary part then this function blows up at either large positive or large negative x , and so is not even in the rigged Hilbert space. Consequently, such a ψ for general complex κ is called a virtual state. Virtual states are sometimes useful because while no state in the Hilbert space may actually be a virtual state, a real state in the Hilbert space may be (at least for finite times in some regions of space) well-approximated by a virtual state and virtual states have very simple time evolution. This may sound odd but the situation is actually familiar from electromagnetism where we know the electromagnetic fields on all space can be expressed in terms of a linear combination of plane waves but in certain regions of space (such as in a box) may be very accurately approximated by spatially or temporally decaying solutions. Because a virtual state $|\psi(t)\rangle$ is like an energy eigenstate with complex energy $\tilde{E}_0$, its time evolution is given by:

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \implies \frac{d|\psi\rangle}{dt} = -\frac{i}{\hbar} \tilde{E}_0 |\psi\rangle \implies |\psi(t)\rangle = e^{-\frac{i}{\hbar} \tilde{E}_0 t} |\psi(0)\rangle = e^{-\frac{i}{\hbar} \text{Re}(\tilde{E}_0) t} e^{\frac{\text{Im}(\tilde{E}_0)}{\hbar} t} |\psi(0)\rangle. \quad (8.9.168)$$

We see that the real part of $\tilde{E}_0$ simply gives oscillations in time in line with the behavior of real states while the imaginary part of $\tilde{E}_0$ gives either exponential growth or decay (depending on its sign) which is very much unlike the behavior of real states. It is useful to introduce the symbol E_0 as the usual real energy and Γ as the decay rate of the virtual state:

$$E_0 = \text{Re}(\tilde{E}_0), \quad \Gamma = -\frac{2\text{Im}(\tilde{E}_0)}{\hbar} \implies |\psi(t)\rangle = e^{-\frac{i}{\hbar} E_0 t} e^{-\frac{\Gamma}{2} t} |\psi(0)\rangle. \quad (8.9.169)$$

Because we are discussing a virtual state, it necessarily has infinite norm. However, we could consider a cutoff (like only integrating over a finite region of space or summing over a finite number of terms, depending on the system) controlled by a parameter Λ so that when $\Lambda \rightarrow \infty$ the full norm is taken but at finite Λ a finite result is achieved (Λ could be the volume of the integration region, for example). Then:

$$\|\psi(t)\|_\Lambda^2 \text{ is finite and } \lim_{\Lambda \rightarrow \infty} \|\psi(t)\|_\Lambda^2 = \infty. \quad (8.9.170)$$

We can see that the complexity of $\tilde{E}_0$ causes the norm of $|\psi(t)\rangle$ to change:

$$\|\psi(t)\|_\Lambda^2 = e^{-\Gamma t} \|\psi(0)\|_\Lambda^2 \quad (8.9.171)$$

which is why Γ (when positive) is identified with the decay rate of the virtual state. Virtual states with positive Γ are for many purposes more interesting than virtual states with negative Γ , because they are often much better approximations of true physical behavior. The reason why is because for positive Γ the virtual state decays and so the fact that a real state can only be approximated locally and for a finite time is compatible with the fact that after a finite time the virtual state is negligible and so the other components of the wavefunction dominant while for negative Γ , the virtual state explodes with time and so necessarily becomes a very poor approximation of the physical state as the part approximated by the virtual state comes to dominate any other components. (However, negative Γ virtual states are interesting for studying instabilities in systems.) Going forward we will assume $\Gamma > 0$ for the applications desired.

When viewed as a decay rate, Γ can also be related to a “lifetime” τ of the state. Let $p(t)$ be defined by:

$$p(t) = 1 - \frac{\|\psi(t)\|_\Lambda^2}{\|\psi(0)\|_\Lambda^2} = 1 - e^{-\Gamma t} \quad (8.9.172)$$

be the fraction of the state’s magnitude which has not decayed after a time t . The instantaneous rate of decay of the state is then $\frac{dp}{dt}$ and the average decay time (meaning average time at which a given amount of state magnitude has decayed), called the lifetime, is:

$$\tau = \int_0^\infty t \frac{dp}{dt} dt = \frac{1}{\Gamma}. \quad (8.9.173)$$

The half-life of the state, meaning the time $\tau_{1/2}$ after which half of the magnitude of the state has decayed is:

$$e^{-\Gamma \tau_{1/2}} \stackrel{!}{=} \frac{1}{2} \implies \tau_{1/2} = \tau \ln 2 = \frac{\ln 2}{\Gamma}. \quad (8.9.174)$$

Because a virtual state corresponds to a “complex eigenvalue eigenstate” of $\hat{H}$ in an extended state

space, it similarly corresponds to a complex pole of $\hat{R}_+(E)$ and $\hat{V}(E)$. We can see this through an analogous calculation to (8.9.167):

$$\frac{\langle \psi | R_+(E) | \psi \rangle_\Lambda}{\|\psi\|_\Lambda^2} = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\|\psi\|_\Lambda^2} \langle \psi | \frac{1}{E - \hat{H} + i\varepsilon} | \psi \rangle_\Lambda = \frac{1}{E - E_0 + \frac{i\hbar\Gamma}{2}}. \quad (8.9.175)$$

Therefore, by exactly the same thinking as in the bound states, **each virtual state of the full theory manifests as a complex energy pole in the transition amplitudes, and each complex energy pole in the transition amplitudes indicates a virtual state in the full theory.**

Many physical observable quantities of interest (such as scattering cross-sections or Fermi's Golden Rule transition rates) depend on the magnitude-squared of transition amplitudes. Suppose $\hat{H}$ has a virtual or bound state so that there is a pole in a particular transition amplitude $T(E)$ (some particular matrix element T_{fi}) when viewed as a function of energy E (through using the $\hat{V}(E)$ operator) at a complex value $E_0 - \frac{i\hbar\Gamma}{2}$, exactly as above. Then because of (8.9.175), for energies in the neighborhood of that value, the transition amplitude will take the form:

$$T(E) = \frac{A}{E - E_0 + \frac{i\hbar\Gamma}{2}} + B(E) \quad (8.9.176)$$

where A is some constant and $B(E)$ is a complex function which is finite at $E = E_0 - \frac{i\hbar\Gamma}{2}$. Suppose that Γ is sufficiently small that $B(E)$ is finite and smooth as a function of E around $E = E_0$ with a radius larger than $\frac{\hbar\Gamma}{2}$ (the state, if virtual, is thus assumed not to decay *too* quickly). Consequently, the magnitude-squared of the transition amplitude becomes:

$$|T(E)|^2 = \frac{|A|^2 - \hbar\Gamma \text{Im}(A^* B(E_0))}{(E - E_0)^2 + \frac{\hbar^2\Gamma^2}{4}} + |B(E_0)|^2 + \mathcal{O}(E - E_0). \quad (8.9.177)$$

We can see that when the full theory has a virtual or bound state, there is a local maximum in the energy dependence of the observable (which depends on E through $|T(E)|^2$) at $E = E_0$. The local maximum value of $|T(E)|^2$ is:

$$M_{\max} = 4 \frac{|A|^2 - \hbar\Gamma \text{Im}(A^* B(E_0))}{\hbar^2\Gamma^2} + |B(E_0)|^2 + \mathcal{O}(E - E_0). \quad (8.9.178)$$

For sufficiently small Γ , this first term dominates the rest so that we may approximate:

$$M_{\max} \approx 4 \frac{|A|^2 - \hbar\Gamma \text{Im}(A^* B(E_0))}{\hbar^2\Gamma^2} \quad (8.9.179)$$

so that nearby the maximum:

$$|T(E)|^2 \approx \frac{\frac{\hbar^2\Gamma^2}{4}}{(E - E_0)^2 + \frac{\hbar^2\Gamma^2}{4}} M_{\max}. \quad (8.9.180)$$

This gives the characteristic profile of the shape of peaks in scattering observables as a function of energy. This profile is known as the **Breit-Wigner distribution**. Conversely, peaks in scattering observables (which are directly experimentally measurable) imply the existence of virtual or bound states in the interacting system. Notice that for a virtual state, the peak is of finite height (and is simply called a resonance) whereas for a bound state ($\Gamma \rightarrow 0$) the peak is of infinite height (and is also called a resonance, but more specifically a pole) as $M_{\max} \rightarrow \infty$. We can give another interpretation to the decay rate in terms of the profile of the resonance. The Full-Width-at-Half-Maximum (FWHM) of a profile is the length $b - a$ of the smallest interval $[a, b]$ which contains the maximum of the profile and so that at each of the endpoints a, b the profile is at half of its maximum value. From (8.9.180), that interval is simply $[E_0 - \frac{\hbar\Gamma}{2}, E_0 + \frac{\hbar\Gamma}{2}]$ so that the FWHM for the Breit-Wigner profile is:

$$\text{FWHM} = \hbar\Gamma. \quad (8.9.181)$$

For further understanding and an example of how a physical state may reasonably be approximated by a virtual state, I like section 16.6 of [3].

8.9.7 Nonrelativistic Single Particle Scattering

Until now we have kept $\hat{H}_0$ completely generic. Let us now be more specific. Consider a single nonrelativistic particle in d spatial dimensions so that our unperturbed Hamiltonian operator is:

$$\hat{H}_0 = \frac{|\hat{p}|^2}{2m}. \quad (8.9.182)$$

Suppose we only have the usual potentials as perturbations so that the total Hamiltonian is of the form:

$$\hat{H} = \frac{|\hat{p} - \vec{K}(\hat{x})|^2}{2m} + U(\hat{x}). \quad (8.9.183)$$

Consequently, the perturbation $\hat{H}_1$ is given by:

$$\hat{H}_1 = \hat{H} - \hat{H}_0 = U(\hat{x}) - \frac{\vec{K} \cdot \hat{p} + \hat{p} \cdot \vec{K}}{2m} + \frac{|\vec{K}|^2}{2m}. \quad (8.9.184)$$

The unperturbed Hamiltonian operator $\hat{H}_0$ has plane waves as eigenstates, which do not decay at large distances, and so they are our scattering states. Thus, we identify the $|\alpha_0\rangle$ states as:

$$\langle \vec{x} | \alpha_0 \rangle = e^{i\vec{k} \cdot \vec{x}} \quad (8.9.185)$$

where now write $|\alpha_0\rangle = |\vec{k}\rangle$, the above plane wave state. We didn't normalize this plane wave the way we often do (such as for momentum eigenstates). This is convention but convenient in cleaning up so annoying factors of 2π . One might naively want to take $\alpha = \vec{k}$ but in order to have the normalization given in (8.9.48) we need $\alpha = N\vec{k}$ for a normalization constant N . In particular:

$$\langle \alpha_0 | \beta_0 \rangle = \langle \alpha_0 | \int |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} | \beta_0 \rangle = \int \langle \vec{k} | \vec{x} \rangle \langle \vec{x} | \vec{k}' \rangle d^d \vec{x} = \int e^{i\vec{x} \cdot (\vec{k} - \vec{k}')} d^d \vec{x} = (2\pi)^d \delta(\vec{k} - \vec{k}') \quad (8.9.186)$$

$$\implies \delta(\alpha - \beta) = (2\pi)^d \delta(\vec{k} - \vec{k}') \quad (8.9.187)$$

$$\implies \delta(N\vec{k} - N\vec{k}') = (2\pi)^d \delta(\vec{k} - \vec{k}') \quad (8.9.188)$$

$$\implies \frac{1}{N^d} \delta(\vec{k} - \vec{k}') = (2\pi)^d \delta(\vec{k} - \vec{k}') \quad (8.9.189)$$

$$\implies N = \frac{1}{2\pi} \implies \alpha = \frac{\vec{k}}{2\pi}. \quad (8.9.190)$$

We can define then the plus and minus wavefunctions as:

$$\psi_{\vec{k}\pm}(\vec{x}) = \langle \vec{x} | \alpha_{\pm} \rangle. \quad (8.9.191)$$

Then, the Lippmann-Schwinger equation becomes:

$$\psi_{\vec{k}\pm}(\vec{x}) = e^{i\vec{k} \cdot \vec{x}} + \lim_{\varepsilon \rightarrow 0^+} \langle \vec{x} | \frac{1}{E_k - \hat{H}_0 \pm i\varepsilon} \hat{H}_1 | \alpha_{\pm} \rangle. \quad (8.9.192)$$

Because $\hat{H}_0 = \frac{|\hat{p}|^2}{2m}$, the unperturbed energy eigenvalues E_k are given by:

$$E_k = \frac{\hbar^2 k^2}{2m} \quad (8.9.193)$$

where $k^2 = |\vec{k}|^2$. Now define the Green's functions from the Green's operators:

$$G_{\pm}(\vec{k}, \vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \langle \vec{x} | \hat{G}_{\pm}(E_k) | \vec{x}' \rangle. \quad (8.9.194)$$

The factor of $\frac{\hbar^2}{2m}$ is convenient for cleaning up the explicit formula we will find for $G_{\pm}$ shortly. By inserting a complete set of position states into the Lippmann-Schwinger equation:

$$\psi_{\vec{k}\pm}(\vec{x}) = e^{i\vec{k} \cdot \vec{x}} + \lim_{\varepsilon \rightarrow 0^+} \int \langle \vec{x} | \frac{1}{E_k - \hat{H}_0 \pm i\varepsilon} | \vec{x}' \rangle \langle \vec{x}' | \hat{H}_1 | \alpha_{\pm} \rangle d^d \vec{x}' \quad (8.9.195)$$

$$= e^{i\vec{k} \cdot \vec{x}} + \frac{2m}{\hbar^2} \int G_{\pm}(\vec{k}, \vec{x}, \vec{x}') \langle \vec{x}' | \hat{H}_1 | \alpha_{\pm} \rangle d^d \vec{x}'. \quad (8.9.196)$$

We can express $G_{\pm}$ as an explicit integral by inserting a complete set of momentum states into its definition:

$$G_{\pm}(\vec{k}, \vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \lim_{\varepsilon \rightarrow 0^+} \langle \vec{x} | \frac{1}{\frac{\hbar^2 k^2}{2m} - \frac{\hat{p}^2}{2m} \pm i\varepsilon} \int |\vec{p}\rangle \langle \vec{p}| d^d \vec{p} | \vec{x}' \rangle \quad (8.9.197)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int \frac{\langle \vec{x} | \vec{p} \rangle \langle \vec{p} | \vec{x}' \rangle}{k^2 - \frac{p^2}{\hbar^2} + \frac{2mi}{\hbar^2} \varepsilon} d^d \vec{p} \quad (8.9.198)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int \frac{e^{i\vec{p} \cdot (\vec{x} - \vec{x}')/\hbar}}{k^2 - \frac{p^2}{\hbar^2} + \frac{2mi}{\hbar^2} \varepsilon} \frac{d^d \vec{p}}{(2\pi\hbar)^d}. \quad (8.9.199)$$

Define the new integration variable $\vec{k}' = \frac{\vec{p}}{\hbar}$. Because we take $\varepsilon \rightarrow 0^+$ we can simply rename the limit variable $\frac{2m}{\hbar^2} \varepsilon$ to ε as it also limits to 0 from above. Then:

$$G_{\pm}(\vec{k}, \vec{x}, \vec{x}') = \lim_{\varepsilon \rightarrow 0^+} \int e^{i\vec{k}' \cdot (\vec{x} - \vec{x}')} \frac{1}{k^2 - k'^2 \pm i\varepsilon} \frac{d^d \vec{k}'}{(2\pi)^d}. \quad (8.9.200)$$

It should now be clear why a prefactor of $\frac{\hbar^2}{2m}$ was included in the definition of the Green's function, as it eliminates any m or $\hbar$ dependence.

For our given form of $\hat{H}_1$:

$$\langle \vec{x}' | \hat{H}_1 | \alpha_{\pm} \rangle = U(\vec{x}') \psi_{\vec{k}\pm}(\vec{x}') + \frac{|\vec{K}(\vec{x}')|^2}{2m} \psi_{\vec{k}\pm}(\vec{x}') + \frac{i\hbar}{2m} (\vec{K}(\vec{x}') \cdot \nabla' \psi_{\vec{k}\pm}(\vec{x}') + \nabla' \cdot (\vec{K}(\vec{x}') \psi_{\vec{k}\pm}(\vec{x}'))). \quad (8.9.201)$$

Then, in terms of the Green's functions the Lippmann-Schwinger equation becomes:

$$\psi_{\vec{k}\pm}(\vec{x}) = e^{i\vec{k} \cdot \vec{x}} + \frac{2m}{\hbar^2} \int G_{\pm}(\vec{k}, \vec{x}, \vec{x}') \left(U(\vec{x}') + \frac{|\vec{K}(\vec{x}')|^2}{2m} + \frac{i\hbar}{2m} (\nabla' \cdot \vec{K}(\vec{x}')) + \frac{i\hbar}{m} \vec{K}(\vec{x}') \cdot \nabla' \right) \psi_{\vec{k}\pm}(\vec{x}') d^d \vec{x}'. \quad (8.9.202)$$

This is well suited for perturbation theory. Directly applying (8.9.93) we have:

$$\psi_{\vec{k}\pm}^{(0)}(\vec{x}) = e^{i\vec{k} \cdot \vec{x}}, \quad (8.9.203)$$

$$\psi_{\vec{k}\pm}^{(n+1)}(\vec{x}) = \frac{2m}{\hbar^2} \int G_{\pm}(\vec{k}, \vec{x}, \vec{x}') \left(U(\vec{x}') + \frac{|\vec{K}(\vec{x}')|^2}{2m} + \frac{i\hbar}{2m} (\nabla' \cdot \vec{K}(\vec{x}')) + \frac{i\hbar}{m} \vec{K}(\vec{x}') \cdot \nabla' \right) \psi_{\vec{k}\pm}^{(n)}(\vec{x}') d^d \vec{x}'. \quad (8.9.204)$$

In order to solve the Lippmann-Schwinger equation we just need to explicitly compute the Green's functions in (8.9.200). The specifics of that integral depend on the spatial dimensions d , so we will save that for when we specify to 1 dimensional or 3 dimensional scattering. (Of course one can also consider scattering in 2 spatial dimensions, but the Green's function is nasty enough we will choose to neglect it.) It is also important to note several special properties of the Green's function. First, there is a nice relationship between G_+ and G_- given by taking the complex conjugate of G_+ :

$$G_+^*(\vec{k}, \vec{x}, \vec{x}') = \lim_{\varepsilon \rightarrow 0^+} \int \frac{e^{-i\vec{k}' \cdot (\vec{x} - \vec{x}')}}{k^2 - k'^2 - i\varepsilon} \frac{d^d \vec{k}'}{(2\pi)^d}. \quad (8.9.205)$$

If we now change the integration variable from $\vec{k}'$ to $-\vec{k}'$, the integration measure is unchanged (as is k'^2) and so:

$$G_+^*(\vec{k}, \vec{x}, \vec{x}') = \lim_{\varepsilon \rightarrow 0^+} \int \frac{e^{i\vec{k}' \cdot (\vec{x} - \vec{x}')}}{k^2 - k'^2 - i\varepsilon} \frac{d^d \vec{k}'}{(2\pi)^d} \quad (8.9.206)$$

$$= G_-(\vec{k}, \vec{x}, \vec{x}'). \quad (8.9.207)$$

Thus, we really only ever need to know G_+ as if we do need G_- it is just given by complex conjugation. Another nice property of the Green's function is that it is symmetric under interchanging $\vec{x}$ and $\vec{x}'$ by the same change of variables of $\vec{k}'$ to $-\vec{k}'$ in the integral:

$$G_+(\vec{k}, \vec{x}', \vec{x}) = \lim_{\varepsilon \rightarrow 0^+} \int \frac{e^{i\vec{k}' \cdot (\vec{x}' - \vec{x})}}{k^2 - k'^2 - i\varepsilon} \frac{d^d \vec{k}'}{(2\pi)^d} \quad (8.9.208)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int \frac{e^{i\vec{k}' \cdot (\vec{x} - \vec{x}')}}{k^2 - k'^2 - i\varepsilon} \frac{d^d \vec{k}'}{(2\pi)^d} \quad (8.9.209)$$

$$= G_+(\vec{k}, \vec{x}, \vec{x}'). \quad (8.9.210)$$

Finally, (but most easily seen) the Green's function only depends on $\vec{k}$ through its magnitude: $k^2 = |\vec{k}|^2$.

The transition matrix (and thus the S matrix) can be cleanly expressed in terms of the Lippmann-Schwinger solution:

$$T_{\beta\alpha} = \langle \beta_0 | \hat{H}_1 | \alpha_+ \rangle \quad (8.9.211)$$

$$\Rightarrow T_{\vec{k}', \vec{k}} = \langle \vec{k}' | \int |\vec{x}\rangle \langle \vec{x}| d^d \vec{x} \hat{H}_1 | \vec{k}_+ \rangle \quad (8.9.212)$$

$$\Rightarrow T_{\vec{k}', \vec{k}} = \int e^{-i\vec{k}' \cdot \vec{x}} \left(U(\vec{x}) + \frac{|\vec{K}(\vec{x})|^2}{2m} + \frac{i\hbar}{2m} (\nabla \cdot \vec{K}(\vec{x})) + \frac{i\hbar}{m} \vec{K}(\vec{x}) \cdot \nabla \right) \psi_{\vec{k}_+}(\vec{x}) d^d \vec{x}. \quad (8.9.213)$$

The S matrix can be simplified now that we have specified $\hat{H}_0$ by using (8.9.128):

$$S_{\vec{k}', \vec{k}} = S_{\beta\alpha} = \delta \left(\frac{\vec{k}'}{2\pi} - \frac{\vec{k}}{2\pi} \right) - 2\pi i T_{\vec{k}', \vec{k}} \delta \left(\frac{\hbar^2 |\vec{k}'|^2}{2m} - \frac{\hbar^2 |\vec{k}|^2}{2m} \right) \quad (8.9.214)$$

$$= (2\pi)^d \delta(\vec{k} - \vec{k}') - 2\pi i T_{\vec{k}', \vec{k}} \frac{2m}{\hbar^2} \delta(|\vec{k}|^2 - |\vec{k}'|^2). \quad (8.9.215)$$

The Dirac delta can be simplified as:

$$\delta(|\vec{k}|^2 - |\vec{k}'|^2) = \frac{\delta(|\vec{k}| - |\vec{k}'|)}{2|\vec{k}|}. \quad (8.9.216)$$

Thus the S matrix becomes:

$$S_{\vec{k}', \vec{k}} = (2\pi)^d \delta(\vec{k} - \vec{k}') + \frac{2\pi m}{i\hbar^2 |\vec{k}|} T_{\vec{k}', \vec{k}} \delta(|\vec{k}'| - |\vec{k}|). \quad (8.9.217)$$

As well, the unitarity of the S matrix becomes:

$$\langle \beta_0 | \hat{S}^\dagger \hat{S} | \alpha_0 \rangle = \delta(\alpha - \beta) \quad (8.9.218)$$

$$\Rightarrow \int \langle \beta_0 | \hat{S}^\dagger | \gamma_0 \rangle \langle \gamma_0 | \hat{S} | \alpha_0 \rangle d\gamma = \delta(\alpha - \beta) \quad (8.9.219)$$

$$\Rightarrow \int S_{\gamma\beta}^* S_{\gamma\alpha} d\gamma = \delta \left(\frac{\vec{k}}{2\pi} - \frac{\vec{k}'}{2\pi} \right) \quad (8.9.220)$$

$$\Rightarrow \int S_{\vec{k}'' \vec{k}}^* S_{\vec{k}'' \vec{k}'} \frac{d^d \vec{k}''}{(2\pi)^d} = (2\pi)^d \delta(\vec{k} - \vec{k}') \quad (8.9.221)$$

$$\Rightarrow \int S_{\vec{k}'' \vec{k}}^* S_{\vec{k}'' \vec{k}'} d^d \vec{k}'' = (2\pi)^{2d} \delta(\vec{k} - \vec{k}'). \quad (8.9.222)$$

8.9.8 Scattering in 1 Spatial Dimension

In 1 spatial dimension, the + Green's function becomes:

$$G_+(k, x, x') = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{k^2 - k'^2 + i\varepsilon} \frac{dk'}{2\pi} \quad (8.9.223)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{(k + \frac{i\varepsilon}{2k})^2 - k'^2 + \frac{\varepsilon^2}{4k^2}} \frac{dk'}{2\pi} \quad (8.9.224)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{(k + i\varepsilon)^2 - k'^2} \frac{dk'}{2\pi} \quad (8.9.225)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{2(k + i\varepsilon)} \left(\frac{1}{k + i\varepsilon - k'} + \frac{1}{k + i\varepsilon + k'} \right) \frac{dk'}{2\pi} \quad (8.9.226)$$

$$= \frac{1}{2k} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} + \frac{1}{2k} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi}. \quad (8.9.227)$$

We can now evaluate each of these integrals by contour integration. Because the Green's function is symmetric under exchange x and x' , we can assume without loss of generality that $x > x'$. Similarly, because it only

depends on $|k|$, we can as well assume $k > 0$. Consider a contour γ which consists of a line segment on the real axis from $-R$ to R with $R > \sqrt{k^2 + \varepsilon^2}$ and a semi-circle in the upper half plane connecting back from R to $-R$. Then, by the residue theorem:

$$\int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} = -ie^{i(k+i\varepsilon)(x-x')}. \quad (8.9.228)$$

As well, decomposing the contour into its two pieces and parameterizing the semi circle by $k' = Re^{i\theta}$ we have:

$$\int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} = \int_{-R}^R \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} - \int_0^{\pi} \frac{e^{iR(x-x')\cos\theta - R(x-x')\sin\theta}}{k + i\varepsilon - Re^{i\theta}} \frac{iRe^{i\theta}}{2\pi} d\theta. \quad (8.9.229)$$

Then, as $R \rightarrow \infty$ the second integrand decays exponentially with R for $x > x'$ and thus goes to 0. So, in the $R \rightarrow \infty$ limit:

$$\int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} = \int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} = -ie^{i(k+i\varepsilon)(x-x')}. \quad (8.9.230)$$

The other integral can be evaluated using the same contour. Though, this time the residue theorem gives:

$$\int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} = 0. \quad (8.9.231)$$

As well, decomposing the contour the same way with the same parameterization we have:

$$\int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} = \int_{-R}^R \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} - \int_0^{\pi} \frac{e^{iR(x-x')\cos\theta - R(x-x')\sin\theta}}{k + i\varepsilon + Re^{i\theta}} \frac{iRe^{i\theta}}{2\pi} d\theta. \quad (8.9.232)$$

The second integrand decays in the same way and so in the $R \rightarrow \infty$ limit:

$$\int_{-\infty}^{\infty} \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} = \int_{\gamma} \frac{e^{ik'(x-x')}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} = 0. \quad (8.9.233)$$

Together then, we have for $x > x'$:

$$G_+(k, x, x') = \frac{1}{2k} \lim_{\varepsilon \rightarrow 0^+} \left(-ie^{i(k+i\varepsilon)(x-x')} \right) + 0 = \frac{e^{ik(x-x')}}{2ik}. \quad (8.9.234)$$

Then, for $x < x'$ as explained we swap x and x' :

$$G_+(k, x, x') = \frac{e^{ik(x'-x)}}{2ik}. \quad (8.9.235)$$

These two cases can be combined as:

$$G_+(k, x, x') = \frac{e^{ik|x-x'|}}{2ik}. \quad (8.9.236)$$

Further, this formula was derived for $k > 0$ and so for general k :

$$\boxed{G_+(k, x, x') = \frac{e^{i|k|(x-x')}}{2i|k|}.} \quad (8.9.237)$$

In one spatial dimension, any vector potential $K(x)$ can be removed by gauge transformation (as every such vector potential can be written as the gradient of a scalar function). So, without loss of generality in $d = 1$ we take $K = 0$. Let us look at the behavior of the Lippmann-Schwinger equation when we are very far away from the origin. Suppose that $k > 0$ so that the incoming wave is moving in the positive x direction. If we are looking very far along the positive x axis then $|x - x'| = x - x'$ and so (8.9.202) becomes:

$$(\text{Very large } x) \quad \psi_{k+}(x) = e^{ikx} + \frac{2m}{\hbar^2} \int_{-\infty}^{\infty} \frac{e^{ik(x-x')}}{2ik} U(x') \psi_{k+}(x') dx' \quad (8.9.238)$$

$$= \left(1 + \frac{m}{i\hbar^2 k} \int_{-\infty}^{\infty} e^{-ikx'} U(x') \psi_{k+}(x') dx' \right) e^{ikx}. \quad (8.9.239)$$

Thus, for x sufficiently large the scattered wavefunction on the positive x axis becomes a plane wave with coefficient:

$$\boxed{t(k) = 1 + \frac{m}{i\hbar^2 |k|} \int_{-\infty}^{\infty} e^{-ikx'} U(x') \psi_{k+}(x') dx'.} \quad (8.9.240)$$

The $|k|$ is put for consistency with the case of $k < 0$. This $t(k)$ is called the transmission coefficient because it gives the amplitude with which the forward wavefunction is transmitted. Alternatively, if we are looking very far along the negative x axis then $|x - x'| = x' - x$ and so (8.9.202) becomes:

$$(\text{Very large } -x) \quad \psi_{k+}(x) = e^{ikx} + \frac{2m}{\hbar^2} \int_{-\infty}^{\infty} \frac{e^{ik(x'-x)}}{2ik} U(x') \psi_{k+}(x') dx' \quad (8.9.241)$$

$$= e^{ikx} + \left(\frac{m}{i\hbar^2 k} \int_{-\infty}^{\infty} e^{ikx'} U(x') \psi_{k+}(x') dx' \right) e^{-ikx}. \quad (8.9.242)$$

Thus, very far along the negative x axis there is our incoming plane wave together with a reflected wave moving in the opposite direction with corresponding coefficient:

$$r(k) = \frac{m}{i\hbar^2 |k|} \int_{-\infty}^{\infty} e^{ikx'} U(x') \psi_{k+}(x') dx'. \quad (8.9.243)$$

By (8.9.213) we see that the reflection and transmission coefficients are related to the transition matrix by:

$$t(k) = 1 + \frac{m}{i\hbar^2 |k|} T_{kk}, \quad r(k) = \frac{m}{i\hbar^2 |k|} T_{-kk}. \quad (8.9.244)$$

Because the only two states of energy eigenvalue E_k in one dimension have wavenumbers k and $-k$, for each $|k|$ the only elements of the transition matrix which appear in the S matrix are T_{kk} and T_{-kk} (and so at each energy level the S matrix is effectively a 2x2 matrix). These two coefficients are completely determined by the reflection and transmission coefficients and thus the S matrix in 1 dimension is completely determined by them as well. By (8.9.217) we have:

$$S_{k'k} = 2\pi\delta(k - k') + \frac{2\pi m}{i\hbar^2 |k|} T_{k'k} \delta(|k'| - |k|). \quad (8.9.245)$$

The Dirac delta can be simplified as:

$$\delta(|k'| - |k|) = \delta(k' - k) + \delta(k' + k). \quad (8.9.246)$$

Thus:

$$S_{k'k} = 2\pi\delta(k - k') + \frac{2\pi m}{i\hbar^2 |k|} T_{k'k} \delta(k' - k) + \frac{2\pi m}{i\hbar^2 |k|} T_{k'k} \delta(k' + k) \quad (8.9.247)$$

$$\implies S_{k'k} = 2\pi \left(1 + \frac{m}{i\hbar^2 |k|} T_{kk} \right) \delta(k' - k) + \frac{2\pi m}{i\hbar^2 |k|} T_{-kk} \delta(k' + k) \quad (8.9.248)$$

$$\implies \boxed{S_{k',k} = 2\pi t(k) \delta(k' - k) + 2\pi r(k) \delta(k' + k)}. \quad (8.9.249)$$

Unitarity of the S matrix then requires (using (8.9.222)):

$$\int_{-\infty}^{\infty} (2\pi t(k') \delta(k'' - k') + 2\pi r(k') \delta(k'' + k'))^* (2\pi t(k) \delta(k'' - k) + 2\pi r(k) \delta(k'' + k)) dk'' = 4\pi^2 \delta(k - k') \quad (8.9.250)$$

$$\implies t(k')^* t(k) \delta(k - k') + t(k')^* r(k) \delta(k' + k) + r(k')^* t(k) \delta(k + k') + r(k')^* r(k) \delta(k' - k) = \delta(k - k') \quad (8.9.251)$$

$$\implies (|t(k)|^2 + |r(k)|^2 - 1) \delta(k - k') + (t(-k)^* r(k) + r(-k)^* t(k)) \delta(k + k') = 0. \quad (8.9.252)$$

Explicitly then, S matrix unitarity demands:

$$\boxed{|t(k)|^2 + |r(k)|^2 = 1, \quad t^*(-k) r(k) + r^*(-k) t(k) = 0.} \quad (8.9.253)$$

8.9.9 Scattering in 3 Spatial Dimensions

We will not compute the 2 dimensional non-relativistic Green's function because it is somewhat nasty (a Hankel function). In 3 spatial dimensions using spherical coordinates with the z axis defined to point along the $\vec{x} - \vec{x}'$ direction and letting $r = |\vec{x} - \vec{x}'|$, the + Green's function becomes:

$$G_+(\vec{k}, \vec{x}, \vec{x}') = \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{e^{ik'r \cos \theta'}}{k^2 - k'^2 + i\varepsilon} \frac{k'^2 \sin \theta' d\varphi' d\theta' dk'}{8\pi^3} \quad (8.9.254)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{8\pi^3} \int_0^{2\pi} d\varphi' \int_0^\infty \frac{k'^2}{k^2 - k'^2 + i\varepsilon} \int_0^\pi e^{ik'r \cos \theta'} \sin \theta' d\theta' dk' \quad (8.9.255)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{8\pi^3} 2\pi \int_0^\infty \frac{k'^2}{k^2 - k'^2 + i\varepsilon} \left(\frac{1}{ik'r} (e^{ik'r} - e^{-ik'r}) \right) dk' \quad (8.9.256)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{4\pi^2} \int_0^\infty \frac{k'^2}{k^2 - k'^2 + i\varepsilon} \frac{1}{k'r} 2 \sin(rk') dk' \quad (8.9.257)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\pi^2 r} \int_0^\infty \frac{k' \sin(rk')}{k^2 - k'^2 + i\varepsilon} dk'. \quad (8.9.258)$$

This integrand is an even function of k' and so we can extend it from $-\infty$ to ∞ :

$$G_+(\vec{k}, \vec{x}, \vec{x}') = \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{k' \sin(rk')}{k^2 - k'^2 + i\varepsilon} dk' \quad (8.9.259)$$

$$= \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{k' \sin(rk')}{\left(k + \frac{i\varepsilon}{2k}\right)^2 - k'^2 + \frac{\varepsilon^2}{4k^2}} dk' \quad (8.9.260)$$

$$= \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{k' \sin(rk')}{(k + i\varepsilon)^2 - k'^2} dk' \quad (8.9.261)$$

$$= \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty k' \sin(rk') \frac{1}{2k'} \left(\frac{1}{k + i\varepsilon - k'} - \frac{1}{k + i\varepsilon + k'} \right) dk' \quad (8.9.262)$$

$$= \frac{1}{8\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{\sin(rk')}{k + i\varepsilon - k'} dk' - \frac{1}{8\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{\sin(rk')}{k + i\varepsilon + k'} dk'. \quad (8.9.263)$$

Changing k' to $-k'$ in the second integral gives:

$$\int_{-\infty}^\infty \frac{\sin(rk')}{k + i\varepsilon + k'} dk' = \int_{-\infty}^\infty \frac{-\sin(rk')}{k + i\varepsilon - k'} dk' = - \int_{-\infty}^\infty \frac{\sin(rk')}{k + i\varepsilon - k'} dk'. \quad (8.9.264)$$

Thus we have:

$$G_+(\vec{k}, \vec{x}, \vec{x}') = \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{\sin(rk')}{k + i\varepsilon - k'} dk' \quad (8.9.265)$$

$$= \frac{1}{4\pi^2 r} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^\infty \frac{1}{k + i\varepsilon - k'} \frac{e^{irk'} - e^{-irk'}}{2i} dk' \quad (8.9.266)$$

$$= \frac{1}{4\pi i r} \lim_{\varepsilon \rightarrow 0^+} \left(\int_{-\infty}^\infty \frac{e^{irk'}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} - \int_{-\infty}^\infty \frac{e^{-irk'}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} \right) \quad (8.9.267)$$

$$= \frac{1}{4\pi i r} \lim_{\varepsilon \rightarrow 0^+} \left(\int_{-\infty}^\infty \frac{e^{irk'}}{k + i\varepsilon - k'} \frac{dk'}{2\pi} - \int_{-\infty}^\infty \frac{e^{irk'}}{k + i\varepsilon + k'} \frac{dk'}{2\pi} \right) \quad (8.9.268)$$

where the last line follows by again changing k' to $-k'$ in the second integral. These are precisely the integrals we evaluated in the 1-dimensional case and so by (8.9.230) and (8.9.233):

$$G_+(\vec{k}, \vec{x}, \vec{x}') = \frac{1}{4\pi i r} (-ie^{ikr} - 0) \quad (8.9.269)$$

$$\Rightarrow \boxed{G_+(\vec{k}, \vec{x}, \vec{x}') = -\frac{e^{i|\vec{k}||\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}.} \quad (8.9.270)$$

Let us look at again study the behavior of the Lippmann-Schwinger equation when we are very far away from the origin. Let $k = |\vec{k}|$, $r = |\vec{x}|$, and $\hat{r} = \frac{\vec{x}}{r}$. For large r , we can make the expansion:

$$|\vec{x} - \vec{x}'| = \sqrt{|\vec{x} - \vec{x}'|^2} = \sqrt{r^2 - 2r\hat{r} \cdot \vec{x}' + |\vec{x}'|^2} = r\sqrt{1 - 2\frac{\hat{r} \cdot \vec{x}'}{r} + \frac{|\vec{x}'|^2}{r^2}} = r - \hat{r} \cdot \vec{x}' + \mathcal{O}\left(\frac{1}{r}\right). \quad (8.9.271)$$

Then, the Green's function becomes:

$$G_+(\vec{k}, \vec{x}, \vec{x}') = -\frac{e^{ik(r - \hat{r} \cdot \vec{x}' + \mathcal{O}(\frac{1}{r}))}}{4\pi(r - \hat{r} \cdot \vec{x}' + \mathcal{O}(\frac{1}{r}))} \quad (8.9.272)$$

$$= -\frac{e^{ikr}}{4\pi r} e^{-ik\hat{r}\cdot\vec{x}'} \frac{e^{\mathcal{O}(\frac{1}{r})}}{1 - \frac{\hat{r}\cdot\vec{x}'}{r} + \mathcal{O}(\frac{1}{r^2})} \quad (8.9.273)$$

$$= -\frac{e^{ikr}}{4\pi r} e^{-ik\hat{r}\cdot\vec{x}'} \left(1 + \mathcal{O}\left(\frac{1}{r}\right) \right) \quad (8.9.274)$$

Then, (8.9.202) becomes:

$$\begin{aligned} \psi_{\vec{k}+}(\vec{x}) &= e^{i\vec{k}\cdot\vec{x}} - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-ik\hat{r}\cdot\vec{x}'} \left(U(\vec{x}') + \frac{|\vec{K}(\vec{x}')|^2}{2m} + \frac{i\hbar}{2m} (\nabla' \cdot \vec{K}(\vec{x}')) + \frac{i\hbar}{m} \vec{K}(\vec{x}') \cdot \nabla' \right) \psi_{\vec{k}+}(\vec{x}') d^3\vec{x}' \\ &\quad + \mathcal{O}\left(\frac{1}{r^2}\right). \end{aligned} \quad (8.9.275)$$

Define then the scattering amplitude $f(\vec{k}, \vec{k}')$:

$$f(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2} \int e^{-i\vec{k}'\cdot\vec{x}} \left(U(\vec{x}) + \frac{|\vec{K}(\vec{x})|^2}{2m} + \frac{i\hbar}{2m} (\nabla \cdot \vec{K}(\vec{x})) + \frac{i\hbar}{m} \vec{K}(\vec{x}) \cdot \nabla \right) \psi_{\vec{k}+}(\vec{x}) d^3\vec{x}. \quad (8.9.276)$$

Then, we have that very far away:

$$\boxed{\psi_{\vec{k}+}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + f(\vec{k}, \vec{k}') \frac{e^{ikr}}{r} + \mathcal{O}\left(\frac{1}{r^2}\right).} \quad (8.9.277)$$

We can see that the scattering amplitude f is directly related to the transition matrix through (8.9.213):

$$f(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2} T_{\vec{k}'\vec{k}}. \quad (8.9.278)$$

The difference in order of arguments is standard convention. From (8.9.217) then we have:

$$\boxed{S_{\vec{k}', \vec{k}} = (2\pi)^3 \delta(\vec{k} - \vec{k}') + \frac{4\pi^2 i}{|\vec{k}|} f(\vec{k}, \vec{k}') \delta(|\vec{k}| - |\vec{k}'|).} \quad (8.9.279)$$

Unitarity then requires by (8.9.222):

$$\int \left(\delta(\vec{k}' - \vec{k}'') - \frac{1}{2\pi i |\vec{k}'|} f(\vec{k}', \vec{k}'') \delta(|\vec{k}'| - |\vec{k}''|) \right)^* \left(\delta(\vec{k} - \vec{k}'') - \frac{1}{2\pi i |\vec{k}|} f(\vec{k}, \vec{k}'') \delta(|\vec{k}| - |\vec{k}''|) \right) d^3\vec{k}'' = \delta(\vec{k} - \vec{k}') \quad (8.9.280)$$

$$\begin{aligned} \implies & \delta(\vec{k} - \vec{k}') + \frac{1}{2\pi i |\vec{k}'|} f^*(\vec{k}', \vec{k}) \delta(|\vec{k}| - |\vec{k}'|) - \frac{1}{2\pi i |\vec{k}|} f(\vec{k}, \vec{k}') \delta(|\vec{k}| - |\vec{k}'|) \\ & + \frac{1}{4\pi^2 |\vec{k}| |\vec{k}'|} \int f^*(\vec{k}', \vec{k}'') f(\vec{k}, \vec{k}'') \delta(|\vec{k}| - |\vec{k}'|) \delta(|\vec{k}| - |\vec{k}''|) d^3\vec{k}'' = \delta(\vec{k} - \vec{k}'). \end{aligned} \quad (8.9.281)$$

To simplify, it is useful to switch to spherical coordinates for $\vec{k}''$ and define:

$$\vec{l}(\theta, \varphi) = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta), \quad d\Omega = \sin \theta d\theta d\varphi \quad (8.9.282)$$

$$\implies d^3\vec{k}'' = (k'')^2 dk'' d\Omega. \quad (8.9.283)$$

With this (8.9.281) becomes:

$$\delta(|\vec{k}| - |\vec{k}'|) \left(\frac{f(\vec{k}, \vec{k}')}{i|\vec{k}|} - \frac{f^*(\vec{k}', \vec{k})}{i|\vec{k}|} - \frac{1}{2\pi |\vec{k}|^2} \int_0^\infty \int_\Omega f^*(\vec{k}', k'' \vec{l}) f(\vec{k}, k'' \vec{l}) \delta(|\vec{k}| - k'') (k'')^2 d\Omega dk'' \right) = 0 \quad (8.9.284)$$

$$\implies \boxed{|\vec{k}| = |\vec{k}'|, \quad f(\vec{k}, \vec{k}') - f^*(\vec{k}', \vec{k}) = \frac{i|\vec{k}|}{2\pi} \int_\Omega f^*(\vec{k}', |\vec{k}| \vec{l}) f(\vec{k}, |\vec{k}| \vec{l}) d\Omega.} \quad (8.9.285)$$

This result is known as the **optical theorem**.

Suppose we have an incident beam coming in from far away which points along the z axis with intensity (particles per unit time per unit area) J_{in} . Those particles will experience the perturbation and be “scattered” to give a resulting distribution of particles going out in all directions with some angular intensity (particles per unit time per unit solid angle) $J_{\text{scattered}}$. We will now relate $J_{\text{scattered}}$ to the S matrix. By (8.6.130), the

charge and current densities of a particle are given by:

$$\rho = q|\psi|^2, \quad \vec{J} = \frac{q\hbar}{m} \text{Im}(\psi^* \vec{\mathcal{D}}\psi). \quad (8.9.286)$$

The number density of that particle is then its charge density divided by its total charge q , and the resulting number current density $\vec{J}_n$ is likewise $\frac{\vec{J}}{q}$ so that:

$$\vec{J}_n = \frac{\hbar}{m} \text{Im}(\psi^* \vec{\mathcal{D}}\psi) \quad (8.9.287)$$

For our incoming beam, the wavefunction is just free particles propagating along the beam axis (in the $\vec{k}$ direction) and they come in from a region in which the vector potential is 0 (so that they are free):

$$\psi_{in}(\vec{x}) = N e^{i\vec{k} \cdot \vec{x}}. \quad (8.9.288)$$

Then, we have:

$$J_{in} = \hat{k} \cdot \vec{J}_n = \hat{k} \cdot \left(\frac{N^2 \hbar}{m} \vec{k} \right) = \frac{N^2 \hbar k}{m}. \quad (8.9.289)$$

For our scattered particles, the wavefunction will then become (8.9.277) (multiplied by N):

$$\psi_{+\vec{k}} = N e^{i\vec{k} \cdot \vec{x}} + N f(\vec{k}, \vec{k}') \frac{e^{ikr}}{r} + \mathcal{O}\left(\frac{1}{r^2}\right). \quad (8.9.290)$$

The first term is just our unscattered beam and so we define $J_{\text{scattered}}$ to only include the contributions from the scattered particles. We can see that the scattered particles are propagating in the $\hat{r}$ direction. So, we have:

$$J_{\text{scattered}} = \lim_{r \rightarrow \infty} r^2 \hat{r} \cdot \vec{J} = \frac{N^2 \hbar k}{m} |f(\vec{k}, \vec{k}')|^2. \quad (8.9.291)$$

The factor of r^2 is because $\vec{J}$ gives particles per unit time per unit cross sectional area but $J_{\text{scattered}}$ was defined as particles per unit time per unit solid angle and so we need the r^2 to account for the fact that the surface area element of a sphere is r^2 times its solid angle element. Then, the differential cross section $\frac{d\sigma}{d\Omega}$ is defined as the outgoing current of scattered particles per unit solid angle per unit incoming current of incident particles per unit beam cross sectional area:

$$\frac{d\sigma}{d\Omega} = \frac{J_{\text{scattered}}}{J_{in}}. \quad (8.9.292)$$

Combining (8.9.289) and (8.9.291) gives that for quantum mechanical scattering:

$$\boxed{\frac{d\sigma}{d\Omega}(\theta, \varphi) = |f(\vec{k}, |\vec{k}| \vec{r}(\theta, \varphi))|^2}. \quad (8.9.293)$$

Thus, the differential cross section is very cleanly given in terms of the scattering amplitude. J_{in} is set by the design of the particle beam and $J_{\text{scattered}}$ is measured in the particle detector. Therefore, the differential cross section is directly experimentally observable and so provides an excellent comparison point between theory and experiment, just as in classical mechanics and in electromagnetism.

Exercises

Problem 8.54: Scattering through a δ -potential. Consider a nonrelativistic quantum particle of mass m experiencing an attractive Dirac delta potential so that the Hamiltonian operator is:

$$\hat{H} = \frac{\hat{p}^2}{2m} - \alpha \delta(\hat{x})$$

(a) Show that the plus Lippmann-Schwinger equation for this system becomes:

$$\psi_{k+}(x) = e^{ikx} + \frac{im\alpha}{\hbar^2 |k|} e^{i|k|x} \psi_{k+}(0).$$

(b) Show that for $k > 0$ the solutions to the plus Lippmann-Schwinger equation give:

$$\psi_{k+}(x) = \begin{cases} e^{ikx} + r(k)e^{-ikx}, & x < 0 \\ t(k)e^{ikx}, & x > 0 \end{cases}$$

where the reflection and transmission coefficients are given by:

$$r(k) = \frac{im\alpha}{\hbar^2 k - im\alpha}, \quad t(k) = \frac{\hbar^2 k}{\hbar^2 k - im\alpha}.$$

Show as well by considering negative k that r and t are both even functions of k .

- (c) Show that the unitarity conditions in (8.9.253) are satisfied by the reflection and transmission coefficients.
- (d) Show that the S matrix (look at $t(k)$) has a pole at the complex value $k = \frac{im\alpha}{\hbar^2}$ and thus energy $E = \frac{\hbar^2 k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$, indicating the presence of a single bound state for this system. Show by explicitly solving the eigenvalue problem for the Hamiltonian operator that this system does have a single bound state given by:

$$\psi(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{-\frac{m\alpha|x|}{\hbar^2}}.$$

Explain how this function is related to $t(k)$ for $k > 0$ having a pole at $k = \frac{im\alpha}{\hbar^2}$.

Problem 8.55: The Born Approximation and Perturbative Unitarity. Consider the total Hamiltonian to be of the form $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$ and take the perturbative expansion of the scattering amplitude in powers of some parameter λ which characterizes the strength of the interaction (and counts powers of $\hat{H}_1$):

$$f(\vec{k}, \vec{k}') = \lambda f^{(1)}(\vec{k}, \vec{k}') + \lambda^2 f^{(2)}(\vec{k}, \vec{k}') + \mathcal{O}(\lambda^3).$$

- (a) Show that the corrections to the scattering amplitude are related to the corrections to the Lippmann-Schwinger equation by:

$$f^{(n)}(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2} \int e^{-i\vec{k}' \cdot \vec{x}} \left(U(\vec{x}) + \frac{|\vec{K}(\vec{x})|^2}{2m} + \frac{i\hbar}{2m} (\nabla \cdot \vec{K}(\vec{x})) + \frac{i\hbar}{m} \vec{K}(\vec{x}) \cdot \nabla \right) \psi_{\vec{k}+}^{(n-1)}(\vec{x}) d^3\vec{x}.$$

- (b) Show that the optical theorem relates scattering amplitude corrections at different orders by:

$$f^{(n)}(\vec{k}, \vec{k}') - f^{(n)*}(\vec{k}', \vec{k}) = \frac{i|\vec{k}|}{2\pi} \int_{\Omega} \sum_{l=1}^{n-1} f^{(l)*}(\vec{k}', |\vec{k}|_l) f^{(n-l)}(\vec{k}, |\vec{k}|_l) d\Omega.$$

Explain how this formula, known as the perturbative optical theorem, can be used to provide a consistency check on calculations of the scattering amplitude. In practice, this formula is very useful for checking for potential errors in your calculations.

Problem 8.56: Forward Scattering and the Optical Theorem. Forward scattering is the limit that the outgoing wave is aligned with the incoming beam. That is, $\vec{k}' \rightarrow \vec{k}$ in $f(\vec{k}, \vec{k}')$. Show, using the optical theorem, (8.9.293), and the definition of the total cross section σ :

$$\sigma = \int_{\Omega} \frac{d\sigma}{d\Omega} d\Omega$$

that the total cross section for scattering of an incoming beam of wavenumber $\vec{k}$ is determined by the imaginary part of the forward scattering amplitude by:

$$\sigma = \frac{4\pi}{|\vec{k}|} \text{Im}(f(\vec{k}, \vec{k})).$$

Problem 8.57: Scalar Potential Scattering. Consider scattering without a vector potential so that $\vec{K} = 0$.

- (a) Show that at lowest order in perturbation theory/in the first Born approximation, the scattering amplitude becomes:

$$f^{(1)}(\vec{k}, \vec{k}') = -\frac{m}{2\pi\hbar^2} \tilde{U}(\vec{k}' - \vec{k})$$

where $\tilde{U}(\vec{q})$ is the Fourier transform of the potential, normalized without any 2π 's:

$$\tilde{U}(\vec{q}) = \int e^{-i\vec{q} \cdot \vec{x}} U(\vec{x}) d^3\vec{x}.$$

- (b) Suppose the potential U is spherically symmetric so that it is a function of r only. Show that the

Fourier transform can be reduced to a single integral:

$$\tilde{U}(\vec{q}) = \frac{4\pi}{|\vec{q}|} \int_0^\infty rU(r) \sin(|\vec{q}|r) dr.$$

(c) Show, recalling that $\vec{k}' = k\vec{u}(\theta, \varphi)$ where $k = |\vec{k}|$:

$$|\vec{k}' - \vec{k}| = 2k \sin \frac{\theta}{2}$$

and that to lowest order in perturbation theory the differential cross section $\frac{d\sigma}{d\Omega}$ for scattering by a spherically symmetric potential can be written:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4E^2 \sin^2 \frac{\theta}{2}} \left(\int_0^\infty rU(r) \sin \left(2kr \sin \frac{\theta}{2} \right) kdr \right)^2 + \text{H.O.T.}$$

where $E = \frac{\hbar^2 k^2}{2m}$ is the energy per particle of the incoming beam.

Problem 8.58: ★ Rutherford Scattering Revisited. An electron interacting with a single proton at distances far from the proton with respect to the proton size is described by experiencing the perturbation:

$$U(r) = -\frac{q_e^2}{4\pi\epsilon_0 r}.$$

The Coulomb potential decays very slowly with distance, and in some sense is as slow as possible while still allowing the requirements of scattering to be achieved. Because it decays very slowly at large r , we will have to treat the large r behavior of integrals with slight care.

(a) Show, for $\varepsilon > 0$ that:

$$\int_0^\infty e^{-\varepsilon r} rU(r) \sin \left(2kr \sin \frac{\theta}{2} \right) kdr = -\frac{q_e^2}{4\pi\epsilon_0} \frac{2k^2 \sin \frac{\theta}{2}}{\varepsilon^2 + 4k^2 \sin^2 \frac{\theta}{2}}.$$

Explain, recalling the definition of the Fourier transform, why this ε damping factor is reasonable to introduce to this integral, so that we conclude:

$$\int_0^\infty rU(r) \sin \left(2kr \sin \frac{\theta}{2} \right) kdr = -\frac{q_e^2}{8\pi\epsilon_0} \frac{1}{\sin^2 \frac{\theta}{2}}.$$

(b) From this, show that the differential cross section for Coulomb scattering at lowest order in perturbation theory is given by:

$$\frac{d\sigma}{d\Omega} = \left(\frac{q_e^2}{16\pi\epsilon_0 E} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}}$$

where $E = \frac{\hbar^2 k^2}{2m}$ is the energy per incoming particle. Recall that when we studied classical Coulomb scattering this was actually the exact result for the differential cross section. In fact, surprisingly even though we derived this in perturbation theory it remains the exact result in quantum mechanics [74]. Show as well that the total cross section of the Coulomb potential diverges. This is because the potential decays so very slowly.

Problem 8.59: Electric Dipole Scattering. Consider the scattering of a charged particle q by an electric dipole potential:

$$\phi(\vec{x}) = \frac{\vec{\wp} \cdot \vec{x}}{4\pi\epsilon_0 |\vec{x}|^3}.$$

(a) Show that in the first Born approximation, the scattering amplitude for the charged particle is given by:

$$f^{(1)}(\vec{k}, \vec{k}') = \frac{imq}{2\pi\hbar^2\epsilon_0} \frac{\vec{\wp} \cdot (\vec{k}' - \vec{k})}{|\vec{k}' - \vec{k}|^2}.$$

(b) Let the plane spanned by the incoming particle's momentum and the electric dipole moment be the xz -plane. Choose (as usual) the incoming particle momentum to be in the z direction with magnitude $\hbar k$. Show that for constants $\wp$ and α the electric dipole moment can be written:

$$\vec{\wp} = \wp(\sin \alpha, 0, \cos \alpha)$$

and show that to leading order in perturbation theory the differential cross section of the charge's

scattering becomes:

$$\frac{d\sigma}{d\Omega} = \left(\frac{mq\varphi}{4\pi\epsilon_0\hbar^2 k} \right)^2 \left(\sin^2 \alpha \cos^2 \varphi \frac{\cos^2 \frac{\theta}{2}}{\sin^2 \frac{\theta}{2}} - \sin(2\alpha) \cos \varphi \frac{\cos \frac{\theta}{2}}{\sin \frac{\theta}{2}} + \cos^2 \alpha \right) + \mathcal{O}(q^3).$$

Note that the total cross section is infinite unless the beam and the dipole moment are perfectly aligned.

Problem 8.60: Magnetic Dipole Scattering and measuring the electron dipole moment. Consider the scattering of a spin-1/2 charged particle q of gyromagnetic ratio γ by a magnetic dipole potential:

$$\vec{A}(\vec{x}) = \frac{\mu_0 \vec{M} \times \vec{x}}{4\pi |\vec{x}|^3}.$$

- (a) Explain that the eigenstates of the free Hamiltonian are labeled by $\vec{k}$ and $\pm$ where $\pm$ indicate whether the spin of the plane wave is aligned or anti-aligned with a particular axis of choice. For this question, choose that axis to be the direction $\vec{M}$. Explain that the scattering amplitude is then a 2x2 matrix $f_{\pm\pm}(\vec{k}, \vec{k}')$ where each $\pm$ indicates the spin alignment of the incoming or outgoing plane wave. Let $\xi_{\pm}$ be constant unit spinors with spins aligned and anti-aligned with $\vec{M}$. Show that:

$$\psi_{(\vec{k}, \pm)_{\text{in}}+}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} \xi_{\pm_{\text{int}}} + \frac{e^{ikr}}{r} (f_{\pm_{\text{in}}+_{\text{out}}} \xi_+ + f_{\pm_{\text{in}}-_{\text{out}}} \xi_-) + \mathcal{O}\left(\frac{1}{r^2}\right).$$

- (b) Show that the magnetic field produced by the given vector potential is:

$$\vec{B}(\vec{x}) = \frac{2}{3} \mu_0 \vec{M} \delta(\vec{x}) + \frac{\mu_0}{4\pi r^3} (3\vec{l}_r \vec{l}_r \cdot \vec{M} - \vec{M}).$$

To do so, recall that $\nabla^2 \frac{1}{r} = -4\pi \delta(\vec{x})$. Show that in the first Born approximation, the scattering amplitude for the charged particle is given by:

$$f_{\pm+}^{(1)} \xi_+ + f_{\pm-}^{(1)} \xi_- = \frac{i\mu_0 q}{2\pi\hbar} \frac{\vec{M} \cdot (\vec{k} \times \vec{k}')}{|\vec{k}' - \vec{k}|^2} \xi_{\pm} - \frac{\mu_0 m \gamma}{2\pi\hbar^2} \left((\vec{l} \cdot \hat{S}_{\xi_{\pm}}) \vec{M} \cdot \vec{l} - \vec{M} \cdot \hat{S}_{\xi_{\pm}} \right)$$

where $\vec{l}$ is the unit vector in the direction of the momentum transfer:

$$\vec{l} = \frac{\vec{k}' - \vec{k}}{|\vec{k}' - \vec{k}|}.$$

- (c) Let the plane spanned by the incoming particle's momentum and the magnetic dipole moment be the xz-plane. Choose (as usual) the incoming particle momentum to be in the z direction with magnitude $\hbar k$. Show that for constants M and α the electric dipole moment can be written:

$$\vec{M} = M(\sin \alpha, 0, \cos \alpha)$$

and show that to leading order in perturbation theory the differential cross section of the charge's scattering (recalling the definition of the g -factor) becomes:

$$\frac{d\sigma}{d\Omega} = \left(\frac{\mu_0 q M}{4\pi\hbar} \right)^2 \left(\frac{\sin^2 \alpha \sin^2 \varphi}{\tan^2 \frac{\theta}{2}} + \left(\frac{g}{2} \right)^2 \left(\cos^2 \frac{\theta}{2} \sin^2 \varphi + \left(\cos \alpha \cos \frac{\theta}{2} \cos \varphi - \sin \alpha \sin \frac{\theta}{2} \right)^2 \right) \right) + \mathcal{O}(M^3).$$

Show that in the limit that the incoming beam is aligned with magnetic dipole moment of the dipole, the cross section simply becomes:

$$\frac{d\sigma}{d\Omega} = \left(\frac{\mu_0 g q M}{8\pi\hbar} \right)^2 \cos^2 \frac{\theta}{2} + \mathcal{O}(M^3).$$

Explain how the angular distribution of scattering particles can be used to determine the values of q and of the g -factor if the dipole moment strength M of the source dipole is known. Thus, using scattering experiments it is possible to measure g for charged particles, such as for the electron.

Problem 8.61: Scattering with time reversal symmetry. Consider scattering in a system with time reversal symmetry by a time reversal pseudo-operator $\hat{T}$ (both the free and full Hamiltonian operator are to have symmetry under this transformation). Suppose the unperturbed eigenstates $|\alpha_0\rangle$ have been chosen to be time reversal symmetric:

$$\hat{T}|\alpha_0\rangle = |\alpha_0\rangle.$$

- (a) Show that the time evolution operator satisfies:

$$\hat{T}\hat{U}(t, t_0)\hat{T}^{-1} = \hat{U}^\dagger(-t_0, -t).$$

Show further that this implies its matrix elements satisfy:

$$\langle \beta_0 | \hat{U}(t, t_0) | \alpha_0 \rangle = \langle \alpha_0 | \hat{U}(-t_0, -t) | \beta_0 \rangle.$$

- (b) Show that the S matrix elements, transition matrix elements, and transition rates satisfy:

$$S_{\beta\alpha} = S_{\alpha\beta}, \quad T_{\beta\alpha} = T_{\alpha\beta}, \quad \Gamma_{\alpha\rightarrow\beta} = \Gamma_{\beta\rightarrow\alpha}.$$

- (c) Show that for 3 dimensional scattering, the scattering amplitude becomes a symmetric function $f(\vec{k}, \vec{k}') = f(\vec{k}', \vec{k})$ and that the optical theorem becomes:

$$\text{Im}f(\vec{k}, \vec{k}') = |\vec{k}| \int_{\Omega} f^*(\vec{k}', |\vec{k}|\vec{l}) f(\vec{k}, |\vec{k}|\vec{l}) \frac{d\Omega}{4\pi}.$$

Problem 8.62: The H-theorem for Fermi's master equation.

- (a) Using the Born rule, explain that $\rho_n(t)$ in the Fermi master equation gives the probability that if the system is ideally measured at the time t it will be approximately in the state $|n\rangle$ after the measurement.
 (b) Let $S(t)$ be the entropy of the distribution of measurement results at time t :

$$S(t) = - \sum_n \rho_n \ln \rho_n.$$

Show that $S(t)$ satisfies:

$$\frac{dS}{dt} = \sum_n \sum_{m \neq n} \Gamma_{m \rightarrow n} (\rho_n - \rho_m) \ln \rho_n.$$

- (c) Suppose the system has time reversal symmetry. Show that $S(t)$ satisfies:

$$\frac{dS}{dt} = \frac{1}{2} \sum_n \sum_{m \neq n} \Gamma_{m \rightarrow n} (\rho_n - \rho_m) (\ln \rho_n - \ln \rho_m).$$

Show that $\frac{dS}{dt} > 0$ for all distributions which are not uniform and that $\frac{dS}{dt} = 0$ for a uniform distribution. Finally then, conclude that under time symmetric evolution by the Fermi master equation, the equilibrium distribution of ρ_n is necessarily uniform. This is known as Boltzmann's H-theorem. Explain how this is consistent with unitary invertible time evolution because the Fermi master equation involves the consistent ignoring of information by neglecting the phases conjugate to the ρ_n .

8.10 Another Big Bold Leap

8.10.1 Trouble with Multi-particle Statistics

We know that Galilean Quantum Mechanics cannot be a perfect theory because we have well established that Galilean symmetry isn't fundamental. However, the wave theory of matter side of what we have done is extremely successful and was able to address the problem of point-particle divergences. As such, the next natural thing to do is to consider a wave theory of matter with Lorentz symmetry, which will be the subject of the next chapter.

Not only are there problems with the Galilean part of Galilean quantum mechanics, there are more fundamental problems associated with the quantum mechanics part, at least the way we have done it so far. We said, without sufficient justification (with the details delayed until chapter 9), that ideal measurements only let us access the state of the quantum system statistically due to its microscopic nature (this led to the Born rule and the the Collapse rule). Galilean Quantum Mechanics is quite successful at describing the statistical behavior of a single particle at small scales experiencing electro and magnetostatic fields while at nonrelativistic velocities. But, it is still unclear how to account for the fact that there exist processes in which the number of particles change, such as when one particle decays into multiple. We had no way to account for this within classical mechanics either. With the wave theory, one might believe that such a process could be explained by considering a wave with multiple separated wave-packets and identifying each wave-packet as a distinct particle. However, this has some problems. In particular, there exist processes in which something charge neutral separates into two particles, one of positive charge and one of negative charge. By our expression for the charge density in equation (8.6.130), the sign of the total charge matches the sign of the charge density everywhere. Therefore, there is no way a charge neutral wave-packet could ever have non-zero charge density in this theory when it splits into different wave-packets. Consequently multiple wave-packets within one wavefunction cannot explain this phenomenon. The only alternative within our framework at this time then is that each particle gets its own wavefunction. But, there is no way to produce more wavefunctions from one within our theory so far. The number of wavefunction is always conserved. This is the same issue which occurred with classical mechanics when a single coordinate would split into multiple coordinates in a decay process.

Another issue is that experimentally there exist "indistinguishable" particles, such as electrons. All electrons we have ever observed have produced the same electric charge, mass, gyromagnetic ratio, and all other physical properties. It seems to us experimentally impossible to tell the difference between any two electrons. This is quite unlike the case in classical physics where we certainly get objects with similar properties, but never apparently exact duplicates. In the wave theory of matter as we have studied it so far, each electron would have a wavefunction. If each electron was represented by an independent function from the others, it would theoretically be allowed to have an independent charge, mass, and gyromagnetic ratio. It seems like a massive unexplained coincidence then that all electrons produce the same values of these parameters. One could assume such a massive coincidence has simply occurred, but it is more than a bit suspicious; such an alignment of parameter values generally in the history of science has indicated that there is an underlying pattern to explain it, that there is some underlying mechanism that *requires* all electrons to be identical. So, we suspect there is something deeper going on to explain the existence of indistinguishable particles which is unexplained by the theory we have discussed so far.

There are further problems with simply treating each particle as having its own wavefunction. Consider a spin-1/2 particle with wavefunction $\psi(t, \vec{x})$. We can define the functions:

$$\psi(t, \vec{x}) = \begin{pmatrix} \psi_+(t, \vec{x}) \\ \psi_-(t, \vec{x}) \end{pmatrix}, \quad \phi(t, \vec{x}) \stackrel{\text{def}}{=} \sqrt{|\psi_+|^2 + |\psi_-|^2}, \quad \chi_{\pm} \stackrel{\text{def}}{=} \frac{\psi_{\pm}}{\phi}, \quad \chi \stackrel{\text{def}}{=} \begin{pmatrix} \chi_+ \\ \chi_- \end{pmatrix} \quad (8.10.1)$$

$$\implies \psi(t, \vec{x}) = \begin{pmatrix} \chi_+(t, \vec{x}) \phi(t, \vec{x}) \\ \chi_-(t, \vec{x}) \phi(t, \vec{x}) \end{pmatrix} = \chi(t, \vec{x}) \phi(t, \vec{x}). \quad (8.10.2)$$

Then, immediately it follows that $|\chi_+|^2 + |\chi_-|^2 = 1$ and so it is possible to define angles $\alpha(t, \vec{x})$, $\theta(t, \vec{x})$, $\varphi(t, \vec{x})$ so that:

$$\chi_+ = e^{i\alpha} e^{-\frac{i}{2}\varphi} \cos \frac{\theta}{2}, \quad \chi_- = e^{i\alpha} e^{\frac{i}{2}\varphi} \sin \frac{\theta}{2}. \quad (8.10.3)$$

In the classical limit, $|\psi|^2 = \phi^2(t, \vec{x})$ becomes localized and so the only values of α, φ, θ which effect experiments are the values near the classical position. That is, in that limit we approximately can treat α, φ, θ as functions of time only with their values being given by evaluating their spatial dependence at $\vec{x}_{cl}(t)$.

Then, the spin angular momentum carried by the wavefunction becomes:

$$\langle \hat{S} \rangle = \langle \psi | \hat{S} | \psi \rangle = \int_{\mathbb{S}} \psi^\dagger \hat{S} \psi d^3 \vec{x} \approx \int_{\mathbb{S}} \phi^2(t, \vec{x}) \chi^\dagger(t) \hat{S} \chi(t) d^3 \vec{x} = \int_{\mathbb{S}} |\psi|^2 d^3 \vec{x} \langle \chi | \hat{S} | \chi \rangle = \langle \chi | \hat{S} | \chi \rangle. \quad (8.10.4)$$

In particular, a simple calculation gives:

$$\vec{S} = \langle \chi | \hat{S} | \chi \rangle = \frac{\hbar}{2} (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \quad (8.10.5)$$

$$\implies |\vec{S}| = \frac{\hbar}{2}. \quad (8.10.6)$$

So a spin-1/2 particle in the classical limit always carries a total spin angular momentum of magnitude $\frac{\hbar}{2}$. Now consider an experiment in which two spin-1/2 particles with wavefunctions essentially in the classical limit interact. After the interaction we measure a component of $\vec{S}$ for one of the particles using a Stern-Gerlach device. If we repeat this experiment many times with the same setup of the initial particles (let's say we have a polarized incoming beams for each) using multiple different orientations of the Stern-Gerlach device for the particle we measure, we can eventually get good statistics to measure $\langle \hat{S} \rangle$ for one of the particles. If we have succeeded in our experimental setup in making it reasonably precise enough that every trial can be treated with the same wavefunction for that particle, then $|\langle \hat{S} \rangle|$ must be $\frac{\hbar}{2}$. However, it is an experimental fact that it is possible in this setup for $|\langle \hat{S} \rangle| \leq \frac{\hbar}{2}$ and in fact can be pushed all the way down to 0 for the right intermediate interaction. There is no wavefunction for a spin-1/2 particle that could produce such a result, and the imprecision of the experimental setup is not significant enough to explain the discrepancy. Therefore, it cannot simply be correct to describe each particle in our theory by a different and completely separate wavefunction. This can be explained by the outgoing particles after the interaction having a beam which is unpolarized (and thus requiring a density matrix) but then it needs to be understood how the interaction of two polarized beams could produced an unpolarized beam, which simply solving equations of motion for interacting but separate wavefunctions will never give.

Thus, there are many issues relating to how quantum mechanics should treat a system of multiple particles which are not adequately addressed by our theory so far. Interestingly all of these problems are statistical, in the sense that they related to how physics is different when we allow multiple particles. Single particle quantum mechanics does seem to successfully describe many microscopic features though and so whatever improved theory we formulate for multi-particle systems will need to reproduce what we have done in this chapter in the case of a single particle.

8.10.2 Quantum Field Theory to the Rescue

Let us remember another puzzle we've encountered previously, the ultraviolet catastrophe. We found in section 5.12 that electromagnetism can be thought of as an infinite number of harmonic oscillators and that when those harmonic oscillators are treated with classical statistical mechanics the resulting thermodynamic quantities all diverge and give unphysical results. The classical density of states of a harmonic oscillator of angular frequency ω is:

$$g_{\text{cl}}(E) = \frac{\vartheta(E)}{\hbar\omega} \quad (8.10.7)$$

where $\hbar$ is used here as the normalization constant introduced in the definition of the phase space density in classical statistical mechanics. This density of states does produce an experimentally accurate spectral radiance $R(T, \omega)$ at large temperatures (compared to $\hbar\omega$). However, this density of states produces an experimentally inaccurate spectral radiance at low temperatures (compared to $\hbar\omega$). Instead, we found in 5.12 that the experimental evidence predicts the density of states:

$$g_{\text{qm}}(E) = \sum_{n=0}^{\infty} \delta(E - n\hbar\omega). \quad (8.10.8)$$

We can understand how this density of states can sometimes be approximated by the first one by noting that if $g(E)$ is integrated against a function $f(E)$ which varies very slowly over a change in energy of $\hbar\omega$ then on each such interval it can be replaced by its average value over that interval:

$$\int_{-\infty}^{\infty} f(E) g_{\text{qm}}(E) dE = \sum_{n=0}^{\infty} f(n\hbar\omega)$$

$$\approx \sum_{n=0}^{\infty} \frac{1}{\hbar\omega} \int_{n\hbar\omega}^{(n+1)\hbar\omega} f(E) dE = \int_{-\infty}^{\infty} f(E) \frac{\vartheta(E)}{\hbar\omega} dE = \int_{-\infty}^{\infty} f(E) g_{\text{cl}}(E) dE. \quad (8.10.9)$$

Therefore, if $\hbar\omega$ is small compared to the scale on which relevant functions change, we can approximate $g_{\text{qm}} \approx g_{\text{cl}}$ as distributions.

Our improved density of states has a striking property. It has discretely separated equally spaced peaks and it must somehow be related to the harmonic oscillator (as electromagnetism is an infinite number of harmonic oscillators). We found in this chapter that the quantum harmonic oscillator written as having Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ has energy eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$. Of course, as always, the zero-point of the energy can be set to be whatever you like by canonical transformation and is unphysical¹³, so we could equally well use the Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{\hbar\omega}{2}\mathbb{1}$, which then has energy eigenvalues $E_n = n\hbar\omega$. One could then write down the spectral density of the quantum harmonic oscillator in this gauge, meaning the function which when integrated over an interval $(a, b]$ gives the number of eigenvalues of the Hamiltonian operator between a and b . Because $E_n = n\hbar\omega$, that function would then precisely be $g_{\text{qm}}(E)$. That is, **the experimentally correct density of states for electromagnetism of a particular frequency at low temperatures is that of a quantum harmonic oscillator.**

With all of these observations, we make a big bold leap, as big as the leap from Galilean symmetry to Lorentz symmetry done in section 3.9, that even more fundamental than the classical field theory of electromagnetism is a **quantum field theory of electromagnetism**. In single particle quantum mechanics (also called first quantization), we replaced our theory of a classical point particle of position $\vec{x}(t)$ with a theory of a complex wavefunction $\psi(t, \vec{x})$ on the space of positions. Our big leap, called quantum field theory (or second quantization) is to now similarly replace the theory of a classical vector potential $A_\mu(t, \vec{x})$ by a theory of a complex wavefunction(al) $\Psi(t)[A]$ on the space of vector potential configurations. This probably looks crazy! The reason to do it at this point is that we want to somehow recover the observed black-body radiation, and that requires that electromagnetism should behave like a quantum harmonic oscillator. However, it turns out that there are countless phenomena producible in experiments that require this theory of quantum electromagnetism. We will give (in my opinion) theoretically more satisfying arguments where quantum field theory comes from in the next chapter.

For now, for quantum electromagnetism we will proceed by analogy to what has been done this chapter. First we need to recall the results of section 4.6 and its homework questions. Classical electromagnetism is described by the Maxwell Lagrangian:

$$\mathcal{L} = \int_{\mathbb{S}} \left(\frac{|\vec{E}|^2 - |\vec{B}|^2}{2} + \vec{J} \cdot \vec{A} - \rho\phi \right) d\mathbb{S}. \quad (8.10.10)$$

After Legendre transformation, this gives the Maxwell Hamiltonian:

$$\mathcal{H} = \int_{\mathbb{S}} \left(\frac{|\vec{P}_A|^2 + |\nabla \times \vec{A}|^2}{2} - \vec{J} \cdot \vec{A} + \phi(\rho + \nabla \cdot \vec{P}_A) \right) d\mathbb{S} \quad (8.10.11)$$

which has ϕ as a Lagrange multiplier giving a constrained canonical system (the constraint is Gauss' law). In Fourier space this Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{K}} \left(\frac{|\vec{P}_A(t, \vec{k})|^2 + |i\vec{k} \times \vec{A}(t, \vec{k})|^2}{2} - \vec{J}^*(t, \vec{k}) \cdot \vec{A}(t, \vec{k}) + \tilde{\phi}^*(t, \vec{k}) \left(\tilde{\rho}(t, \vec{k}) + i\vec{k} \cdot \vec{P}_A(t, \vec{k}) \right) \right) d^3\vec{k}. \quad (8.10.12)$$

Let $\vec{\xi}_0(\vec{k}) = i\frac{\vec{k}}{|\vec{k}|}$, $\vec{\xi}_1(\vec{k})$, $\vec{\xi}_{-1}(\vec{k})$ be the longitudinal and transverse polarization vectors defined in problem 4.40 so that:

$$i\vec{k} \times \vec{\xi}_m = m|\vec{k}|\vec{\xi}_m, \quad \vec{\xi}_m^*(-\vec{k}) = \vec{\xi}_m(\vec{k}), \quad \vec{\xi}_m^\dagger \vec{\xi}_{m'} = \delta_{mm'}, \quad \sum_{m=-1}^1 \vec{\xi}_m \vec{\xi}_m^\dagger = \mathbb{1}. \quad (8.10.13)$$

¹³Some readers may believe that the zero-point of energy is physical and can be observed, for example in the Casimir effect. This is incorrect. It has been understood for a half-century [105] that the Casimir effect can be derived fully without reference to zero-point energy, does not measure zero-point energy, and that in calculations that make it look like it is doing so it is because it is actually measuring the difference between two simultaneously imposed conflicting conventions on setting the zero-point energy and so is a measure of an energy difference.

A Fourier transformed vector field $\vec{F}$ can be decomposed into the helicity basis according to $\vec{F}_m = \vec{\xi}_m^\dagger \vec{F}$. In the helicity basis the electromagnetic Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{K}} \left(\sum_{h \in \{-1, 1\}} \left(\frac{|\tilde{P}_{Ah}|^2 + |\vec{k}|^2 |\tilde{A}_h|^2}{2} - \tilde{J}_h^* \tilde{A}_h \right) + \frac{|\tilde{P}_{A0}|^2}{2} - \tilde{J}_0^* \tilde{A}_0 + \tilde{\phi}^* (\tilde{\rho} - |\vec{k}| \tilde{P}_{A0}) \right) d^3 \vec{k} \quad (8.10.14)$$

and has the Poisson brackets:

$$\{\tilde{A}_m(t, \vec{k}), \tilde{A}_{m'}(t, \vec{k}')\} = 0, \quad (8.10.15)$$

$$\{\tilde{A}_m(t, \vec{k}), \tilde{P}_{Am'}(t, \vec{k}')\} = \delta_{mm'} \delta(\vec{k} + \vec{k}'), \quad (8.10.16)$$

$$\{\tilde{P}_{Am}(t, \vec{k}), \tilde{P}_{Am'}(t, \vec{k}')\} = 0. \quad (8.10.17)$$

As well, the gauge transformation becomes:

$$\tilde{\phi}' = \tilde{\phi} - \frac{\partial \tilde{f}}{\partial t}, \quad \tilde{A}'_{-1} = \tilde{A}_{-1}, \quad \tilde{A}'_0 = \tilde{A}_0 + |\vec{k}| \tilde{f}, \quad \tilde{A}'_1 = \tilde{A}_1. \quad (8.10.18)$$

Thus only the longitudinal mode of the vector potential is not gauge invariant. For the transverse modes, (8.10.14) is precisely the Hamiltonian of a driven harmonic oscillator. However, for the longitudinal modes there are still constraints to be handled for gauge invariance. We can clean up (8.10.14) by introducing “John’s Quantum Map” coordinates just as in (8.2.3) or analogously just like in our analysis of the quantum harmonic oscillator. Define $\omega(\vec{k}) = |\vec{k}|$ and the mode vector $\vec{a}(t, \vec{k})$ for $h \in \{-1, 1\}$:

$$\vec{a}(t, \vec{k}) = a_{-1}(t, \vec{k}) \vec{\xi}_{-1}(\vec{k}) + a_1(t, \vec{k}) \vec{\xi}_1(\vec{k}) \quad (8.10.19)$$

$$a_h(t, \vec{k}) = \sqrt{\frac{\omega}{2\hbar}} \tilde{A}_h(t, \vec{k}) + \frac{i}{\sqrt{2\omega\hbar}} \tilde{P}_{Ah}(t, \vec{k}). \quad (8.10.20)$$

Inverting these and returning them to the Hamiltonian gives:

$$\tilde{A}_h(t, \vec{k}) = \sqrt{\frac{\hbar}{2\omega}} \left(a_h(t, \vec{k}) + a_h^*(t, -\vec{k}) \right), \quad \tilde{P}_{Ah}(t, \vec{k}) = \frac{1}{i} \sqrt{\frac{\hbar\omega}{2}} \left(a_h(t, \vec{k}) - a_h^*(t, -\vec{k}) \right) \quad (8.10.21)$$

$$\mathcal{H} = \int_{\mathbb{K}} \left(\sum_h \left(\hbar\omega(\vec{k}) a_h^* a_h - \sqrt{\frac{2\hbar}{\omega}} \text{Re}(\tilde{J}_h^* a_h) \right) + \frac{|\tilde{P}_{A0}|^2}{2} - \tilde{J}_0^* \tilde{A}_0 + \tilde{\phi}^* (\tilde{\rho} - |\vec{k}| \tilde{P}_{A0}) \right) d^3 \vec{k} \quad (8.10.22)$$

$$\{a_h(t, \vec{k}), a_{h'}(t, \vec{k}')\} = 0, \quad \{a_h(t, \vec{k}), a_{h'}^*(t, \vec{k}')\} = -\frac{i}{\hbar} \delta_{hh'} \delta(\vec{k} - \vec{k}'), \quad \{a_h, \tilde{A}_0\} = \{a_h, \tilde{P}_{A0}\} = 0. \quad (8.10.23)$$

The Gauss’ law constraint on the longitudinal modes requires:

$$\tilde{P}_{A0} = \frac{\partial \tilde{A}_0}{\partial t} + |\vec{k}| \tilde{\phi} = \frac{\tilde{\rho}}{|\vec{k}|}. \quad (8.10.24)$$

Let $\Lambda(t, \vec{x})$ be a function whose Laplacian matches the divergence of the vector potential:

$$\nabla^2 \Lambda = \nabla \cdot \vec{A}. \quad (8.10.25)$$

Such a function is guaranteed to exist for vector potentials which decay at infinity due to the existence of solutions to the Poisson equation. Then, we have:

$$\tilde{A}_0 = |\vec{k}| \tilde{\Lambda} \quad (8.10.26)$$

and that Λ is completely arbitrary under gauge transformation:

$$\Lambda' = \Lambda + f(t, \vec{x}). \quad (8.10.27)$$

Thus, Λ is fully unphysical and undetermined by the dynamics (it is pure gauge). Using these constraints, the electromagnetic Hamiltonian becomes:

$$\mathcal{H} = \int_{\mathbb{K}} \sum_h \left(\hbar\omega(\vec{k}) a_h^* a_h - \sqrt{\frac{2\hbar}{\omega}} \text{Re}(\tilde{J}_h^* a_h) \right) d^3 \vec{k} + \int_{\mathbb{S}, \mathbb{S}} \frac{\rho(t, \vec{x}) \rho(t, \vec{x}')}{8\pi |\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' - \int_{\mathbb{S}} \vec{J} \cdot \nabla \Lambda d^3 \vec{x}. \quad (8.10.28)$$

These last two terms do not at all depend on the dynamical degrees of freedom. They are necessary for managing Lorentz and gauge invariance together, but are not dynamically independent. In terms of Λ and the a_h , the potentials (and $\tilde{P}_A$) can be written:

$$\phi(t, \vec{x}) = -\frac{\partial \Lambda}{\partial t} + \int_{\mathbb{S}} \frac{\rho(t, \vec{x}')}{4\pi |\vec{x} - \vec{x}'|} d^3 \vec{x}' \quad (8.10.29)$$

$$\vec{A}(t, \vec{x}) = \nabla \Lambda + \operatorname{Re} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \vec{a}(t, \vec{k}) \sqrt{\frac{2\hbar}{\omega}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} \quad (8.10.30)$$

$$\vec{P}_A(t, \vec{x}) = \nabla \int \frac{\rho(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d^3 \vec{x}' + \operatorname{Im} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \vec{a}(t, \vec{k}) \sqrt{2\hbar\omega} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}}. \quad (8.10.31)$$

Thus, all of classical electromagnetism can be expressed in terms of a fully arbitrary function $\Lambda(t, \vec{x})$ and the gauge invariant functions $a_{\pm 1}(t, \vec{k})$ which represent the physical degrees of freedom of the system.

In the quantum theory of electromagnetism, the classical physical degrees of freedom $a_{\pm 1}(t, \vec{k})$ will be given by the operator summary of appropriate operators $\hat{a}_{\pm 1}(\vec{k})$ on an appropriate Hilbert space $\mathbb{H}$ with respect to the system's state vector $|\Psi(t)\rangle$:

$$a_{\pm 1}(t, \vec{k}) = \langle \Psi(t) | \hat{a}_{\pm 1}(\vec{k}) | \Psi(t) \rangle. \quad (8.10.32)$$

Λ does not receive an operator because it is just an arbitrary function, not a degree of freedom of the theory. By theorem (8.5), if the classical quantities $a_{\pm 1}(t, \vec{k})$ are to satisfy the Poisson brackets in (8.10.23), the operators $\hat{a}_{\pm 1}$ must satisfy the commutators:

$$[\hat{a}_h(\vec{k}), \hat{a}_{h'}(\vec{k}')] = 0, \quad [\hat{a}_h(\vec{k}), \hat{a}_h^\dagger(\vec{k}')] = \delta_{hh'} \delta(\vec{k} - \vec{k}'). \quad (8.10.33)$$

If the classical quantities $a_{\pm 1}(t, \vec{k})$ are to have the correct classical equations of motion (those given by the Hamiltonian (8.10.28)) then because those are simply the driven harmonic oscillator equations of motion and we know that the quantum harmonic oscillator gives the classical harmonic oscillator equations of motion for the operator summaries, we simply take the Hamiltonian operator of quantum electromagnetism to be:

$$\hat{H} = \int_{\mathbb{K}} \sum_h \left(\hbar\omega(\vec{k}) \hat{a}_h^\dagger \hat{a}_h - \sqrt{\frac{2\hbar}{\omega}} \operatorname{Sa}(\tilde{J}_h^* \hat{a}_h) \right) d^3 \vec{k} + \int_{\mathbb{S}, \mathbb{S}} \frac{\rho(t, \vec{x}) \rho(t, \vec{x}')}{8\pi|\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' \mathbb{1} - \int_{\mathbb{S}} \vec{J} \cdot \nabla \Lambda d^3 \vec{x} \mathbb{1} \quad (8.10.34)$$

where Sa indicates the self-adjoint part of an operator (define as well As as the anti-self-adjoint part):

$$\operatorname{Sa} \hat{O} = \frac{\hat{O} + \hat{O}^\dagger}{2}, \quad \operatorname{As} \hat{O} = \frac{\hat{O} - \hat{O}^\dagger}{2i} \quad (8.10.35)$$

$$\implies \hat{O} = \operatorname{Sa}(\hat{O}) + i \operatorname{As}(\hat{O}), \quad (\operatorname{Sa}(\hat{O}))^\dagger = \operatorname{Sa}(\hat{O}), \quad (\operatorname{As}(\hat{O}))^\dagger = -\operatorname{As}(\hat{O}). \quad (8.10.36)$$

It is useful for calculations to repackage the $\hat{a}_{\pm 1}(\vec{k})$ commutators into commutators explicitly in terms of $\hat{a}(\vec{k})$. Using (8.10.13) with $\hat{a}_b(\vec{k})$ meaning component b of $\hat{a}(\vec{k})$:

$$[\hat{a}_a(\vec{k}), \hat{a}_b(\vec{k}')] = 0, \quad [\hat{a}_a(\vec{k}), \hat{a}_b^\dagger(\vec{k}')] = \perp_{ab}(\vec{k}) \delta(\vec{k} - \vec{k}') \mathbb{1} \quad (8.10.37)$$

where $\perp_{ab}(\vec{k})$ is a projector onto the space orthogonal to $\vec{k}$:

$$\perp_{ab}(\vec{k}) = \delta_{ab} - \frac{k_a k_b}{|\vec{k}|^2}. \quad (8.10.38)$$

Because the classical quantities $\phi, \vec{A}, \vec{P}_A$ depend at most linearly on the $a_{\pm 1}(t, \vec{k})$ and the $a_{\pm 1}(t, \vec{k})$ are given by operator summaries, it is natural to define the operators:

$$\hat{\phi}(t, \vec{x}) = -\frac{\partial \Lambda}{\partial t} \mathbb{1} + \int_{\mathbb{S}} \frac{\rho(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d^3 \vec{x}' \mathbb{1} \quad (8.10.39)$$

$$\hat{\vec{A}}(t, \vec{x}) = \nabla \Lambda \mathbb{1} + \operatorname{Sa} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \hat{\vec{a}}(\vec{k}) \sqrt{\frac{2\hbar}{\omega}} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} \quad (8.10.40)$$

$$\hat{\vec{P}}_A(t, \vec{x}) = \nabla \int \frac{\rho(t, \vec{x}')}{4\pi|\vec{x} - \vec{x}'|} d^3 \vec{x}' \mathbb{1} + \operatorname{As} \int_{\mathbb{K}} e^{i\vec{k} \cdot \vec{x}} \hat{\vec{a}}(\vec{k}) \sqrt{2\hbar\omega} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} \quad (8.10.41)$$

where $\hat{\vec{a}}$ is given by:

$$\hat{\vec{a}}(\vec{k}) = \hat{a}_1(\vec{k}) \vec{\xi}_1(\vec{k}) + \hat{a}_{-1}(\vec{k}) \vec{\xi}_{-1}(\vec{k}). \quad (8.10.42)$$

Then, the classical potentials and conjugate momenta can be expressed as operator summaries of these operators in the natural way:

$$\phi(t, \vec{x}) = \langle \Psi(t) | \hat{\phi}(t, \vec{x}) | \Psi(t) \rangle, \quad \vec{A}(t, \vec{x}) = \langle \Psi(t) | \hat{\vec{A}}(t, \vec{x}) | \Psi(t) \rangle, \quad \vec{P}_A(t, \vec{x}) = \langle \Psi(t) | \hat{\vec{P}}_A(t, \vec{x}) | \Psi(t) \rangle. \quad (8.10.43)$$

Similarly, in the classical theory $\vec{E}(t, \vec{x})$ is given by $-\vec{P}_A(t, \vec{x})$ and $\vec{B}(t, \vec{x})$ by $\nabla \times \vec{A}(t, \vec{x})$. So, it is natural to define the electric and magnetic field operators:

$$\hat{\vec{E}} = -\hat{\vec{P}}_A, \quad \hat{\vec{B}} = \nabla \times \hat{\vec{A}}. \quad (8.10.44)$$

Again due to the linearity of these expressions in the relevant operators, the classical electric and magnetic fields are then given by:

$$\vec{E}(t, \vec{x}) = \langle \Psi(t) | \hat{\vec{E}}(t, \vec{x}) | \Psi(t) \rangle, \quad \vec{B}(t, \vec{x}) = \langle \Psi(t) | \hat{\vec{B}}(t, \vec{x}) | \Psi(t) \rangle. \quad (8.10.45)$$

By using these definitions, together with the Schrödinger equation for $|\Psi\rangle$ under the Hamiltonian operator in (8.10.34) and the commutators in (8.10.33), one finds that **Maxwell's equations are exactly maintained in quantum electromagnetism**. The difference between classical and quantum electromagnetism is that in classical electromagnetism the potentials $\phi, \vec{A}$ contain all of the data in the theory but in quantum electromagnetism it is possible to consider more complicated objects such as $\langle \hat{A}_x(t_1, \vec{x}_1) \hat{A}_z(t_2, \vec{x}_2) \rangle$ and other operator summaries of operator products which are quantities not found in the classical theory. Quantum electromagnetism contains all of classical electromagnetism but it also includes many many other degrees of freedom, due to fundamentally being described by a wavefunctional $|\Psi(t)\rangle$ on an enormous Hilbert space.

The free Hamiltonian operator of quantum electromagnetism (meaning without any applied charges or currents) is (by simply setting $\rho = 0, \vec{J} = 0$ in (8.10.34)):

$$\hat{H}_0 = \int_{\mathbb{K}} \sum_h \hbar \omega \hat{a}_h^\dagger \hat{a}_h d^3 \vec{k}. \quad (8.10.46)$$

From (8.10.33) we see that $\hat{a}_h(\vec{k})$ has the canonical commutation relations of the annihilation operator (with $\hat{a}_h^\dagger$ being the creation operator) for a harmonic oscillator. Let $|0\rangle$ be the normalized ground state of $\hat{H}_0$, which because it is a sum of harmonic oscillators correspond to the state which is annihilated by $\hat{a}_h(\vec{k})$ for all h and $\vec{k}$:

$$\hat{a}_h(\vec{k})|0\rangle = 0. \quad (8.10.47)$$

This $|0\rangle$ state is often called the “vacuum” state. However, it is dangerous (read: incorrect) to think of the vacuum state as a state in which there is nothing going on. To see why it is useful to do two simple calculations (simple in theory, somewhat tedious in practice). For the first, let us compute the electric field in vacuum:

$$\langle 0 | \hat{\vec{E}}(\vec{x}) | 0 \rangle = \frac{1}{2i} \int_{\mathbb{K}} \left(e^{i\vec{k} \cdot \vec{x}} \langle 0 | \hat{\vec{a}} | 0 \rangle - e^{-i\vec{k} \cdot \vec{x}} \langle 0 | \hat{\vec{a}}^\dagger | 0 \rangle \right) \sqrt{2\hbar\omega} \frac{d^3 \vec{k}}{(2\pi)^{\frac{3}{2}}} = 0. \quad (8.10.48)$$

Both $\langle 0 | \hat{\vec{a}} | 0 \rangle$ and $\langle 0 | \hat{\vec{a}}^\dagger | 0 \rangle$ are 0 because $\hat{\vec{a}}$ annihilates $|0\rangle$ in the first and $\langle 0 | \hat{\vec{a}}^\dagger = (\hat{\vec{a}}|0\rangle)^\dagger = 0$ in the second. For the second, let us compute the summary of a product of electric field components in vacuum:

$$\langle 0 | \hat{E}_a(\vec{x}) \hat{E}_b(\vec{x}') | 0 \rangle = - \int_{\mathbb{K}, \mathbb{K}'} \frac{\hbar \sqrt{\omega \omega'}}{16\pi^3} \langle 0 | \left(e^{i\vec{k} \cdot \vec{x}} \hat{a}_a(\vec{k}) - e^{-i\vec{k} \cdot \vec{x}} \hat{a}_a^\dagger(\vec{k}) \right) \left(e^{i\vec{k}' \cdot \vec{x}'} \hat{a}_b(\vec{k}') - e^{-i\vec{k}' \cdot \vec{x}'} \hat{a}_b^\dagger(\vec{k}') \right) | 0 \rangle d^3 \vec{k} d^3 \vec{k}'. \quad (8.10.49)$$

Because $\hat{\vec{a}}$ annihilates $|0\rangle$ and $\hat{\vec{a}}^\dagger$ annihilates $\langle 0|$, only one of the four terms in the product survives, giving:

$$\langle 0 | \hat{E}_a(\vec{x}) \hat{E}_b(\vec{x}') | 0 \rangle = \int_{\mathbb{K}, \mathbb{K}'} \frac{\hbar \sqrt{\omega \omega'}}{16\pi^3} e^{i\vec{k} \cdot \vec{x} - \vec{k}' \cdot \vec{x}'} \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_b^\dagger(\vec{k}') | 0 \rangle d^3 \vec{k} d^3 \vec{k}'. \quad (8.10.50)$$

The final surviving summary inside the integral can be evaluated using the commutation relations:

$$\langle 0 | \hat{a}_a(\vec{k}) \hat{a}_b^\dagger(\vec{k}') | 0 \rangle = \langle 0 | (\hat{a}_a(\vec{k}) \hat{a}_b^\dagger(\vec{k}') - \hat{a}_b^\dagger(\vec{k}') \hat{a}_a(\vec{k}) + \hat{a}_b^\dagger(\vec{k}') \hat{a}_a(\vec{k})) | 0 \rangle \quad (8.10.51)$$

$$= \langle 0 | [\hat{a}_a(\vec{k}), \hat{a}_b(\vec{k}')] | 0 \rangle + \langle 0 | \hat{a}_b^\dagger(\vec{k}') \hat{a}_a(\vec{k}) | 0 \rangle \quad (8.10.52)$$

$$= \langle 0 | \perp_{ab}(\vec{k}) | 0 \rangle + 0 \quad (8.10.53)$$

$$= \perp_{ab}(\vec{k}) \delta(\vec{k} - \vec{k}'). \quad (8.10.54)$$

Returning this to (8.10.50) gives:

$$\langle 0 | \hat{E}_a(\vec{x}) \hat{E}_b(\vec{x}') | 0 \rangle = \int_{\mathbb{K}} \hbar |\vec{k}| \perp_{ab}(\vec{k}) e^{i\vec{k} \cdot (\vec{x} - \vec{x}')} \frac{d^3 \vec{k}}{16\pi^3}. \quad (8.10.55)$$

The remaining integration can be completed to give the right-hand side an explicit distributional form, though

it isn't very insightful. What is insightful is that this is a nonzero quite complicated object. Even in the vacuum state, there are nontrivial correlations in quantum field theory.

Because the eigenstates of a single harmonic oscillator can be written all by acting the creation operator some number of times on the ground state, the eigenstates of $\hat{H}_0$ here can be written by acting the creation operator (for possibly many pairs of helicity and wavenumber) some number of times on $|0\rangle$. That is, we can take as an eigenbasis of $\hat{H}_0$ the states constructed by the following. Let D be a nonnegative integer and let $(n_1, h_1, \vec{k}_1), \dots, (n_D, h_D, \vec{k}_D)$ be a list of D triplets of a nonnegative integer n , a helicity h , and a wavenumber $\vec{k}$ with no triplets sharing simultaneously their values of h and $\vec{k}$. Define the state $|n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D\rangle$ by:

$$|n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D\rangle = \frac{(\hat{a}_{h_1}^\dagger(\vec{k}_1))^{n_1}}{\sqrt{n_1!}} \dots \frac{(\hat{a}_{h_D}^\dagger(\vec{k}_D))^{n_D}}{\sqrt{n_D!}} |0\rangle. \quad (8.10.56)$$

Ranging over all possible lists α for a given D and then all values of D produces an eigenbasis of $\hat{H}_0$. The eigenvalues of $\hat{H}_0$ are found by directly applying the canonical commutation relations and that $|0\rangle$ is the ground state:

$$\hat{H}_0 |n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D\rangle = \sum_{d=1}^D \hbar \omega(\vec{k}_d) n_d |n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D\rangle. \quad (8.10.57)$$

This eigenvalue spectrum precisely is exactly the distribution corresponding to the density of states necessary to derive the black-body formula, as we hoped. We can now understand how unwieldy the Hilbert space of quantum electromagnetism is by expressing a general state $|\Psi\rangle$ in this basis. Defining the components:

$$\Psi_{(n_1 h_1, \dots, n_D h_D)}(\vec{k}_1, \dots, \vec{k}_D) = \langle n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D | \Psi \rangle \quad (8.10.58)$$

and using that these form a complete basis, we have that an arbitrary $|\Psi\rangle$ can be written as:

$$|\Psi\rangle = \sum_{D=0}^{\infty} \sum_{n_1=0}^{\infty} \sum_{h_1 \in \pm 1} \int_{\mathbb{K}_1} \dots \sum_{n_D=0}^{\infty} \sum_{h_D \in \pm 1} \int_{\mathbb{K}_D} \Psi_{(n_1 h_1, \dots, n_D h_D)}(\vec{k}_1, \dots, \vec{k}_D) |n_1 h_1 \vec{k}_1, \dots, n_D h_D \vec{k}_D\rangle d^3 \vec{k}_1 \dots d^3 \vec{k}_D. \quad (8.10.59)$$

This is the unfortunate generic form for a state in the Hilbert space of quantum electromagnetism.

In the free theory (under evolution by $\hat{H}_0$), of course each eigenstate simply evolves by a phase determined by its eigenvalue. Consequently, the occupation numbers $n_1, \dots, n_D$ are constant in the free theory. We can get somewhat of an intuition of what is going on with $|\Psi\rangle$, at least in the free theory, by looking at the subspaces of the Hilbert space of different occupation numbers. The total occupation number is of a state of definite number simply given by eigenvalue of the total number operator $\hat{N}$, which as always for each species of a harmonic oscillator is given by $\hat{a}^\dagger \hat{a}$ and so in total is giving by summing over such species. Therefore:

$$\hat{N} = \int_{\mathbb{K}} \sum_{h \in \pm 1} \hat{a}_h^\dagger(\vec{k}) \hat{a}_h(\vec{k}) d^3 \vec{k}. \quad (8.10.60)$$

The subspace with all occupation numbers as 0 is simply the vacuum $|0\rangle$. A generic state $|\Psi\rangle_1$ with total occupation number 1 can be written as a linear combination of occupation 1 eigenstates of $\hat{H}_0$. Under the free evolution given by $\hat{H}_0$, an occupation 1 state remains occupation 1 (because $\hat{N}$ commutes with $\hat{H}_0$) so takes the form:

$$|\Psi(t)\rangle_1 = \int_{\mathbb{K}} (\psi_1(t, \vec{k}) \hat{a}_1^\dagger(\vec{k}) + \psi_{-1}(t, \vec{k}) \hat{a}_{-1}^\dagger(\vec{k})) |0\rangle d^3 \vec{k} = \int_{\mathbb{K}} \vec{\psi}(t, \vec{k}) \cdot \hat{\vec{a}}^\dagger(\vec{k}) |0\rangle d^3 \vec{k} \quad (8.10.61)$$

for some functions $\psi_{\pm 1}(t, \vec{k})$ or equivalently $\vec{\psi}(t, \vec{k})$ defined so that:

$$\vec{\psi}(t, \vec{k}) = \psi_1(t, \vec{k}) \vec{\xi}_1(\vec{k}) + \psi_{-1}(t, \vec{k}) \vec{\xi}_{-1}(\vec{k}). \quad (8.10.62)$$

Such a $\vec{\psi}(t, \vec{k})$ can also be thought of as an arbitrary vector function satisfying:

$$\vec{k} \cdot \vec{\psi}(t, \vec{k}) = 0 \quad \text{or equivalently} \quad \perp_a \vec{b}(\vec{k}) \psi^b(t, \vec{k}) = \psi^a(t, \vec{k}). \quad (8.10.63)$$

The normalization of $|\Psi\rangle_1$ requires:

$$1 = \langle \Psi | \Psi \rangle_1 = \int_{\mathbb{K} \mathbb{K}'} \psi^{*a}(t, \vec{k}) \psi^b(t, \vec{k}') \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_b^\dagger(\vec{k}') | 0 \rangle d^3 \vec{k} d^3 \vec{k}' \quad (8.10.64)$$

$$= \int_{\mathbb{K} \mathbb{K}'} \psi^{*a}(t, \vec{k}) \psi^b(t, \vec{k}') \perp_{ab}(\vec{k}) \delta(\vec{k} - \vec{k}') d^3 \vec{k} d^3 \vec{k}' \quad (8.10.65)$$

$$= \int_{\mathbb{K}} |\psi(t, \vec{k})|^2 d^3 \vec{k}. \quad (8.10.66)$$

Therefore, $\vec{\psi}(t, \vec{k})$ must be normalized as a wavefunction on wavenumber space. We can find the explicit time evolution of $\vec{\psi}(t, \vec{k})$ using the Schrödinger equation:

$$i\hbar \frac{d|\Psi(t)\rangle_1}{dt} = \hat{H}_0 |\Psi\rangle_1 \quad (8.10.67)$$

$$\implies i\hbar \int_{\mathbb{K}} \frac{\partial \vec{\psi}(t, \vec{k})}{\partial t} a^\dagger(\vec{k}) |0\rangle d^3 \vec{k} = \int_{\mathbb{K}} \hbar \omega(\vec{k}) \vec{\psi}(t, \vec{k}) \cdot \hat{\vec{a}}^\dagger |0\rangle d^3 \vec{k} \quad (8.10.68)$$

$$\implies i\hbar \frac{\partial \vec{\psi}(t, \vec{k})}{\partial t} = \hbar \omega(\vec{k}) \vec{\psi}(t, \vec{k}). \quad (8.10.69)$$

This is precisely the Schrödinger equation for a single particle wavefunction written in wavenumber space with Hamiltonian operator $\hbar \omega(\vec{k})$ (where $\vec{k}$ would be the wavenumber operator for that single particle quantum system). Define then the Hilbert space $\mathbb{H}_1$ of states of $\vec{\psi}(t, \vec{k})$ so that we now write $|\psi(t)\rangle$, with Hamiltonian operator $\hat{H}_1 = \hbar \omega(\vec{k})$ and $|\vec{k}_\pm\rangle$ the wavenumber eigenstates of helicity ± 1 . Then, we can write:

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}_1 |\psi\rangle, \quad \psi_{\pm 1}(t, \vec{k}) = \langle \vec{k}_\pm | \psi(t) \rangle. \quad (8.10.70)$$

As well, for any operator $\hat{\mathcal{O}}$, the operator summary in the state $|\Psi\rangle_1$ can be reduced to an operator summary on the Hilbert space of configurations of $\vec{\psi}(t, \vec{k})$:

$$\langle \Psi | \hat{\mathcal{O}} | \Psi \rangle_1 = \int_{\mathbb{K}\mathbb{K}'} \psi^{*a}(t, \vec{k}) \psi^b(t, \vec{k}') \langle 0 | \hat{a}_a(\vec{k}) \hat{\mathcal{O}} \hat{a}_b^\dagger(\vec{k}') | 0 \rangle d^3 \vec{k} d^3 \vec{k}' = \langle \psi | \hat{\mathcal{O}}_1 | \psi \rangle \quad (8.10.71)$$

where $\hat{\mathcal{O}}_1$ is defined by:

$$\hat{\mathcal{O}}_1 = \int_{\mathbb{K}\mathbb{K}'} \sum_{h \in \pm 1} \sum_{h' \in \pm 1} |\vec{k}_h\rangle \langle 0 | \hat{a}_h(\vec{k}) \hat{\mathcal{O}} \hat{a}_{h'}^\dagger(\vec{k}') | 0 \rangle \langle \vec{k}_{h'} | d^3 \vec{k} d^3 \vec{k}'. \quad (8.10.72)$$

Therefore, **the subspace of occupation number one reduces to just single particle quantum mechanics**. The particle (meaning wave-packet, not point-particle) created by a single application of the electromagnetic creation operator is called the **photon**. Because of this, we call the occupation number the particle number (and in the case of electromagnetism, the **photon number**) and say that $|\Psi\rangle_1$ is a single photon state. We could even define a wavefunction $\vec{\psi}(t, \vec{x})$ on position space by Fourier transforming $\vec{\psi}(t, \vec{k})$ in the usual way to give an even more direct look at a single photon wavefunction if we like. **Quantum field theory contains single particle quantum mechanics**.

The subspace of photon number one is just single particle quantum mechanics with a particular Hamiltonian operator. What is the subspace of photon number two? Let us proceed similarly to find out. A state of photon number two will involve acting two creation operators on the vacuum state in a generic linear combination. Again the photon number is conserved by the free Hamiltonian, so under such evolution a generic state will be characterized by some coefficients $\psi_{\pm 1 \pm 1}(t, \vec{k}, \vec{k}')$ in the form:

$$|\Psi(t)\rangle_2 = \frac{1}{\sqrt{2}} \int_{\mathbb{K}\mathbb{K}'} \sum_{hh'} \psi_{hh'}(t, \vec{k}, \vec{k}') \hat{a}_h^\dagger(\vec{k}) \hat{a}_{h'}^\dagger(\vec{k}') | 0 \rangle d^3 \vec{k} d^3 \vec{k}'. \quad (8.10.73)$$

We can just as well define the bivector with components $\psi^{ab}(t, \vec{k}, \vec{k}')$ by:

$$\psi^{ab}(t, \vec{k}, \vec{k}') = \sum_{hh'} \psi_{hh'}(t, \vec{k}, \vec{k}') \xi_h^a(\vec{k}) \xi_{h'}^b(\vec{k}'). \quad (8.10.74)$$

Because $\hat{a}_a^\dagger(\vec{k})$ and $\hat{a}_b^\dagger(\vec{k}')$ commute, $\psi^{ab}(t, \vec{k}, \vec{k}')$ is automatically a symmetric under interchanging the order of photon creation (because it is defined simply as whatever coefficients are in (8.10.73):

$$\psi^{ba}(t, \vec{k}', \vec{k}) = \psi^{ab}(t, \vec{k}, \vec{k}'). \quad (8.10.75)$$

The normalization of $|\Psi\rangle_2$ requires:

$$1 = \langle \Psi | \Psi \rangle_2 = \frac{1}{2} \int_{\mathbb{K}\mathbb{K}'\mathbb{K}''\mathbb{K}'''} \psi^{*ab}(t, \vec{k}, \vec{k}') \psi^{cd}(t, \vec{k}'', \vec{k}''') \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_b(\vec{k}') \hat{a}_c^\dagger(\vec{k}'') \hat{a}_d^\dagger(\vec{k}''') | 0 \rangle d^3 \vec{k} d^3 \vec{k}' d^3 \vec{k}'' d^3 \vec{k}'''. \quad (8.10.76)$$

We can simplify by sufficient use of the commutation relations:

$$\begin{aligned} \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_b(\vec{k}') \hat{a}_c^\dagger(\vec{k}'') \hat{a}_d^\dagger(\vec{k}''') | 0 \rangle &= \langle 0 | \hat{a}_a(\vec{k}) (\hat{a}_c^\dagger(\vec{k}'') \hat{a}_b(\vec{k}') + \perp_{bc}(\vec{k}') \delta(\vec{k}' - \vec{k}'')) \hat{a}_d^\dagger(\vec{k}''') | 0 \rangle \\ &= \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_c^\dagger(\vec{k}'') \hat{a}_b(\vec{k}') \hat{a}_d^\dagger(\vec{k}''') | 0 \rangle + \perp_{bc}(\vec{k}') \delta(\vec{k}' - \vec{k}'') \langle 0 | \hat{a}_a(\vec{k}) \hat{a}_d^\dagger(\vec{k}''') | 0 \rangle \\ &= \perp_{ac}(\vec{k}) \perp_{bd}(\vec{k}) \delta(\vec{k} - \vec{k}'') \delta(\vec{k}' - \vec{k}''') + \perp_{ad}(\vec{k}) \perp_{bc}(\vec{k}') \delta(\vec{k} - \vec{k}''') \delta(\vec{k}' - \vec{k}''). \end{aligned}$$

Now returning this to the normalization and using the symmetry of ψ^{ab} :

$$\int_{\mathbb{K}\mathbb{K}'} \psi_{ab}^*(t, \vec{k}, \vec{k}') \psi^{ab}(t, \vec{k}, \vec{k}') d^3\vec{k} d^3\vec{k}' = 1. \quad (8.10.77)$$

Therefore, ψ is like a normalized wavefunction on the Hilbert space $\mathbb{H}_2$ which is formed by the symmetric elements of the tensor product of the Hilbert space $\mathbb{H}_1$ with another copy of $\mathbb{H}_1$. We express this by:

$$\mathbb{H}_2 = \text{Sym}(\mathbb{H}_1 \otimes \mathbb{H}_1). \quad (8.10.78)$$

Very interestingly and very importantly, $\mathbb{H}_2$ is not simply two copies of $\mathbb{H}_1$. That is, a state of photon number two is not the same as a pair of states of photon number one. If we had two states $|\Psi\rangle_1$ and $|\Psi'\rangle_1$ of photon number one (with corresponding single particle wavefunctions $\vec{\psi}(t, \vec{k})$ and $\vec{\psi}'(t, \vec{k})$), then we could form a state of photon number two by considering the creation of a photon with wavefunction $\vec{\psi}(t, \vec{k})$ and then the creation of another photon with wavefunction $\vec{\psi}'(t, \vec{k})$. That is, we could define:

$$|\Psi\rangle_{1,1} = N \int_{\mathbb{K}\mathbb{K}'} \vec{\psi}(t, \vec{k}) \cdot \hat{a}^\dagger(\vec{k}) \vec{\psi}'(t, \vec{k}') \cdot \hat{a}^\dagger(\vec{k}') | 0 \rangle d^3\vec{k} d^3\vec{k}'. \quad (8.10.79)$$

where N is some normalization factor. This is a two photon state with two photon wavefunction:

$$\psi_{1,1}^{ab}(t, \vec{k}, \vec{k}') = \frac{N}{\sqrt{2}} (\psi^a(t, \vec{k}) \psi'^b(t, \vec{k}') + \psi'^a(t, \vec{k}) \psi^b(t, \vec{k}')). \quad (8.10.80)$$

This does not represent a generic state of $\mathbb{H}_2$. In fact, the linear combination of two states of this form with linearly independent single photon wavefunctions does not produce a state in this form. Therefore, **the state space of a two photon system is significantly larger than two independent copies of the state space of a single photon system**. If the two photon state can be written in the form of (8.10.80) it is said to be **separable**. Otherwise, it is said to be **entangled**. It should be stressed that entanglement is the generic much more common case and separability is highly restrictive.

Just like in the single photon case, under the evolution given by $\hat{H}_0$ it is possible to define a reduced effective Hamiltonian operator for $\psi^{ab}(t, \vec{k}, \vec{k}')$. Inserting (8.10.73) into the Schrödinger equation with $\hat{H}_0$ as the Hamiltonian operator we find:

$$i\hbar \frac{d|\Psi\rangle_2}{dt} = \hat{H}_0 |\Psi\rangle_2 \quad (8.10.81)$$

$$\implies i\hbar \frac{\partial \psi^{ab}(t, \vec{k}, \vec{k}')}{\partial t} = (\hbar\omega(\vec{k}) + \hbar\omega(\vec{k}')) \psi^{ab}(t, \vec{k}, \vec{k}'). \quad (8.10.82)$$

Therefore the effective two photon Hamiltonian operator $\hat{H}_2$ on $\mathbb{H}_2$ is simply $\hat{H}_2 = \hbar\omega(\vec{k}) + \hbar\omega(\vec{k}')$. It is important to notice that if the initial two photon wavefunction is separable then it remains separable under the time evolution given by $\hat{H}_2$. However, under a more general time evolution (suppose there was some sort of interaction present so that we did not reduce from $\hat{H}_0$ but instead from $\hat{H}_0$ + a term that causes the two photons to interact) even an initially separable wavefunction will become entangled dynamically. This is analogous to (and related to) how initially statistically independent quantities in statistical mechanics lose their statistical independence when they interact with each other. So, quantum field theory also *defines* two particle quantum mechanics as living on the Hilbert space of the tensor product of two Hilbert spaces of single particle quantum mechanics (the symmetrization is because as we have considered it both particles are the same species, photons).

Also just like the single photon case, it is possible to reduce operator summaries involving $|\Psi\rangle_2$ to operator summaries involving only $\psi^{ab}(t, \vec{k}, \vec{k}')$:

$$\langle \Psi | \hat{O} | \Psi \rangle_2 = \int_{\mathbb{K}^4} \sum_{hh'h''h'''} \psi_{hh'}^*(t, \vec{k}, \vec{k}') \psi_{h''h'''}(t, \vec{k}'', \vec{k}''') \langle 0 | \hat{a}_h(\vec{k}) \hat{a}_{h'}(\vec{k}') \hat{a}_{h''}^\dagger(\vec{k}'') \hat{a}_{h'''}^\dagger(\vec{k}''') | 0 \rangle d^3\vec{k} d^3\vec{k}' d^3\vec{k}'' d^3\vec{k}''' \quad (8.10.83)$$

$$= \langle \psi | \hat{O}_2 | \psi \rangle \quad (8.10.84)$$

$$\hat{\mathcal{O}}_2 = \int_{\mathbb{K}^4} \sum_{hh'h''h'''} |\vec{k}_h\rangle \otimes |\vec{k}'_{h'}\rangle \langle 0 | \hat{a}_h(\vec{k}) \hat{a}_{h'}(\vec{k}') \hat{a}_{h''}^\dagger(\vec{k}'') \hat{a}_{h'''}^\dagger(\vec{k}''') | 0 \rangle \langle \vec{k}''_{h''} | \otimes \langle \vec{k}'''_{h'''} | d^3\vec{k} d^3\vec{k}' d^3\vec{k}'' d^3\vec{k}'''. \quad (8.10.85)$$

It should be no surprise that at each photon number N it is possible to define an effective N photon wavefunction of N different wavenumbers and helicities which is fully symmetric, evolves under a Schrödinger type equation, and for which it is possible to define reduced operators for operator summaries in an N photon state. Because $\mathbb{H}_N$ is formed from a (symmetrized) tensor product of $\mathbb{H}_1$'s rather than simply a direct sum (which would be a list of N copies of $\mathbb{H}_1$), there are many independent quantities in an N photon state which have no single photon description. So, quantum field theory defines N particle quantum mechanics by a wavefunction on the tensor product space of each of the constituent particles. The full Hilbert space $\mathbb{H}$ of the quantum field theory is consists of the direct sum of the Hilbert spaces of each particle number:

$$\mathbb{H} = \mathbb{H}_1 \oplus \mathbb{H}_2 \oplus \mathbb{H}_3 \oplus \dots \quad (8.10.86)$$

as a general state in $\mathbb{H}$ can be formed by linear combinations of states of various $D, n, h, \vec{k}$ as defined in (8.10.56). Such a Hilbert space constructed out of the direct sum of individual Hilbert spaces of various particle numbers is called a Fock space.

An N photon state remains an N photon state under the free Hamiltonian operator $\hat{H}_0$. What happens if we use the full interacting $\hat{H}$ in (8.10.34)? Well, the number operator $\hat{N}$ does not commute with $\hat{H}$ so an N photon state will not remain an N photon state. The commutator of $\hat{N}$ with $\hat{H}$ gives:

$$\frac{1}{i\hbar} [\hat{N}, \hat{H}] = \int_{\mathbb{K}} \sum_h \sqrt{\frac{2}{\hbar\omega}} \text{As}(\tilde{J}_h^* \hat{a}_h) d^3\vec{k}. \quad (8.10.87)$$

The easiest way to see that the presence of a current changes the number of photons is to simply look at what $\hat{H}$ does to the vacuum state. Suppose for simplicity we consider a nonzero current but a charge density of 0, and that we choose $\Lambda = 0$ by definition. Then, suppose we begin initially in the vacuum state $|0\rangle$ at $t = 0$. The resulting initial time derivative of $|\Psi\rangle$ at $t = 0$ is given by:

$$i\hbar \left. \frac{d|\Psi\rangle}{dt} \right|_{t=0} = \hat{H}|0\rangle = \int_{\mathbb{K}} \sum_h \sqrt{\frac{\hbar}{2\omega}} \tilde{J}_h(\vec{k}) \hat{a}_h^\dagger(\vec{k}) |0\rangle d^3\vec{k} \quad (8.10.88)$$

which is a linear combination of one photon states. Therefore, an arbitrarily short application of the current will cause a transition from the vacuum state to a linear combination of the vacuum state and one photon states (and as time passes the full $|\Psi\rangle$ generically becomes a linear combination of photon states are arbitrarily high and different numbers). Therefore, **interactions cause particle production**. As well, if we began in a state with a nonzero number of photons, the current can drive transitions to state of a lower number of photons (because $\tilde{J}_h^*(\vec{k})$ multiplies the annihilation operator $\hat{a}_h(\vec{k})$ in the Hamiltonian operator).

The properties of quantum field theory we have seen in this section are not unique to electromagnetism. By theorem 8.2, the lowest order Hamiltonian of any stable classical field theory can be put into the form of creation and annihilation fields (as ψ in the Schrödinger equation satisfies the canonical Poisson brackets with ψ^* appropriate for creation and annihilation fields). So, when “quantized”, meaning that classical field theory Hamiltonian is replaced with an analogous quantum field theory Hamiltonian operator, its free Hamiltonian operator (the lowest order quadratic part) will be the Hamiltonian operator of an infinite number of quantum harmonic oscillators and it will produce the subspaces of different particle numbers seen here for electromagnetism. The inclusion of interaction terms (anything beyond that minimal harmonic oscillator Hamiltonian operator) will generically cause transitions between the subspaces of different particle numbers. Therefore, if we describe matter by quantum field theory then we can explain the experimental fact that particles can be created and destroyed through interactions. Similarly, we could explain the existence of indistinguishable particles (as they would simply be particles formed from the same set of creation and annihilation operators). Finally, we could even explain the odd statistical properties we observed earlier this section about the two electron system. If we take electrons to be particles created by an appropriate electron creation operator, then a single electron system would have a two component (due to being spin-1/2) wavefunction $\psi^a(t, \vec{x})$ but a two electron system would have a four component (due to the tensor product of two spin-1/2 spaces) wavefunction $\psi^{ab}(t, \vec{x}, \vec{x}')$. The observation that no single electron wavefunction can explain the single electron spin statistics observed in a two electron system is completely explained by the fact that $\psi^{ab}(t, \vec{x}, \vec{x}')$ will generically be entangled and so there will be no single electron wavefunction appropriate for either individual electron.

Quantum field theory explains all of the problems we found with single particle quantum mechanics. Therefore, even though we just began studying our wave theory of matter this chapter, we know what more powerful theory will replace it. The Schrödinger equation for a single electron just describes the one electron subspace of a quantum field theory in which electrons are created and annihilated by appropriate operators. This theory will recover single particle quantum mechanics on that one particle subspace but will give a richer and more fundamental theory in general. Quantum field theory is not just a formalism for electromagnetism, it is a formalism for everything. Ultimately, all species of matter of all interactions are described by interacting quantum field theory.

Perhaps surprisingly at first, many particle quantum mechanics of a fixed number and species of particles is inherently a nonrelativistic theory. This is because approximately the same energy scale determines whether a particle is relativistic as well as whether particles of that species can be created in an interaction. For a localized relativistic wave-packet, we have approximately $E \approx \sqrt{|\vec{p}|^2 + m^2}$ in Lorentz natural units. If $|\vec{p}| \ll m$ then the nonrelativistic approximation is appropriate. However, if $|\vec{p}|$ is of the same order as m or larger, a special relativistic treatment is necessary. Consequently, at energies of order $E = 2m$, relativity is important. But, an energy of $2m$ is enough energy to transition from a state with a single particle of mass m to two particles of mass m . Therefore, particle creation has the same characteristic energy scale as relativistic effects. Generically, the Hamiltonian of an interacting system will allow particle creation and annihilation and so it is not possible to maintain a fixed number of particles of fixed species when the particles have relativistic energies.

We will learn many things from quantum field theory but one of the broadest lessons which we have already seen in play is that when you have one quantum system described by a wavefunction in Hilbert space $\mathbb{H}_1$ and you bring it to interact with another quantum system described by a wavefunction in Hilbert space $\mathbb{H}_2$, then the appropriate Hilbert space of the combined system is $\mathbb{H}_1 \otimes \mathbb{H}_2$. This is reflected in the fact that the two particle Hilbert space is given by the tensor product of single particle Hilbert spaces. Or, in the fact that if there were two sets of field operators (say a field for electromagnetism and another field for the electron), then the wavefunctional Ψ would depend on the vector potential and the electron field, which as a function space is the tensor product of the space of functionals of just the vector potential and functionals of just the electron field. Thus, whenever we combine two quantum systems this tensor product structure will appear again.

Exercises

Problem 8.63: Compton Scattering. Consider a physical process in which a nonrelativistic electron and a single photon scatter off of each other but no particles are created or destroyed. This process is known as Compton scattering. Assume that in both the initial and final states the electron and photon are each sufficiently localized wave-packets for the purposes of relevant approximations.

- (a) Based on the analysis of this section, explain that when they are far from each other the electron and photon energy can be written as:

$$E_e = \sqrt{c^2|\vec{p}_e|^2 + m_e^2 c^4}, \quad E_\gamma = \hbar c |\vec{k}_\gamma|$$

where $\vec{p}_e$ is the momentum of the electron and $\vec{k}_\gamma$ is the wavenumber of the photon.

- (b) Let us work in the frame in which the electron is initially at rest. Let λ be the initial wavelength of the photon and λ' be its final wavelength. Let θ be the scattering angle of the photon, meaning the angle between its initial and final directions of propagation. Show using the conservation of energy and linear momentum that:

$$\lambda' - \lambda = \frac{2\pi\hbar}{m_e c} (1 - \cos \theta).$$

Thus, the color of light scattered off of an electron is shifted.

Problem 8.64: Statistics of a two particle system. Consider two distinguishable spin-1/2 particles that are each approximately localized well enough that we can treat each of them as at some position with some spinor describing their polarization at that position. Let $\mathbb{H}_1$ (or $\mathbb{H}_2$) be the Hilbert space of the spinor of particle 1 (or particle 2) with basis vectors $|+1\rangle$ and $|-1\rangle$ (or $|+2\rangle$ and $|-2\rangle$) indicating the spin eigenvectors aligned and anti-aligned with z -axis.

- (a) Explain that a state vector describing the interacting system of the two particles at a single time is of

the form:

$$|\psi\rangle = \psi_{++}|+1\rangle \otimes |+2\rangle + \psi_{+-}|+1\rangle \otimes |-2\rangle + \psi_{-+}|-1\rangle \otimes |+2\rangle + \psi_{--}|-1\rangle \otimes |-2\rangle.$$

- (b) Show that $|\psi\rangle$ is separable (meaning each particle has a well-defined wavefunction) if and only if:

$$\psi_{++}\psi_{--} = \psi_{+-}\psi_{-+}.$$

Show that in this case and only in this case, with $|\psi_1\rangle$ (or $|\psi_2\rangle$) the state vector of particle 1 (or particle 2):

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle. \quad (8.10.89)$$

- (c) Consider the state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+1+2\rangle + |-1-2\rangle).$$

Show that in this state the total spin of each particle is 0:

$$\vec{S}_1 = \langle \hat{S}_1 \otimes \mathbb{1}_2 \rangle = \vec{S}_2 = \langle \hat{\mathbb{1}}_1 \otimes \hat{S}_2 \rangle = 0.$$

Thus this state is consistent with the results of the experiment described in the section.

- (d) Consider a generic state vector for which $\vec{S}_1 = \vec{S}_2 = 0$. Show that (after absorbing the meaningless overall phase of the wavefunction) for real parameters θ, α, β the wavefunction can be written as:

$$|\psi\rangle = \frac{\cos\theta}{\sqrt{2}}(e^{i\alpha}|+1+2\rangle + e^{-i\alpha}|-1-2\rangle) + \frac{\sin\theta}{\sqrt{2}}(e^{i\beta}|+1-2\rangle - e^{-i\beta}|-1+2\rangle).$$

Show that the parameters θ, α, β can be determined from the values of the correlation matrix:

$$M^{ab} = \langle \psi | \hat{S}_1^a \otimes \hat{S}_2^b | \psi \rangle.$$

Show further that if this matrix is required to be rotationally invariant then up to an overall phase the wavefunction must be:

$$|\psi\rangle = \frac{|+1-2\rangle - |-1+2\rangle}{\sqrt{2}}.$$

Thus this is the only spherically symmetric state vector for the spins of two spin-1/2 particles.

Problem 8.65: Addition of Angular Momentum for Spin-1/2 Particles. Consider a quantum system of two interacting spin-1/2 particles which are well localized. Let $\mathbb{H}_1$ be the Hilbert space of the spinor of particle 1 and $\mathbb{H}_2$ be the Hilbert space of the spinor of particle 2.

- (a) Let $\vec{S}$ be the total (free) spin angular momentum of the two particles. Show that $\vec{S} = \langle \hat{S} \rangle$ where the operator $\hat{S}$ is given by:

$$\hat{S} = \hat{S}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{S}_2$$

and $\hat{S}_1$ and $\hat{S}_2$ are the spin operators of particles 1 and 2.

- (b) Show that the components of $\hat{S}$ satisfy the usual $\mathfrak{su}(2)$ commutation relations:

$$[\hat{S}_a, \hat{S}_b] = i\hbar\epsilon_{abc}\hat{S}_c.$$

Explain based on theorem 8.11 that this means the Hilbert space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ can be decomposed into a direct sum of Hilbert spaces so that on each component of the direct sum $\hat{S}$ acts in an irreducible representation of $\mathfrak{su}(2)$.

- (c) Compute how $\hat{S}_a$ acts on each of the basis states $|+1+2\rangle, |+1-2\rangle, |-1+2\rangle, |-1-2\rangle$.
 (d) From the results of the previous part, diagonalize $\hat{S}_z$ and $\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$. Show that $\mathbb{H}$ decomposes specifically as:

$$\mathbb{H} = \mathbb{H}_0 \oplus \mathbb{H}_1$$

where for states in $\mathbb{H}_0$ $\hat{S}$ acts as the irreducible spin-0 representation and for states in $\mathbb{H}_1$ $\hat{S}$ acts as the irreducible spin-1 representation. Let $|s, m\rangle$ be the eigenstates of $\hat{S}^2, \hat{S}_z$ with spin s and z -component eigenvalue $\hbar m$. Show that the eigenstates of total spin are related to the individual particle bases by:

$$|0, 0\rangle = \frac{|+1-2\rangle - |-1+2\rangle}{\sqrt{2}}, \quad |1, 1\rangle = |+1+2\rangle, \quad |1, 0\rangle = \frac{|+1-2\rangle + |-1+2\rangle}{\sqrt{2}}, \quad |1, -1\rangle = |-1-2\rangle.$$

Problem 8.66: Interaction of Spin-1/2 Particles. Consider the interaction of two localized spin-1/2 particles according to the Hamiltonian operator:

$$\hat{H} = \frac{\omega}{\hbar} \hat{S}_1 \cdot \hat{S}_2$$

for some constant ω .

- (a) Let $\hat{S}$ be the generating operator of the total spin of the two particles. Show that $\hat{H}$ can be rewritten as:

$$\hat{H} = \frac{\omega}{2\hbar} (\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2).$$

- (b) Show that the $|s, m\rangle$ basis constructed in the previous question diagonalizes this Hamiltonian operator and show that the eigenvalues are:

$$\hat{H}|s, m\rangle = \frac{\hbar\omega}{4} (2s^2 + 2s - 3) |s, m\rangle.$$

Problem 8.67: ★ Addition of Angular Momentum in general. Consider two quantum systems, the first in an irreducible representation of angular momentum j_1 and the second in an irreducible representation of angular momentum j_2 . Label a basis of states of system 1 by $|m_1\rangle$, where $\hbar m_1$ is the eigenvalue of $\hat{J}_{1z}$ and of system 2 by $|m_2\rangle$, where $\hbar m_2$ is the eigenvalue of $\hat{J}_{2z}$.

- (a) Let $\vec{J}$ be the total angular momentum of the two systems. Show that $\vec{J} = \langle \vec{J} \rangle$ where the operator $\hat{J}$ is given by:

$$\hat{J} = \hat{J}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{J}_2$$

and $\hat{J}_1$ and $\hat{J}_2$ are the angular momentum operators of the two systems.

- (b) Show that the components of $\hat{J}$ satisfy the usual $\mathfrak{su}(2)$ commutation relations:

$$[\hat{J}_a, \hat{J}_b] = i\hbar \epsilon_{abc} \hat{J}_c.$$

Explain based on theorem 8.11 that this means the Hilbert space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ can be decomposed into a direct sum of Hilbert spaces so that on each component of the direct sum $\hat{J}$ acts in an irreducible representation of $\mathfrak{su}(2)$.

- (c) Let $|j, m\rangle$ be a state in total angular momentum representation j with $\hat{J}_z$ eigenvalue $\hbar m$. Explain that there exist some coefficients $C_{m_1 m_2}^{jm}$ so that:

$$|j, m\rangle = \sum_{m_1 m_2} C_{m_1 m_2}^{jm} |m_1\rangle \otimes |m_2\rangle.$$

These coefficients, known as Clebsch-Gordan coefficients do also depend on j_1 and j_2 , but because those are fixed in this question we suppress the visibility of that dependence to keep notation condensed.

- (d) Define the operators $\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$ and compute $\hat{J}_{\pm}|j, m\rangle$ following the calculations of section 8.7. Show that the Clebsch-Gordan coefficients satisfy the recurrence relation:

$$\begin{aligned} \sqrt{j(j+1) - m(m+1)} C_{m_1 m_2}^{j(m+1)} &= \sqrt{j_1(j_1+1) - m_1(m_1+1)} C_{(m_1+1)m_2}^{jm} \\ &+ \sqrt{j_2(j_2+1) - m_2(m_2+1)} C_{m_1(m_2+1)}^{jm}. \end{aligned}$$

- (e) By using the definition of $\hat{S}_z$, show that $C_{m_1 m_2}^{jm} = 0$ unless $m = m_1 + m_2$. Consequently, show that the maximum value of j is $j_1 + j_2$. Then, show that the dimension of the direct sum of Hilbert spaces of irreducible representations of angular momenta $|j_1 - j_2|$, $|j_1 - j_2| + 1$, ..., $j_1 + j_2$ equals the dimension of the tensor product Hilbert space of $\mathbb{H}_1 \otimes \mathbb{H}_2$.

- (f) For simplicity, assume we have labeled the systems so that $j_1 \geq j_2$. Explain that using $\hat{J}_-$, if we know all of the coefficients for $C_{m_1(j-m_1)}^{jj}$ we can determine all of $C_{m_1 m_2}^{jm}$. Then, using the recurrence relation, show that:

$$C_{(m_1-1)(j-m_1+1)}^{jj} = -\sqrt{\frac{j_2(j_2+1) - (j-m_1)(j-m_1+1)}{j_1(j_1+1) - m_1(m_1-1)}} C_{m_1(j-m_1)}^{jj}.$$

Then, solve this recurrence relation and normalize $|j, j\rangle$ with the convention that $(\langle j_1| \otimes \langle j-j_1|)|jj\rangle$ be

real and greater than 0. Use this to show that the Clebsch-Gordan coefficients for $m \geq 0$ are given by:

$$C_{m_1 m_2}^{jm} = \delta_{m_1+m_2}^m \sqrt{\frac{(2j+1)(j+j_1-j_2)!(j-j_1+j_2)!(j_1+j_2-j)!}{(j_1+j_2+j+1)!}} \\ \times \sqrt{(j+m)!(j-m)!(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!} \\ \times \sum_k \frac{(-1)^k}{k!(j_1+j_2-j-k)!(j_1-m_1-k)!(j_2+m_2-k)!(j-j_2+m_1+k)!(j-j_1-m_2+k)!}$$

where the range of k in the sum is over all integers for which the arguments of all factorials involved are nonnegative.

- (g) Show that the coefficients for $m < 0$ can be determined by:

$$C_{m_1 m_2}^{jm} = (-1)^{j-j_1-j_2} C_{(-m_1)(-m_2)}^{j(-m)}.$$

In a general context, we will write $C_{j_1 m_1 j_2 m_2}^{jm}$ for the Clebsch-Gordan coefficients. As well, for symmetry convenience, it is typical to define the coefficients for $j_1 < j_2$ by:

$$C_{j_1 m_1 j_2 m_2}^{jm} = (-1)^{j-j_1-j_2} C_{j_2 m_2 j_1 m_1}^{jm}.$$

- (h) Let $\mathbb{H}_j$ indicate the Hilbert space of states in the irreducible representation of angular momentum j . Show that all of the results of this question together imply:

$$\mathbb{H}_{j_1} \otimes \mathbb{H}_{j_2} = \mathbb{H}_{|j_1-j_2|} \oplus \mathbb{H}_{|j_1-j_2|+1} \oplus \dots \oplus \mathbb{H}_{j_1+j_2-1} \oplus \mathbb{H}_{j_1+j_2}.$$

The collective results of this question are known as the Clebsch-Gordan theorem.

Problem 8.68: Wigner-Eckart Theorem. Let $\hat{R}(\vec{\theta})$ be a generic 3x3 rotation matrix, with components R^a_b . As we have previously defined, a rank N rotational tensor T is an object with components $T^{a_1 \dots a_N}$ which under a rotation transform according to:

$$T'^{a_1 \dots a_N} = R^{a_1}_{b_1} \dots R^{a_N}_{b_N} T^{b_1 \dots b_N}.$$

- (a) Let $\mathbb{V}$ be the vector space of 3 dimensional vectors. Explain why the vector space of rank N rotational tensors is simply the N fold tensor product of $\mathbb{V}$ with itself, i.e. $\mathbb{V} \otimes \mathbb{V} \otimes \dots \otimes \mathbb{V}$ with N factors of $\mathbb{V}$.
 (b) Explain why $\mathbb{V}$ is exactly the Hilbert space of the irreducible angular momentum 1 representation of $\text{su}(2)$.
 (c) Consider the irreducible angular momentum j representation of $\text{su}(2)$. Define the matrix $D_{m'm}^j(\vec{\theta})$, known as Wigner's D -matrix by:

$$D_{m'm}^j(\vec{\theta}) = \langle j, m' | e^{-\frac{i}{\hbar} \vec{\theta} \cdot \hat{J}} | j, m \rangle.$$

Explain how $D_{m'm}^j$ completely characterizes the j angular momentum representation of rotations. Explicit formulas exist for $D_{m'm}^j$, but they are extremely complicated. Let $|v\rangle$ be a state vector in the Hilbert space of irreducible angular momentum j representation of $\text{su}(2)$ with components v_m so that:

$$|v\rangle = \sum_{m=-j}^j v_m |j, m\rangle.$$

Show that under a rotation the components of $|v\rangle$ transform as:

$$v'_m = \sum_{m'=-j}^j D_{mm'}^j v_{m'}.$$

- (d) Using the Clebsch-Gordan theorem, explain why the vector space of rank N rotational tensors is not an irreducible representation of angular momentum and in fact actually contains a tower of representations of different angular momenta. Show that there exists a subspace of the vector space of rank N rotational tensors which is an irreducible representation of $\text{su}(2)$ with angular momentum N . A rank N tensor which is in this subspace is called a rank N spherical tensor.
 (e) Let $T^{(N)}$ be a rank N spherical tensor. Explain that there exist $2N+1$ rank N spherical tensors $M_k^{(N)}$ with the label k running from $-N$ to N which form a basis for such tensors and components $T_k^{(N)}$ so

that $T^{(N)}$ can be written as:

$$T^{(N)} = \sum_{k=-N}^N T_k^{(N)} M_k^{(N)}$$

and so that under a rotation the $T_k^{(N)}$ transform like:

$$T_k'^{(N)} = \sum_{m=-N}^N D_{km}^N T_m^{(N)}.$$

- (f) In quantum mechanics, a spherical tensor operator of rank N is an operator $\hat{T}^{(N)}$ so that $\langle \hat{T}^{(N)} \rangle$ is a spherical tensor of rank N . Show that this requirement implies:

$$[\hat{T}_k^{(N)}, \hat{J}_a] = \sum_{m=-j}^j \langle N, k | \hat{J}_a | N, m \rangle \hat{T}_m^{(N)}.$$

Equivalently, show that this requires:

$$[\hat{T}_k^{(N)}, \hat{J}_{\pm}] = \hbar \sqrt{N(N+1) - k(k \mp 1)} \hat{T}_{k \mp 1}^{(N)}, \quad [\hat{T}_k^{(N)}, \hat{J}_z] = \hbar k \hat{T}_k^{(N)}.$$

- (g) From the above commutators, show that the matrix elements of components of a spherical tensor operator satisfy $\langle j, m | \hat{T}_k^{(N)} | j', m' \rangle = 0$ unless $m' = m + k$ and also satisfy the recurrence relation:

$$\begin{aligned} \sqrt{j'(j'+1) - m'(m' \pm 1)} \langle j, m | \hat{T}_k^{(N)} | j', m' \pm 1 \rangle &= \sqrt{j(j+1) - m(m \mp 1)} \langle j, m \mp 1 | \hat{T}_k^{(N)} | j', m' \rangle \\ &+ \sqrt{N(N+1) - k(k \mp 1)} \langle j, m | \hat{T}_{k \mp 1}^{(N)} | j', m' \rangle. \end{aligned}$$

- (h) Show that the matrix elements of a spherical tensor operator satisfy all of the same conditions as the Clebsch-Gordan coefficients except for the normalization condition, and thus based on the Clebsch-Gordan theorem show that the matrix elements of the components of a spherical tensor operator satisfy:

$$\langle j, m | \hat{T}_k^{(N)} | j', m' \rangle = T_{jj'}^{(N)} C_{jmNk}^{j'm'}$$

where $C_{j_1 m_1 j_2 m_2}^{j m}$ are the Clebsch-Gordan coefficients and $T_{jj'}^{(N)}$ are called the Wigner-Eckart reduced matrix elements of $\hat{T}^{(N)}$. The fact that the matrix elements of spherical tensor operators take this simple factorized form is known as the Wigner-Eckart theorem.

8.11 Summary and Additional Reading

Important homework questions from this chapter (highly recommended to do them):

- **Problem 8.3: Silver Bullet Solution to the Schrödinger equation** and
- **Problem 8.7: The Time Evolution Operator** establish the basics of how to solve the time evolution of a general quantum mechanical system.
- **Problem 8.9: Ehrenfest's Theorem and the Quantum Noether Theorem** derives the special form that Noether's theorem takes in quantum mechanics.
- **Problem 8.10: Active vs. Passive Picture** introduces the active description of quantum mechanics, in which the state vector of the system is constant and all of the time evolution is shuffled into the operators and shows that it is equivalent to the more typical passive picture, in which the state vector is dynamical and satisfies the Schrödinger equation.
- **Problem 8.11: Commutators becoming derivatives** shows how commutators of an operator with a variable effectively differentiates that operator with respect to the conjugate to that variable.
- **Problem 8.12: Restoring factors of $\hbar$** explains how to remove and how to restore factors of $\hbar$ when going between natural units in which $\hbar = 1$ and unnatural unit systems in which it is not.
- **Problem 8.20: The Baker–Campbell–Hausdorff formula** derives the extent to which the operators in the exponents of a product of operator exponentials fail to add, which turns out to be an extremely useful formula for calculations in quantum mechanics.
- **Problem 8.22: First Look at Coherent States** introduces coherent states, which are states that are “maximally classical”, in the sense of being simultaneously as localized as possible in both position and momentum space.
- **Problem 8.25: Double-Slit Experiment Revisited** explains the experimental results of the high-rate double slit experiment in terms of the wavefunction, resolving the experimental mystery noticed in Chapter 4.
- **Problem 8.30: The Aharonov-Bohm Effect** derives experimental consequences which involve the direct interaction of the wavefunction with the vector potential, not simply its gauge invariant byproducts, thus demonstrating unambiguously that the vector potential is genuinely physical.
- **Problem 8.31: Generator of Gauge Transformations** derives the canonical structure of gauge transformations in the interacting theory of a single electrically charged Schrödinger particle with electromagnetism.
- **Problem 8.32: The Quantum Harmonic Oscillator (QHOI) - Creation and Annihilation Operators** and
- **Problem 8.33: QHOII - Moment Evolution Equations** and
- **Problem 8.34: QHOIII - Evolution of Coherent States and Evolutor** and
- **Problem 8.35: QHOIV - Driven Oscillations** and
- **Problem 8.36: QHOV - Multivariable Oscillator** derive all of the basic properties of quantum harmonic oscillators, which are one of the most important and commonly recurring quantum systems.
- **Problem 8.45: Solving the Hydrogen Atom** shows how the spectrum of the hydrogen atom is directly determined by the Schrödinger equation, in excellent agreement with experiment.
- **Problem 8.46: Atomic Spectral Lines and Measuring $\hbar$** shows how the atomic spectra can be measured experimentally and how the placement of spectral lines can be used to infer the value of $\hbar$ in unnatural units or calibrate the units of the action (so that $\hbar = 1$) in natural units.
- **Problem 8.47: The Photoelectric Effect** gives another way of measuring $\hbar$ and derives the photoelectric effect, which is an experimental phenomenon that is not explained by classical mechanics.
- **Problem 8.48: The Fine-Structure Constant** introduces the fine-structure constant α , which is a fundamental unitless physical constant that determines the strength of the electromagnetic interaction. From α , we defined the elementary electric charge e .
- **Problem 8.50: The Stern-Gerlach Experiment** describes and explains how the spin of electrons can be measured and how the presence of an inhomogeneous magnetic field prevents the classical limit from being a good approximation for the dynamics of an electron wave-packet.
- **Problem 8.58: Rutherford Scattering Revisited** shows that the scattering of one charged particle off of another leads to exactly the same differential cross section in both classical mechanics and quantum mechanics.
- **Problem 8.67: Addition of Angular Momentum in general** defines the Clebsch-Gordan coefficients and explains how to construct the total angular momentum Hilbert space when two different

systems in their own angular momentum representations are brought together into one system in quantum mechanics.

In this chapter we developed the theory of single particle quantum mechanics. This theory replaced the description of matter by point-particles by a wave description, giving us a classical field theory for a single particle. That classical field, the wavefunction, satisfies the Schrödinger equation. Because that classical field is not perfectly localized, it has finite interactions with electromagnetism, fixing the problem of point particle divergences. In section 8.1, we introduced the Dirac equation and the concept of a Hilbert space to help us cast classical field theory in the language of linear algebra. This perspective is extremely useful for clear notation and thinking, as well as performing calculations. In section 8.2, we showed that a generic stable lowest order classical field theory when put into the right coordinates simply becomes the Schrödinger equation with some self-adjoint Hamiltonian operator. We also introduced $\hbar$ as a constant that relates the energy of normalized waves to their angular frequency, we discussed the relationship between Hermiticity and self-adjointness, we proved the spectral theorem, and we showed that projective intensities (in many sources called “quantum probabilities”) are the adiabatic invariants of quantum mechanics. In section 8.3 we proved Wigner’s theorem, which gives the form of canonical transformations in quantum mechanics. Specifically, we showed that time nonreversing canonical transformations are implemented by a unitary transformation and time reversing canonical transformations are implemented by a unitary transformation and a complex conjugation. In section 8.4 we showed the form that continuous transformations and the Poisson bracket take in quantum mechanics. We also showed how quantum tomography can be used to reconstruct the entire wavefunction up to an overall phase from operator summaries. In section 8.5 we found that position and momentum operators as the natural quantities which track the center of mass of the wavefunction and the total linear momentum of the wavefunction respectively. We also showed some basic mathematical properties of operator spreads, such as the uncertainty theorem, we showed the basics of how the classical limit arises and how from it we can infer what is the meaning and purposes of $\hbar$, and we introduced the basics of the Born rule although at this time without explanation. In section 8.6 we finally found the specific Hamiltonian operator appropriate for a nonspinning nonrelativistic quantum particle interacting with electromagnetism. We also studied the geometry of gauge transformations and found that the vector potential is a deeply geometric quantity that provides the connection (analogously to the Christoffel symbols) on the internal complex space on which the wavefunction lives; the electric and magnetic fields are then the curvature of that space. In section 8.7 we derived the basic facts of the quantum theory of angular momentum. We found that the group $SU(2)$ is the appropriate group for understanding how rotations act on the wavefunction. We classified all irreducible representations of $SU(2)$, computed explicit forms of the angular momentum operators in each representation, and found explicit formulas for the spherical harmonics. In section 8.8 we found the specific Hamiltonian operator appropriate for a spin-1/2 nonrelativistic quantum particle interacting with electromagnetism. In section 8.9 we derived the basics of the theory of scattering in quantum systems. Because the time scales of quantum evolution tend to be extremely short compared to our experimental resolution, scattering theory is fundamental to our experimental access to quantum systems. In section 8.10 we discussed various experimental troubles faced by naive applications of single particle quantum mechanics and we found that these troubles as well as our previous confusion around black-body radiation can all be explained by quantum field theory. Whereas in single particle quantum mechanics there are operators ($\hat{x}$ and $\hat{p}$) whose summaries in the classical limit become the classical variables of a single particle, in quantum field theory there are operators (which are fields) whose summaries in the classical limit become the classical fields of a classical field theory. The deep properties of quantum field theory will be the subject of the rest of our studies.

This chapter is by no means a complete treatment of essential topics in single particle quantum mechanics. Refer to [3], [69], [92] [98], [108], [127] for general treatments. For more on single particle quantum mechanics as a classical field theory, refer to [45]. For more on the interpretative elements on quantum mechanics (which we will also discuss thoroughly in the next chapter), refer to [76]. There are many more specialized and technical topics in basic quantum mechanics not covered much in any of these. Because nonrelativistic quantum mechanics of one or a few particles remains actively important for scientific research and is so young as a discipline compared to classical mechanics, there are far too many specialized applications for any one book to cover.

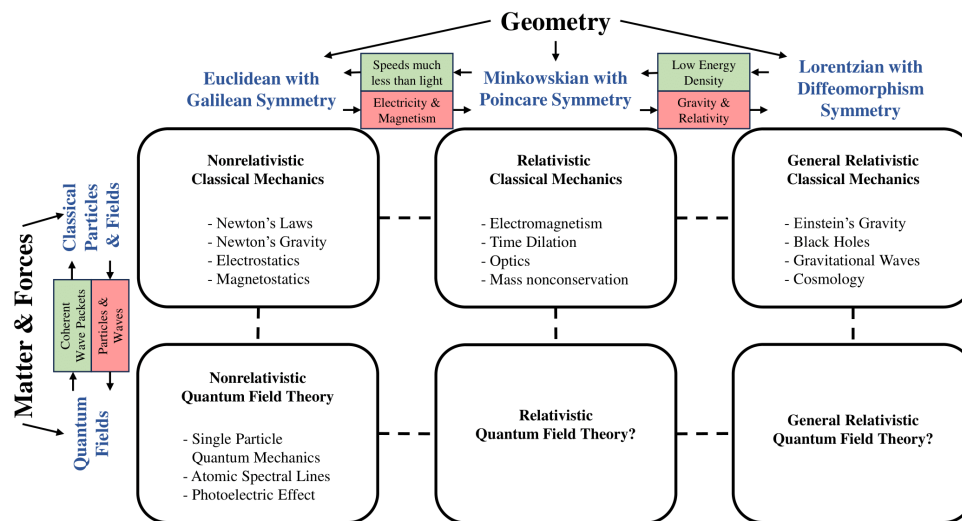


Figure 8.1: Our perspective on physics as of the end of this chapter. Replacing our point particle theory of matter with a wave theory has completely solved the problem of point particle divergences. However, so far only did so using Galilean symmetry and naturally must next work on combining Lorentz symmetry with our wave theory of matter. As well, we found that our wave theory of matter was not quite right for the statistics of multiple particles and that quantum field theory, which we haven't yet studied, is its necessary generalization to get these statistics right.

Chapter 9

Quantum Mechanics in General

Ever since the advent of modern quantum mechanics in the late 1920's, the idea has been prevalent that the classical laws of probability cease, in some sense, to be valid in the new theory. More or less explicit statements to this effect have been made in large number and by many of the most eminent workers in the new physics. Some authors have even gone farther and stated that the formal structure of logic must be altered to conform to the terms of reference of quantum physics. Such a thesis is surprising, to say the least, to anyone holding more or less conventional views regarding the positions of logic, probability, and experimental science: many of us have been apt – perhaps too naively – to assume that experiments can lead to conclusions only when worked up by means of logic and probability, whose laws seem to be on a different level from those of physical science. The primary object of this presentation is to show that the thesis in question is entirely without validity and is the product of a confused view of the laws of probability.

– Bernard Koopman [58]

Something [is] rotten in the eigenstate of Denmark.

– Adam Becker [5]

Niels Bohr brain-washed a whole generation of physicists into believing that the problem had been solved fifty years ago.

– Murray Gell-Mann [47]

We discovered at the end of the last chapter that quantum mechanics is a more general concept than simply replacing our point particle theory of matter with a wave theory. In this chapter we will understand that quantum mechanics is actually a second branch of possibilities that we sped past all the way back in chapter 1, though I did warn you. In order to get there, we need to go all the way back and remember our line of thinking in section 1.3. This second branch of possibilities combined with the principles of locality and relativity will lead naturally to quantum field theory, which is the formalism that is at the foundation of our status quo understanding of physics.

9.1 Why Quantum Mechanics?

9.1.1 Quantum Ex Nihilo

There is another way of arriving at exactly the same Lagrangian and Hamiltonian as in section 8.2 but by apparently very different thinking. In section 1.3 we found that all of our dynamical variables and transformation generators can be encoded in linear operators (for example an operator $\hat{F}$) so that under the transformation generated by some other generator (say $\hat{G}$, with transformation parameter β):

$$\frac{d\hat{F}}{d\beta} = [\hat{G}, \hat{F}]. \quad (9.1.1)$$

In section 1.4 we found a representation of this formalism through real valued variables and functions known as the Poisson representation. However, this is not the only possible representation. In fact, it should be clear that the Poisson representation is not a faithful representation of the linear operators. In particular, if the linear operators $\hat{F}$ and $\hat{G}$ do not commute, then $\hat{F}\hat{G}$ and $\hat{G}\hat{F}$ are of course different objects while if $\hat{F}$ and $\hat{G}$ are represented by phase space functions f and g in the Poisson representation, then the products fg and gf are the same as they are simply real valued functions. We will prove more directly and explicitly later that there is no bijection between our linear operators and real valued functions that is compatible with the Lie bracket. In the rest of this section we will discuss a faithful representation of the objects of section 1.3.

The generators as written in (9.1.1) are normalized the way mathematicians typically normalize them¹. However, for physics that normalization is inconvenient. Let us label the generators as mathematicians normalize them with a subscript L , short for Lie:

$$\frac{d\hat{F}_L}{d\beta} = [\hat{G}_L, \hat{F}_L]. \quad (9.1.2)$$

The coordinate operators $\hat{Q}^a$ of section 1.3 were defined so that when acting on a function of the coordinates at a particular coordinate value they simply multiply by the coordinate value. Suppose we have d coordinate operators $\hat{Q}^1, \dots, \hat{Q}^d$. Due to the commutativity of multiplication, these coordinate operators automatically commute with each other and due to the use of real coordinates, these coordinate operators are automatically self-adjoint. Then, consider a Dirac delta centered at coordinates Q^a , which as usual we write as a vector using the Dirac notation $|Q\rangle$. Then, at the coordinate center $\hat{Q}^a|Q\rangle = Q^a|Q\rangle$ because the coordinate operators multiply the coordinate value by definition and away from the coordinate center the Dirac delta vanishes and so both sides of this equation evaluate to 0. Thus:

$$\hat{Q}^a|Q\rangle = Q^a|Q\rangle, \quad [\hat{Q}^a, \hat{Q}^b] = 0, \quad \hat{Q}^{a\dagger} = \hat{Q}^a. \quad (9.1.3)$$

Hence these coordinate operators $\hat{Q}^a$ are exactly like the $\hat{x}^a$ operators found in the previous chapter. Automatically then we can recycle the identities:

$$\langle Q|Q'\rangle = \delta(Q - Q'), \quad \int |Q\rangle\langle Q| d^d Q = \mathbb{1}, \quad \hat{Q}^a = \int Q^a |Q\rangle\langle Q| d^d Q. \quad (9.1.4)$$

If $|\Psi\rangle$ is a function of Q represented as a vector, then we can also recycle:

$$|\Psi\rangle = \int \Psi(Q) |Q\rangle d^d Q, \quad \Psi(Q) = \langle Q|\Psi\rangle. \quad (9.1.5)$$

The momentum operators of section 1.3 are generators and so we write them as $\hat{P}_{La}$ and they were defined so that they differentiate functions of the coordinates with respect to the appropriate coordinate. Written in the Dirac notation, this is simply:

$$\langle Q|\hat{P}_{La}|\Psi\rangle = \frac{\partial \Psi(Q)}{\partial Q^a}. \quad (9.1.6)$$

Thus the $\hat{P}_{La}$ are not quite exactly like the $\hat{p}_a$ operators of the previous chapter. As defined, $\hat{P}_{La}$ is anti-self-adjoint as it is equal to the negative of its own adjoint (the derivative picks up a negative sign under integration by parts). If we include an i in the definition of the momentum operators, then like the $\hat{p}_a$ of the previous chapter they will be self-adjoint. Thus, we introduce the physicist normalization (which we write without a subscript) by:

$$\hat{G}_a = -i\hbar \hat{G}_{La} \quad (9.1.7)$$

for a generic transformation generator $\hat{G}_a$. The factor of $\hbar$ is there to control units of the action. The momentum conjugate to a coordinate Q has units of action divided by the units of Q while the mathematician's momentum operator $\hat{P}_{La}$ has units of $\frac{1}{Q}$, thus effectively being a convention in which the action is unitless. The choice of the value of $\hbar$ as some specific real number implicitly defines the units of the action or conversely so. So, we write the momentum operators $\hat{P}_a$ so that:

$$\langle Q|\hat{P}_a|\Psi\rangle = -i\hbar \frac{\partial \Psi(Q)}{\partial Q^a}. \quad (9.1.8)$$

¹There are possible convention differences by a minus sign between sources.

From this we can automatically recycle:

$$\hat{P}_a = \int |Q\rangle \left(-i\hbar \frac{\partial}{\partial Q^a} \right) \langle Q| d^d Q, \quad [\hat{Q}^a, \hat{P}_b] = i\hbar \delta_b^a \mathbb{1}, \quad [\hat{P}_a, \hat{P}_b] = 0, \quad \hat{P}_a^\dagger = \hat{P}_a. \quad (9.1.9)$$

As well, we already know we can diagonalize the $\hat{P}_a$ operators and how to do so:

$$|P\rangle = \int \frac{e^{\frac{i}{\hbar} Q^a P_a}}{(2\pi\hbar)^{\frac{d}{2}}} |Q\rangle d^d Q, \quad \langle P|P'\rangle = \delta(P - P'), \quad \int |P\rangle \langle P| d^d P = \mathbb{1}, \quad \hat{P}_a = \int P_a |P\rangle \langle P| d^d P. \quad (9.1.10)$$

Using the physicist normalization for generators, equation (9.1.1) becomes:

$$\frac{d\hat{F}}{d\beta} = \frac{1}{i\hbar} [\hat{F}, \hat{G}]. \quad (9.1.11)$$

So, we can reorganize the generating operators of section 1.3 into a form that looks suggestive and familiar to quantum mechanics, but that isn't exactly the same as arriving at quantum mechanics. The next step is where the real magic happens. So far we have been discussing these abstract mathematical objects of linear operators. Experimenters do not read out linear operators from their equipment; they measure numbers. Therefore, somehow these linear operators have to map somehow to a number that represents the physical property the experimenter desires to measure. That is, there must be some map from our operators into an appropriate space of numbers (we will take that space to be the complex numbers $\mathbb{C}$, as they contain the usual real numbers and sometimes provide convenient additional structure) with the output numerical value of this map meant to represent the experimentally relevant number assigned to the linear operator under consideration. Let the map from the operators into complex numbers be denoted $\langle \cdot \rangle$ so that $\langle \hat{F} \rangle$ is a complex number. We will call $\langle \hat{F} \rangle$ the summary of $\hat{F}$. This notation obviously references the operator summary notation used in the last chapter, but pretend you don't know what an operator summary means in that way for the time being.

Many of our quantities of interest are vectors in some vector space (such as literal spatial vectors or 4-vectors, higher rank tensors, et cetera) and so we express them as linear combinations of basis vectors in whatever appropriate space. The summary map maps operators into complex numbers. So, the natural definition for a summary of a vector of operators is to make it the vector whose components are the summary of each of those respective operators. That is:

$$\hat{\vec{F}} = \hat{F}^a \vec{t}_a \implies \langle \hat{\vec{F}} \rangle \stackrel{\text{def}}{=} \langle \hat{F}^a \rangle \vec{t}_a. \quad (9.1.12)$$

Under a change of basis for some real coefficients M^a_b :

$$\vec{t}_a = M^b_a \vec{t}'_b. \quad (9.1.13)$$

$$\hat{\vec{F}} = \hat{F}^a \vec{t}_a = \hat{F}^b M^a_b \vec{t}'_a = \hat{F}'^a \vec{t}'_a \quad (9.1.14)$$

$$\implies \hat{F}'^a = \hat{F}^b M^a_b. \quad (9.1.15)$$

A vector in a vector space is the same object whatever basis is used. Therefore, to respect the vector space structure, we need the summary of a vector to be independent of the basis chosen. Thus:

$$\langle \hat{\vec{F}} \rangle = \langle \hat{F}^a \rangle \vec{t}_a \stackrel{!}{=} \langle \hat{F}'^a \rangle \vec{t}'_a \quad (9.1.16)$$

$$\implies \langle \hat{F}'^a \rangle \vec{t}'_a = \langle \hat{F}^a \rangle \vec{t}_a \quad (9.1.17)$$

$$\implies \langle \hat{F}^b M^a_b \rangle \vec{t}'_a = \langle \hat{F}^b \rangle M^a_b \vec{t}'_a \quad (9.1.18)$$

$$\implies \langle \hat{F}^b M^a_b \rangle = \langle \hat{F}^b \rangle M^a_b. \quad (9.1.19)$$

This must be true for all change of basis coefficients M^a_b . Component by component this is just the linearity property. That is, in order for the summary map to respect the basis independence of vectors, it must be linear over complex numbers:

$$\langle a\hat{F} + b\hat{G} \rangle = a\langle \hat{F} \rangle + b\langle \hat{G} \rangle. \quad (9.1.20)$$

Thus, we will require linearity of the summary map going forward.

The linear operators which we are taking the summary of act on some complex vector space (for example, on some appropriate set of functions of the coordinates Q). Let us call the associated vector space $\mathbb{H}$. We can equip that vector space with a complex inner product (for functions on the coordinates, the usual integral expression for the inner product of complex valued functions). Then, with that inner product, we can develop

an orthonormal basis of vectors $|n\rangle$ for $\mathbb{H}$ with usual adjoint vectors $\langle n|$. Due to our desire to be able to take limits in physics, we require $\mathbb{H}$ to be complete, and thus we have that $\mathbb{H}$ is a Hilbert space. Then, the orthonormality and completeness relations read:

$$\langle n|m\rangle = \delta_{nm}, \quad \sum_n |n\rangle\langle n| = \mathbb{1}. \quad (9.1.21)$$

As well, for any operator $\hat{F}$ we can define the matrix elements of that operator by:

$$F_{nm} \stackrel{\text{def}}{=} \langle n|\hat{F}|m\rangle. \quad (9.1.22)$$

Then, any operator may be expressed as:

$$\hat{F} = \sum_n |n\rangle\langle n|\hat{F} \sum_m |m\rangle\langle m| = \sum_{nm} |n\rangle\langle n|\hat{F}|m\rangle\langle m| = \sum_{nm} F_{nm} |n\rangle\langle m|. \quad (9.1.23)$$

It is useful to define the trace of an operator by:

$$\text{Tr}(\hat{F}) \stackrel{\text{def}}{=} \sum_n \langle n|\hat{F}|n\rangle = \sum_n F_{nn}. \quad (9.1.24)$$

Naively it appears that the trace is a basis dependent quantity. However, consider a new basis $|n'\rangle$ which is also orthonormal and complete. Then, this basis must have some expansion in terms of the old basis elements:

$$|n'\rangle = \sum_m C_{n'm} |m\rangle. \quad (9.1.25)$$

Define the change of basis operator $\hat{U}$ so that it has matrix elements $C_{n'm}$:

$$U_{mn} = \langle m|\hat{U}|n\rangle = C_{n'm} \quad (9.1.26)$$

$$\implies |n'\rangle = \sum_m |m\rangle\langle m|\hat{U}|n\rangle = \mathbb{1}\hat{U}|n\rangle = \hat{U}|n\rangle. \quad (9.1.27)$$

Then the orthonormality condition becomes:

$$\langle m'|n'\rangle = \langle m|\hat{U}^\dagger\hat{U}|n\rangle = \delta_{mn} \stackrel{!}{=} \langle m|n\rangle \quad (9.1.28)$$

$$\implies \langle m|(\hat{U}^\dagger\hat{U} - \mathbb{1})|n\rangle = 0 \quad (9.1.29)$$

$$\implies \sum_{mn} |m\rangle\langle m|(\hat{U}^\dagger\hat{U} - \mathbb{1})|n\rangle\langle n| = 0 \quad (9.1.30)$$

$$\implies \hat{U}^\dagger\hat{U} = \mathbb{1}. \quad (9.1.31)$$

The completeness condition becomes:

$$\sum_n |n'\rangle\langle n'| \stackrel{!}{=} \mathbb{1} \quad (9.1.32)$$

$$\implies \sum_n \hat{U}|n\rangle\langle n|\hat{U}^\dagger = \mathbb{1} \quad (9.1.33)$$

$$\implies \hat{U}\hat{U}^\dagger = \mathbb{1}. \quad (9.1.34)$$

Hence, $\hat{U}$ must be a unitary operator. For such a change of basis, the transformed trace is then:

$$\text{Tr}(\hat{F})' = \sum_n \langle n'|\hat{F}|n'\rangle = \sum_n \langle n|\hat{U}^\dagger\hat{F}\hat{U}|n\rangle = \sum_{nm} \langle n|\hat{U}^\dagger|m\rangle\langle m|\hat{F}\hat{U}|n\rangle \quad (9.1.35)$$

$$= \sum_{nm} \langle m|\hat{F}\hat{U}|n\rangle\langle n|\hat{U}^\dagger|m\rangle = \sum_m \langle m|\hat{F}\hat{U}\mathbb{1}\hat{U}^\dagger|m\rangle = \sum_n \langle n|\hat{F}|n\rangle = \text{Tr}(\hat{F}). \quad (9.1.36)$$

So, the trace of an operator is in fact basis independent. There is a subtlety here. In an infinite dimensional vector space, change of basis and the trace both involve infinite series which may or may not converge or may only converge conditionally. Because of this, there may be ways to rearrange the series by infinite rearrangements so that the result of the trace operation appears basis dependent. If it is possible to do so with an operator, then there exists a basis in which the trace operation would give an infinite sum and there exist rearrangements of the series which can reach infinitely many different values. Because of this, for such operators we say the trace is not well-defined. We only are allowed to properly apply the trace to so-called trace-class operators, which are operators for which there are no convergence issues with these series/integrals. Going forward if we take the trace of an operator, we will always be assuming it is trace-class.

Another important property of the trace is cyclicity. For any three operators $\hat{A}, \hat{B}, \hat{C}$:

$$\begin{aligned}\text{Tr}(\hat{A}\hat{B}\hat{C}) &= \sum_n \langle n | \hat{A}\hat{B}\hat{C} | n \rangle = \sum_{nml} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | l \rangle \langle l | \hat{C} | n \rangle = \sum_{nml} \langle l | \hat{C} | n \rangle \langle n | \hat{A} | m \rangle \langle m | \hat{B} | l \rangle \\ &= \sum_{nml} \langle n | \hat{C} | m \rangle \langle m | \hat{A} | l \rangle \langle l | \hat{B} | n \rangle = \text{Tr}(\hat{C}\hat{A}\hat{B}).\end{aligned}\quad (9.1.37)$$

Due to (9.1.20), $\langle \hat{F} \rangle$ is a linear functional of $\hat{F}$. Because $\hat{F}$ depends linearly on its matrix elements and $\langle \hat{F} \rangle$ depends linearly on $\hat{F}$, $\langle \hat{F} \rangle$ also depends linearly on the matrix elements of $\hat{F}$. So, for some coefficients ρ^{nm} which are independent of $\hat{F}$:

$$\langle \hat{F} \rangle = \sum_{nm} \rho^{nm} F_{mn}. \quad (9.1.38)$$

Define then the operator $\hat{\rho}$ called the density matrix to have matrix elements ρ^{nm} :

$$\rho^{nm} = \langle n | \hat{\rho} | m \rangle \quad (9.1.39)$$

$$\implies \langle \hat{F} \rangle = \sum_{nm} \langle n | \hat{\rho} | m \rangle \langle m | \hat{F} | n \rangle = \sum_n \langle n | \hat{\rho} \hat{F} | n \rangle = \text{Tr}(\hat{\rho} \hat{F}). \quad (9.1.40)$$

Hence, there must be some distinguished operator $\hat{\rho}$ which characterizes the summary map so that the summary of any operator can always be written as:

$$\boxed{\langle \hat{F} \rangle = \text{Tr}(\hat{\rho} \hat{F})}. \quad (9.1.41)$$

This is an essential discovery. The entire relationship between our abstract operator formalism and the numbers we wish to measure is characterized by this single operator $\hat{\rho}$. Let us now study its properties.

Consider the identity operator. Because the identity operator is always 1 when acting on any vector or multiplied on any operator, its effective numerical value is necessarily 1. Thus, its summary must be 1:

$$\langle \mathbb{1} \rangle = \text{Tr}(\hat{\rho} \mathbb{1}) = \text{Tr}(\hat{\rho}) \stackrel{!}{=} 1. \quad (9.1.42)$$

And so, the density matrix must have a trace of 1.

Consider our self-adjoint coordinate operators $\hat{Q}^a$. Because they are intended to represent real-valued coordinates, they must have real-valued operator summaries. However, physics knows nothing about what coordinates we choose to describe it with, so any other choice of self-adjoint coordinate operators must also have real-valued operator summaries. Consider some unspecified self-adjoint generator $\hat{G}$ and the transformation given by using $\hat{G}$ as a generator:

$$\frac{d\hat{Q}^a}{d\beta} = \frac{1}{i\hbar} [\hat{Q}^a, \hat{G}], \quad \frac{d\hat{P}_a}{d\beta} = \frac{1}{i\hbar} [\hat{P}_a, \hat{G}]. \quad (9.1.43)$$

Because $\hat{Q}^a$ and $\hat{G}$ are self-adjoint, automatically so is $\frac{1}{i\hbar} [\hat{Q}^a, \hat{G}]$ by a very short calculation. Therefore, $\frac{d\hat{Q}^a}{d\beta}$ is self-adjoint and so the transformed coordinate is always self-adjoint. Thus, the operator summary of $\frac{d\hat{Q}^a}{d\beta}$ must be real-valued for any choice of $\hat{G}$, as that represents a valid coordinate transformation. For a given value of a (say 1), the actual operator on the right hand side defining $\frac{d\hat{Q}^1}{d\beta}$ can be made to be any self-adjoint operator by appropriate choice of $\hat{G}$. Therefore, for $\frac{d\hat{Q}^1}{d\beta}$ to have real operator summary for any choice of self-adjoint $\hat{G}$, it must be the case that the operator summary of any self-adjoint operator is itself real.

Let $\hat{F}$ be an operator, not necessarily self-adjoint, and split it into its self-adjoint and anti-self-adjoint parts:

$$\text{Sa}(\hat{F}) = \frac{\hat{F} + \hat{F}^\dagger}{2}, \quad \text{As}(\hat{F}) = \frac{\hat{F} - \hat{F}^\dagger}{2i} \implies \hat{F} = \text{Sa}(\hat{F}) + i\text{As}(\hat{F}). \quad (9.1.44)$$

Automatically both $\text{Sa}(\hat{F})$ and $\text{As}(\hat{F})$ are self-adjoint and so as reasoned they have real-valued operator summaries:

$$\langle \text{Sa}(\hat{F}) \rangle^* = \langle \text{Sa}(\hat{F}) \rangle, \quad \langle \text{As}(\hat{F}) \rangle^* = \langle \text{As}(\hat{F}) \rangle. \quad (9.1.45)$$

From this and linearity it immediately follows that:

$$\langle \hat{F} \rangle^* = \langle (\text{Sa}(\hat{F}) + i\text{As}(\hat{F})) \rangle^* = \langle \text{Sa}(\hat{F}) \rangle - i\langle \text{As}(\hat{F}) \rangle = \langle \hat{F}^\dagger \rangle \quad (9.1.46)$$

Let us now look at this in components:

$$\langle \hat{F} \rangle = \sum_{mn} \rho^{nm} F_{mn} \quad (9.1.47)$$

$$\implies \langle \hat{F} \rangle^* = \sum_{mn} (\rho^{nm})^* F_{mn}^*, \quad \langle \hat{F}^\dagger \rangle = \sum_{mn} \rho^{nm} F_{nm}^*. \quad (9.1.48)$$

Equating these two:

$$\sum_{mn} (\rho^{nm})^* F_{mn}^* = \sum_{mn} \rho^{mn} F_{mn}^* \quad (9.1.49)$$

$$\implies \sum_{mn} (\rho^{mn} - (\rho^{nm})^*) F_{mn}^* = 0, \quad \forall F_{mn} \quad (9.1.50)$$

$$\implies \rho^{mn} = (\rho^{nm})^* \quad (9.1.51)$$

$$\implies \hat{\rho} = \hat{\rho}^\dagger. \quad (9.1.52)$$

Hence, the requirement that $\langle \hat{Q}^a \rangle$ be real for any choice of coordinates demands that the density matrix $\hat{\rho}$ is self adjoint.

Finally let us consider a nonnegative function of our coordinates $f(\hat{Q})$. That is, $f(Q)$ is a function such that for any real valued Q , $f(Q) \geq 0$. Because $\langle f(\hat{Q}) \rangle$ is intended to represent the physical value of this function and this function is nonnegative, we need $\langle f(\hat{Q}) \rangle$ to be nonnegative. Because this f may be any nonnegative function and we may perform arbitrary coordinate transformations of our coordinates which keep the coordinate operators self-adjoint, we really need $\langle \hat{F} \rangle \geq 0$ for every nonnegative operator $\hat{F}$. Because $\hat{\rho}$ is self-adjoint, the spectral theorem guarantees it is diagonalizable. Let $|\rho; n\rangle$ denote an orthonormal eigenbasis of $\hat{\rho}$, with n a label, and let ρ_n indicate the eigenvalues of $\hat{\rho}$:

$$\hat{\rho}|\rho; n\rangle = \rho_n|\rho; n\rangle, \quad \langle \rho; n|\rho; n'\rangle = \delta_{nn'}, \quad \sum_n |\rho; n\rangle\langle \rho; n| = \mathbb{1} \implies \hat{\rho} = \sum_n \rho_n |\rho; n\rangle\langle \rho; n|. \quad (9.1.53)$$

The operator $|\rho; n\rangle\langle \rho; n|$ is automatically nonnegative for each n because for any vector $|\psi\rangle$:

$$\langle \psi | (|\rho; n\rangle\langle \rho; n|) | \psi \rangle = |\langle \psi | \rho; n \rangle|^2 \geq 0. \quad (9.1.54)$$

Thus, we need $\langle |\rho; n\rangle\langle \rho; n| \rangle$ to be nonnegative:

$$0 \leq \langle |\rho; n\rangle\langle \rho; n| \rangle = \text{Tr}(\hat{\rho}|\rho; n\rangle\langle \rho; n|) = \rho_n. \quad (9.1.55)$$

Therefore, the eigenvalues of $\hat{\rho}$ are nonnegative. Consequently, for any vector $|\psi\rangle$:

$$\langle \psi | \hat{\rho} | \psi \rangle = \sum_n \rho_n |\langle \psi | \rho; n \rangle|^2 \geq 0 \quad (9.1.56)$$

and so $\hat{\rho}$ is a necessarily a nonnegative operator.

The operator Lie bracket formalism is the most general way to write down continuous transformations. In that formalism every quantity is associated with a linear operator. The requirement that experiments yield numbers demands that there exists a map from those operators into the complex numbers which we call the operator summary. The requirement that the summary of a vector transforms according to the change of basis formula for a vector demands that the summary depends linearly on the operator one is taking the summary of. This linearity requirement implies that the summary can be written as a trace of the product of the operator in question with a distinguished operator called the density matrix $\hat{\rho}$. The requirement that the summary of a constant number be that constant implies that the density matrix has trace 1. The requirement that the summary of a self-adjoint operator be real implies that the density matrix is self-adjoint. The requirement that the summary of a nonnegative operator be nonnegative implies that the density matrix is nonnegative. So, we have:

$$\langle \hat{F} \rangle = \text{Tr}(\hat{\rho}\hat{F}), \quad \forall \hat{F} \quad (9.1.57)$$

$$\text{Tr}(\hat{\rho}) = 1 \quad (9.1.58)$$

$$\hat{\rho} = \hat{\rho}^\dagger \quad (9.1.59)$$

$$\langle \psi | \hat{\rho} | \psi \rangle \geq 0, \quad \forall |\psi\rangle. \quad (9.1.60)$$

Time is itself a continuous parameter and so time evolution is a continuous transformation with some generator which we call $\hat{H}_A$, the Hamiltonian operator in the active picture. Because time is a real valued parameter its generator is real valued and so $\hat{H}_A$ must be self-adjoint. Then, any operator corresponding to a

generator (call it $\hat{F}_A$) within our system evolves in time according to (9.1.11):

$$\frac{d\hat{F}_A}{dt} = \frac{1}{i\hbar}[\hat{F}_A, \hat{H}_A]. \quad (9.1.61)$$

This is precisely the evolution equation for an operator in the active picture of quantum mechanics. Define the operator $\hat{U}(t, t_0)$, called the time evolution operator, by the conditions:

$$\hat{U}(t_0, t_0) = \mathbb{1}, \quad i\hbar \frac{d\hat{U}(t, t_0)}{dt} = \hat{U}(t, t_0) \hat{H}_A(t). \quad (9.1.62)$$

Then, we can see that at $t = t_0$ the operator $\hat{U}$ is unitary:

$$\hat{U}^\dagger(t_0, t_0) \hat{U}(t_0, t_0) = \mathbb{1}, \quad \hat{U}(t_0, t_0) \hat{U}^\dagger(t_0, t_0) = \mathbb{1}. \quad (9.1.63)$$

As well, we can see that unitarity is preserved by the equation of motion:

$$\frac{d}{dt} (\hat{U} \hat{U}^\dagger) = \frac{d\hat{U}}{dt} \hat{U}^\dagger + \hat{U} \frac{d\hat{U}^\dagger}{dt} = \left(\frac{1}{i\hbar} \hat{U} \hat{H}_A \right) \hat{U}^\dagger + \hat{U}^\dagger \left(\frac{1}{i\hbar} \hat{U} \hat{H}_A \right)^\dagger = -\frac{1}{i\hbar} \hat{U} \hat{H}_A \hat{U}^\dagger + \frac{1}{i\hbar} \hat{U} \hat{H}_A \hat{U}^\dagger = 0. \quad (9.1.64)$$

$$\frac{d}{dt} (\hat{U}^\dagger \hat{U}) = \frac{d\hat{U}^\dagger}{dt} \hat{U} + \hat{U}^\dagger \frac{d\hat{U}}{dt} = \left(\frac{1}{i\hbar} \hat{U} \hat{H}_A \right)^\dagger \hat{U} + \hat{U}^\dagger \frac{1}{i\hbar} \hat{U} \hat{H}_A = -\frac{1}{i\hbar} \hat{H}_A \hat{U}^\dagger \hat{U} + \frac{1}{i\hbar} \hat{U}^\dagger \hat{U} \hat{H}_A = 0 \quad (9.1.65)$$

The first one is 0 automatically using that $\hat{H}_A$ is self-adjoint. The second is 0 because we see that $\hat{U}^\dagger \hat{U} - \mathbb{1}$ satisfies a linear homogeneous equation of motion in terms of itself and that combination is initially 0 and thus remains 0 for all time under homogeneous linear evolution. So, $\hat{U}(t, t_0)$ is unitary for all t, t_0 . By recalling the active picture, we can immediately define the passive picture Hamiltonian operator $\hat{H}(t)$ written without a subscript:

$$\hat{H}(t) = \hat{U}(t, t_0) \hat{H}_A(t) \hat{U}^\dagger(t, t_0). \quad (9.1.66)$$

Then, automatically:

$$\hat{H}(t) \hat{U}(t, t_0) = \hat{U}(t, t_0) \hat{H}_A(t). \quad (9.1.67)$$

So, (9.1.62) can equivalently be written as:

$$i\hbar \frac{d\hat{U}(t, t_0)}{dt} = \hat{H}(t) \hat{U}(t, t_0). \quad (9.1.68)$$

Recycling (8.9.45) we can in principle explicitly solve for $\hat{U}(t, t_0)$ using the time ordering transformation:

$$\hat{U}(t, t_0) = \mathcal{T} : e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt'}. \quad (9.1.69)$$

For an operator $\hat{F}_A(t)$ representing some generator within our system evolving with time we see that:

$$\frac{d}{dt} (\hat{U}(t, t_0) \hat{F}_A(t) \hat{U}^\dagger(t, t_0)) = \frac{d\hat{U}}{dt} \hat{F}_A \hat{U}^\dagger + \hat{U} \frac{d\hat{F}_A}{dt} \hat{U}^\dagger + \hat{U} \hat{F}_A \frac{d\hat{U}^\dagger}{dt} \quad (9.1.70)$$

$$= \frac{1}{i\hbar} \hat{U} \hat{H}_A \hat{F}_A \hat{U}^\dagger + \hat{U} \frac{1}{i\hbar} (\hat{F}_A \hat{H}_A - \hat{H}_A \hat{F}_A) \hat{U}^\dagger - \frac{1}{i\hbar} \hat{F}_A \hat{H}_A \hat{U}^\dagger \quad (9.1.71)$$

$$= 0. \quad (9.1.72)$$

So, this combination is constant. At $t = t_0$ we see:

$$\hat{U}(t_0, t_0) \hat{F}_A(t_0) \hat{U}^\dagger(t_0, t_0) = \mathbb{1} \hat{F}_A(t_0) \mathbb{1} = \hat{F}_A(t_0) \quad (9.1.73)$$

$$\implies \hat{U}(t, t_0) \hat{F}_A(t) \hat{U}^\dagger(t, t_0) = \hat{F}_A(t_0) \quad (9.1.74)$$

$$\implies \hat{F}_A(t) = \hat{U}^\dagger(t, t_0) \hat{F}_A(t_0) \hat{U}(t, t_0). \quad (9.1.75)$$

Hence, the time evolution operator explicitly solves the evolution of any generator within our system by this form. This is precisely the evolution of an operator in the active picture, and so we can honestly interpret $\hat{F}_A(t)$ with this time dependence as the active picture operator and define $\hat{F} = \hat{F}_A(t_0)$ as the passive picture operator.

As we have discussed the density matrix so far, it simply exists to define the summary map $\langle \cdot \rangle$ and so is not a dynamical quantity; all the dynamics have been carried in the active picture operators. Going forward, when viewing the density matrix this way, we will call that static density matrix $\hat{\rho}_A$. However, when we reorganize to the passive picture, the linear operators representing properties of our system are stripped of their time dependence, and we repackage that time dependence into the density matrix. We call the passive

picture density matrix simply $\hat{\rho}(t)$. Looking at the operator summary and using the cyclicity of the trace:

$$\langle \hat{F}_A(t) \rangle = \text{Tr}(\hat{F}_A(t)\hat{\rho}_A) = \text{Tr}(\hat{U}^\dagger(t, t_0)\hat{F}\hat{U}(t, t_0)\hat{\rho}_0) = \text{Tr}(\hat{F}\hat{U}(t, t_0)\hat{\rho}_0\hat{U}^\dagger(t, t_0)). \quad (9.1.76)$$

Thus, if we define the passive picture density matrix $\hat{\rho}(t)$ by:

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}_A\hat{U}^\dagger(t, t_0) \quad (9.1.77)$$

we have that:

$$\text{Tr}(\hat{F}_A(t)\hat{\rho}_A) = \text{Tr}(\hat{F}\hat{\rho}) \quad (9.1.78)$$

and so we can equivalently capture all of the dynamical information of the theory in the time evolving density matrix while keeping all of the generator operators $\hat{F}$ constant. Thus, in the passive picture, **the density matrix contains the entire state of the system**. By construction, the operator summaries in the active picture using $\hat{\rho}_A$ exactly match the operator summaries in the passive picture using $\hat{\rho}$ and so nothing is lost or gained in either approach.

We can find a nice equation of motion for the density matrix by differentiating (9.1.77) in time:

$$\frac{d\hat{\rho}}{dt} = \frac{\partial \hat{U}}{\partial t}\hat{\rho}_0\hat{U}^\dagger + \hat{U}\hat{\rho}_0\frac{d\hat{U}^\dagger}{dt} = \frac{1}{i\hbar}\hat{H}\hat{U}\hat{\rho}_0\hat{U}^\dagger - \frac{1}{i\hbar}\hat{U}\hat{\rho}_0\hat{U}^\dagger\hat{H} \quad (9.1.79)$$

$$\Rightarrow \boxed{\frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar}[\hat{\rho}, \hat{H}] = 0.} \quad (9.1.80)$$

Equation (9.1.80) is known as the **von Neumann equation** and we see that it gives the fundamental equation of motion of the density matrix, and thus of the entire state of our system. The von Neumann equation perfectly reproduces Ehrenfest's theorem; to see this consider a generator $\hat{F}(t)$ which in the passive picture we allow for generality to possibly have some explicit time dependence:

$$\frac{d\langle \hat{F} \rangle}{dt} = \frac{d}{dt}\text{Tr}(\hat{\rho}\hat{F}) = \text{Tr}\left(\frac{d\hat{\rho}}{dt}\hat{F} + \hat{\rho}\frac{\partial \hat{F}}{\partial t}\right) = \text{Tr}\left(\frac{1}{i\hbar}(\hat{H}\hat{\rho} - \hat{\rho}\hat{H})\hat{F}\right) + \langle \frac{\partial \hat{F}}{\partial t} \rangle = \left\langle \left(\frac{\partial \hat{F}}{\partial t} + \frac{1}{i\hbar}[\hat{F}, \hat{H}]\right) \right\rangle \quad (9.1.81)$$

using the cyclicity of the trace.

9.1.2 Why Density Matrices?

All of this density matrix formalism is mathematically interesting, but how is it quantum mechanics? Previously when we studied quantum mechanics, the state of the system was represented by a state vector $|\Psi\rangle$. The density matrix can be seen as a strict generalization of the state vector description. Consider the special case that there exists at some particular time t_0 a state vector $|\Psi_0\rangle$ so that $\hat{\rho}$ can be written in the form:

$$\hat{\rho}(t_0) = |\Psi_0\rangle\langle\Psi_0|. \quad (9.1.82)$$

Then, at a general time t the density matrix can be written as:

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t, t_0) = (\hat{U}(t, t_0)|\Psi_0\rangle)(\langle\Psi_0|\hat{U}^\dagger(t, t_0))^\dagger = |\Psi(t)\rangle\langle\Psi(t)| \quad (9.1.83)$$

where we have defined the time dependent state vector $|\Psi(t)\rangle$ by:

$$|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi_0\rangle \quad (9.1.84)$$

which then automatically satisfies the Schrödinger equation by differentiation:

$$i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle. \quad (9.1.85)$$

Thus the state vector description of quantum mechanics and the Schrödinger equation emerge as the special case that the density matrix ever takes the specific form of (9.1.82). Such a density matrix is called a **pure state**. Otherwise, it is called a **mixed state**. There is a simple basis independent way to tell if a density matrix is a mixed state or a pure state. For a pure state:

$$1 = \text{Tr}(\hat{\rho}) = \sum_n \langle n|\Psi\rangle\langle\Psi|n\rangle = \langle\Psi|\Psi\rangle \quad (9.1.86)$$

and thus $|\Psi\rangle$ is normalized. Then:

$$\text{Tr}(\hat{\rho}^2) = \sum_n \langle n|\Psi\rangle\langle\Psi|\Psi\rangle\langle\Psi|n\rangle = \langle\Psi|\Psi\rangle = 1. \quad (9.1.87)$$

Hence, for a pure state $\text{Tr}(\hat{\rho}^2) = 1$. Alternatively, for a mixed state, we can still diagonalize $\hat{\rho}$:

$$\hat{\rho} = \sum_n \rho_n |\rho; n\rangle \langle \rho; n|. \quad (9.1.88)$$

Because $\text{Tr}(\rho) = 1$, the ρ_n sum to 1:

$$1 = \text{Tr}(\rho) = \sum_n \rho_n \langle \rho; n | \rho; n \rangle = \sum_n \rho_n. \quad (9.1.89)$$

And, because $\hat{\rho}$ is nonnegative, each of its eigenvalues is nonnegative. Thus, each eigenvalue must be less than or equal to 1 and if any of the eigenvalues is 1, all of the rest must be 0. If one of the ρ_n is 1 and the rest are 0 then $\hat{\rho}$ is a pure state. Consequently, for a mixed state:

$$0 < \rho_n < 1. \quad (9.1.90)$$

Multiplying by ρ_n :

$$0 < \rho_n^2 < \rho_n \quad (9.1.91)$$

and so for a mixed state:

$$\text{Tr}(\hat{\rho}^2) = \sum_{nml} \langle n | \rho_m | \rho; m \rangle \langle \rho; m | \rho_l | \rho; l \rangle \langle \rho; l | n \rangle = \sum_{ml} \delta_{ml} \rho_m \rho_l \langle \rho; l | \rho; m \rangle = \sum_n \rho_n^2 < \sum_n \rho_n = \text{Tr}(\hat{\rho}) = 1. \quad (9.1.92)$$

Therefore, for all states $\text{Tr}(\hat{\rho}^2) \leq 1$ with equality if and only if $\hat{\rho}$ is a pure state.

The density matrix description is more general than the state vector description and so it doesn't hurt to take interest in, but more fundamentally there are several reasons it is actually necessary for doing quantum mechanics in general. In a real experiment, many trials have to be done and statistics have to be collected. Consequently, the "same" state has to be attempted to be prepared many times (at least same within some experimental equivalence class). As well, when state preparation is attempted, we do not actually know everything about the state of the system we are preparing due to the enormity of variables in the world beyond our control. Thus, in any real experimental setup there will be some probability distribution on the state of the system at the time of setup. This is just a repeat of the logic used before for classical statistical mechanics, and really is the gateway into quantum statistical mechanics. Suppose we believed in a description of quantum mechanics using only state vectors and suppose we had a probability distribution in our experiment so that we prepare state $|\Psi_n\rangle$ with probability p_n (these $|\Psi_n\rangle$ are normalized but we assume nothing about how they relate to each other). Then, let $G = \langle \Psi | \hat{G} | \Psi \rangle$ be some generator of experimental interest. The expected value of this quantity in our experiment is:

$$\mathbb{E}(G) = \sum_n p_n G_n = \sum_n p_n \langle \Psi_n | \hat{G} | \Psi_n \rangle. \quad (9.1.93)$$

It would be mathematically convenient if we could identify a state vector $|\tilde{\Psi}\rangle$ so that $\mathbb{E}(G) = \langle \tilde{\Psi} | \hat{G} | \tilde{\Psi} \rangle$ with $|\tilde{\Psi}\rangle$ independent of $\hat{G}$ as then this $|\tilde{\Psi}\rangle$ would contain all of the information of statistical expectations in our experiment. However, this is almost never possible. Notice though that we can write:

$$\mathbb{E}(G) = \text{Tr} \left(\hat{G} \sum_n p_n |\Psi_n\rangle \langle \Psi_n| \right) \quad (9.1.94)$$

and thus can define the effective density matrix $\hat{\rho}$:

$$\hat{\rho} = \sum_n p_n |\Psi_n\rangle \langle \Psi_n| \quad (9.1.95)$$

so that:

$$\mathbb{E}(G) = \text{Tr}(\hat{G} \hat{\rho}). \quad (9.1.96)$$

Quite short calculations reveal that $\hat{\rho}$ as defined here is self-adjoint, has trace 1, is nonnegative, and satisfies the von Neumann equation. Thus, whenever the quantum state is imperfectly known or prepared over a distribution of state vectors, there is generally no effective state vector that describes the system statistically. However, there is always a density matrix which does so.

The density matrix structure is also self-reproducing. If we consider a distribution of probabilities p_n

over possible density matrices $\hat{\rho}_n$ then we can still assign an effective density matrix to the statistics:

$$\mathbb{E}(G) = \sum_n p_n G_n = \sum_n p_n \text{Tr}(\rho_n \hat{G}) = \text{Tr} \left(\hat{G} \sum_n p_n \hat{\rho}_n \right) \stackrel{!}{=} \text{Tr}(\hat{G} \hat{\rho}) \quad \forall \hat{G} \implies \hat{\rho} = \sum_n p_n \hat{\rho}_n. \quad (9.1.97)$$

Again, short calculations reveal that $\hat{\rho}$ as defined here is self-adjoint, has trace 1, is nonnegative, and satisfies the von Neumann equation. Thus when combining quantum mechanics with statistical mechanics a density is absolutely necessary. Because probabilities themselves can be cast in the form of statistical expectations, we know that in a statistical context the expectation map $\mathbb{E}$ contains all statistical information. Because the expectation of operator summaries is characterized by a density matrix, in quantum statistical mechanics, the state of the system remains a density matrix. Interestingly, when considering a single quantum system or a distribution over quantum systems, the state is just a density matrix. Technically, this is only true when the only quantities of interest are the expectations of operator summaries. The distribution p_n and constituent density matrices $\hat{\rho}_n$ contain more information than $\hat{\rho}$ itself when considering quantities beyond the expectations of operator summaries. Expectations of operator summaries happen to be the relevant quantities of interest in quantum statistical mechanics, allowing $\hat{\rho}$ to be sufficiently descriptive for it to be the only thing we care about.

It is extremely important to note here a subtle point of interpretation which is often gotten wrong. We see that when one has a probability distribution on the density matrix one can identify an effective density matrix for the distribution that is the probability weighted sum of density matrices in that distribution where the weights are nonnegative and sum to 1. Such a sum is called a convex linear combination. The result is the effective density matrix in the sense that it produces all the correct statistical expectations. However, any given density matrix that is not a pure state can be written infinitely many ways as a convex sum. So, if one has a density matrix $\hat{\rho}$ that can be written in the form $\sum_n p_n \hat{\rho}_n$ where the p_n are a mathematically valid probability distribution and the $\hat{\rho}_n$ are each a mathematically valid density matrix that does **NOT** mean that p_n is the probability the density matrix of a single instance of the system is $\hat{\rho}_n$. For example, on a two dimensional Hilbert space the density matrix $\hat{\rho} = \frac{1}{2} \mathbb{1}$ can be written as $\hat{\rho} = \frac{1}{2}(|+_z\rangle\langle+_z| + |-_z\rangle\langle-_z|)$ where $|+_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|-_z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Naively interpreting in the way I am telling you not to would suggest that this means $\hat{\rho}$ comes from a source which in half of experiments is in the state $|+_z\rangle\langle+_z|$ and in the other half is in the state $|-_z\rangle\langle-_z|$. However, it is also possible to decompose $\hat{\rho}$ as $\hat{\rho} = \frac{1}{2}(|+_x\rangle\langle+_x| + |-_x\rangle\langle-_x|)$ where $|+_x\rangle = \frac{|+_z\rangle + |-_z\rangle}{\sqrt{2}}$ and $|-_x\rangle = \frac{|+_z\rangle - |-_z\rangle}{2}$. Naively interpreting this decomposition instead would suggest that $\hat{\rho}$ comes from a source which in half of experiments is in the state $|+_x\rangle\langle+_x|$ and in the other half is in the state $|-_x\rangle\langle-_x|$. This interpretation is clearly inconsistent with the previous interpretation because none of these states match each other. So, absolutely plainly you can **NOT** reverse engineer the distribution p_n and constituent density matrices $\hat{\rho}_n$ that go into forming the average density matrix $\hat{\rho}$ that describes statistical expectations of operator summaries from the final average density matrix $\hat{\rho}$ alone.

It is a common misconception that density matrices are only useful or necessary for describing statistical ensembles of quantum systems. However, the density matrix is also necessary outside of quantum statistical mechanics. Suppose we have one quantum system which has operators acting on a Hilbert space $\mathbb{H}_1$ and another quantum system which has operators acting on another Hilbert space $\mathbb{H}_2$. Then, what is the appropriate Hilbert space of the combined interacting system? When we realized quantum field theory was necessary, we learned that the two particle Hilbert space is given by the tensor product of each of the individual particle Hilbert spaces (in the case that the particles were the same species, like photons, we also saw that indistinguishability reflected in the Hilbert space, in that case by symmetrization). This is because in general, when two quantum systems are combined, the combined Hilbert space is $\mathbb{H}_1 \otimes \mathbb{H}_2$. This is called a bipartite quantum system. This tensor product structure is automatically necessary when the ability to select two properties independently is combined with the linearity structure of quantum mechanics. Now suppose we have two quantum systems which we join together and allow to interact. Then, the combined system will have some state on the space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$. If we were to commit to a state vector description, then letting $|n_1\rangle$ be an orthonormal basis for $\mathbb{H}_1$ and $|n_2\rangle$ be an orthonormal basis for $\mathbb{H}_2$, the state vector $|\Psi\rangle$ on $\mathbb{H}$ would take the form:

$$|\Psi\rangle = \sum_{mn} \Psi_{mn} |m_1\rangle \otimes |n_2\rangle. \quad (9.1.98)$$

Now consider the value of a quantity associated with the first system. Let $\hat{A}$ be a linear operator associated to some generator on $\mathbb{H}_1$. On $\mathbb{H}$ there is then some operator $\hat{F}$ to represent this quantity. Because this quantity is intended to only be a property of system 1, its value should be independent of system 2. As

well, $\hat{F}$ should reduce to just $\hat{A}$ on system 1. So, $\hat{F}$ should be given by:

$$\hat{F} = \hat{A} \otimes \mathbb{1} \quad (9.1.99)$$

so that it acts with $\hat{A}$ on system 1 and does not affect system 2 at all. Then, the summary value of $\hat{F}$ is given by:

$$\langle \Psi | \hat{F} | \Psi \rangle = \sum_{mn} \Psi_{mn}^* \langle m_1 n_2 | \hat{A} \otimes \mathbb{1} \sum_{m'n'} \Psi_{m'n'} | m'_1 n'_2 \rangle = \sum_{mnm'n'} \Psi_{mn}^* \Psi_{m'n'} \langle m_1 | \hat{A} | m'_1 \rangle \langle n_2 | \mathbb{1} | n'_2 \rangle \quad (9.1.100)$$

$$= \sum_{nmnm'n'} \Psi_{mn}^* \Psi_{m'n'} A_{mm'} \delta_{nn'} = \sum_{mm'} A_{mm'} \sum_n \Psi_{mn}^* \Psi_{m'n}. \quad (9.1.101)$$

If we define the operator $\hat{\rho}_1$ on $\mathbb{H}_1$ by:

$$\langle m'_1 | \hat{\rho}_1 | m_1 \rangle = \sum_n \Psi_{m'n} \Psi_{mn}^* \quad (9.1.102)$$

$$\implies \langle \Psi | \hat{F} | \Psi \rangle = \sum_{mm'} A_{mm'} \langle m'_1 | \hat{\rho}_1 | m_1 \rangle = \sum_{mm'} \langle m_1 | \hat{A} | m'_1 \rangle \langle m'_1 | \hat{\rho}_1 | m_1 \rangle = \text{Tr}(\hat{\rho}_1 \hat{A}). \quad (9.1.103)$$

There is in general no Ψ_1 so that $\langle \Psi | \hat{F} | \Psi \rangle$ is given by $\langle \Psi_1 | \hat{A} | \Psi_1 \rangle$ for all $\hat{A}$ and corresponding $\hat{F}$. But, there is a density matrix $\hat{\rho}_1$ so that the properties of system 1 are described by that density matrix no matter the state of the combined system (again the basic properties of trace 1, self-adjointness, and positivity can be checked directly). We see that even if a combined quantum system's full state is described by a state vector, there is no guarantee that any of its subsystems can be described by a state vector. In general, a subsystem of a quantum system *must* be described by a density matrix. This argument has nothing to do with the dynamics of a quantum subsystem, which we will discuss later. The density matrix is necessitated simply by considering a subsystem. However, every system in the universe other than the whole universe itself is a subsystem. Therefore, every system ever relevant experimentally is necessarily a subsystem and thus demands a density matrix. It is essentially an occasional accident that the state vector description ever gives correct results; to consistently be correct a density matrix is mandatory.

In this subsystem description, the density matrix structure again reproduces itself. Consider a system with state density matrix $\hat{\rho}$ and Hilbert space $\mathbb{H}_1 \otimes \mathbb{H}_2$. Then, consider the same $\hat{F}$ and $\hat{A}$ structure as previously. The operator summary of $\hat{F}$ gives:

$$\langle \hat{F} \rangle = \text{Tr}(\hat{F} \hat{\rho}) = \sum_{mn} \langle m_1 n_2 | (\hat{A} \otimes \mathbb{1}) \hat{\rho} | m_1 n_2 \rangle = \sum_{mm'n} \langle m_1 | \hat{A} | m'_1 \rangle \langle m'_1 n_2 | \hat{\rho} | m_1 n_2 \rangle. \quad (9.1.104)$$

If we define the operator $\hat{\rho}_1$ on $\mathbb{H}_1$ by:

$$\langle m'_1 | \hat{\rho}_1 | m_1 \rangle = \sum_n \langle m'_1 n_2 | \hat{\rho} | m_1 n_2 \rangle \quad (9.1.105)$$

$$\implies \langle \hat{F} \rangle = \sum_{mm'} \langle m_1 | \hat{A} | m'_1 \rangle \langle m'_1 | \hat{\rho}_1 | m_1 \rangle = \text{Tr}(\hat{A} \hat{\rho}_1). \quad (9.1.106)$$

Thus there remains an effective density matrix for the subsystem. By using the density matrix description, every subsystem of a quantum system has a well-defined state. We can see that the structure in (9.1.105) keeps the system 1 labels (m_1 and m'_1) fixed while summing over a basis of system 2 (the n_2 labels). This is called a partial trace. In particular, $\hat{\rho}_1$ is the partial trace of $\hat{\rho}$ when traced over system 2 and is called the reduced density matrix of system 1. This is written as (and defined properly by):

$$\hat{\rho}_1 = \text{Tr}_2(\hat{\rho}) = \sum_{mm'n} |m_1\rangle \langle m_1 n_2 | \hat{\rho} | m'_1 n_2 \rangle \langle m'_1|. \quad (9.1.107)$$

9.1.3 Entanglement

When the state of a quantum system is a state vector in a bipartite Hilbert space $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ yet it is not possible to describe the effective state on either $\mathbb{H}_1$ or $\mathbb{H}_2$ by a state vector, then two subsystems are said to be entangled (otherwise, they are separable). It is relatively simple to determine whether a state vector of a bipartite quantum system is entangled or separable. Consider a state vector of a bipartite quantum system:

$$|\Psi\rangle = \sum_{mn} \Psi_{mn} |m_1\rangle \otimes |n_2\rangle. \quad (9.1.108)$$

By definition if and only if the state is separable, the density matrix $\hat{\rho}_1$ is a pure state and we can assign a state vector $|\Psi_1\rangle$ to system 1. That is:

$$\hat{\rho}_1 = |\Psi_1\rangle\langle\Psi_1|, \quad |\Psi_1\rangle = \sum_m \Psi_m^{(1)} |m_1\rangle \quad (9.1.109)$$

for some coefficients $\Psi_m^{(1)}$. Using (9.1.102), we have automatically that for a separable state:

$$\sum_n \Psi_{mn} \Psi_{m'n}^* = \Psi_m^{(1)} \Psi_{m'}^{(1)*}. \quad (9.1.110)$$

This is the equation that defines the $\Psi_m^{(1)}$ coefficients and clearly we can redefine all of these coefficients by multiplying by a single overall phase with no effect. For $m' = m$:

$$|\Psi_m^{(1)}| = \sqrt{\sum_n |\Psi_{mn}|^2}. \quad (9.1.111)$$

Let m_0 be a value of m for which $|\Psi_m^{(1)}| \neq 0$. Such an m must exist because $\hat{\rho}_1 \neq 0$. Choose the arbitrary overall phase so that $\Psi_{m_0}^{(1)} = |\Psi_{m_0}^{(1)}|$. Thus, using (9.1.110) with $m' = m_0$:

$$\Psi_m^{(1)} = \frac{\sum_n \Psi_{mn} \Psi_{m_0 n}^*}{\sqrt{\sum_n |\Psi_{m_0 n}|^2}}. \quad (9.1.112)$$

Returning this expression to (9.1.110), renaming m_0 to m'' and simplifying gives:

$$\left(\sum_n \Psi_{mn} \Psi_{m'n}^* \right) \left(\sum_n |\Psi_{m''n}|^2 \right) = \left(\sum_n \Psi_{mn} \Psi_{m''n}^* \right) \left(\sum_n \Psi_{m''n} \Psi_{m'n}^* \right). \quad (9.1.113)$$

While originally derived for m'' such that $\sum_n |\Psi_{m''n}|^2 \neq 0$, it is automatically also true if this condition is not met as then both sides are automatically 0. Thus, for and only for a separable state, this equation holds for all m, m', m'' . Whether a state is separable can then be determined by computing and comparing the two sides of this equation. For a separable state, now evaluate the above at $m' = m$ and then rename m'' to m' to give:

$$\left(\sum_n |\Psi_{mn}|^2 \right) \left(\sum_n |\Psi_{m'n}|^2 \right) = \left| \sum_n \Psi_{mn} \Psi_{m'n}^* \right|^2. \quad (9.1.114)$$

Define the vectors $|\Phi_m\rangle \in \mathbb{H}_2$ by:

$$|\Phi_m\rangle = \sum_n \Psi_{mn} |n_2\rangle. \quad (9.1.115)$$

Then (9.1.114) can be written simply as:

$$\langle\Phi_m|\Phi_m\rangle\langle\Phi_{m'}|\Phi_{m'}\rangle = |\langle\Phi_m|\Phi_{m'}\rangle|^2. \quad (9.1.116)$$

This is the saturated case of the Cauchy-Schwarz inequality for each m and m' . Thus, all of the $|\Phi_m\rangle$ must be colinear and we can define a vector $|\Phi\rangle$ (which we take to be normalized by definition) and coefficients A_m so that:

$$|\Phi_m\rangle = A_m |\Phi\rangle, \quad \langle\Phi|\Phi\rangle = 1. \quad (9.1.117)$$

Let $|\Phi\rangle$ have coefficients B_n :

$$|\Phi\rangle = \sum_n B_n |n_2\rangle. \quad (9.1.118)$$

Then, the definition of $|\Phi_m\rangle$ yields:

$$\Psi_{mn} = A_m B_n. \quad (9.1.119)$$

Automatically, by equation (9.1.102):

$$\Psi_{m'}^{(1)} \Psi_m^{(1)*} = A_{m'} A_m^*. \quad (9.1.120)$$

Because this is the only restriction on $\Psi_m^{(1)}$, we can take $A_m = \Psi_m^{(1)}$. Then, it automatically follows similarly that $\hat{\rho}_2$ is a pure state with state vector $|\Phi\rangle$ and so we can take $B_n = \Psi_n^{(2)}$. Thus, a separable state vector

$|\Psi\rangle$ is simply a tensor product of the form:

$$|\Psi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \quad (9.1.121)$$

for some $|\Psi_1\rangle, |\Psi_2\rangle$. The converse that a state of such form is separable is automatically true by a one line calculation.

For a two component quantum system with a pure state density matrix $\hat{\rho} = |\Psi\rangle\langle\Psi|$, entanglement represents the extent to which the density matrices of the components of the system fail to contain all of the information of the density matrix of the full system. Let $\hat{F} = \hat{A} \otimes \hat{B}$ where $\hat{A}$ is an operator on $\mathbb{H}_1$ and $\mathbb{H}_2$ is an operator on $\mathbb{H}_2$. For $|\Psi\rangle$ separable, we can write $|\Psi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle$ and so:

$$\langle\hat{F}\rangle = \langle\Psi|\hat{F}|\Psi\rangle = \langle\Psi_1|\hat{A}|\Psi_1\rangle\langle\Psi_2|\hat{B}|\Psi_2\rangle = \langle\hat{A}\rangle_1\langle\hat{B}\rangle_2. \quad (9.1.122)$$

Alternatively, if $|\Psi\rangle$ is entangled, then there is a some minimum number $K > 1$ of terms, normalized wavefunctions $|\Psi_1^{(k)}\rangle, \dots, |\Psi_2^{(k)}\rangle$, and coefficients c_k so that:

$$|\Psi\rangle = \sum_{k=1}^K c_k |\Psi_1^{(k)}\rangle \otimes |\Psi_2^{(k)}\rangle \quad (9.1.123)$$

and so:

$$\langle\hat{F}\rangle = \sum_{k=1}^K \sum_{k'=1}^K c_k c_{k'}^* \langle\Psi_1^{(k')}\rangle \langle\hat{A}|\Psi_1^{(k)}\rangle \langle\Psi_2^{(k')}\rangle \langle\hat{B}|\Psi_2^{(k)}\rangle. \quad (9.1.124)$$

Thus for an entangled system it is not possible to reduce the summary of a joint operator to the subsystem summaries of terms in the joint operator. In this way, the density matrix $\hat{\rho}$ contains information about the joint properties of the two subsystem which is not contained in either of the subsystem density matrices $\hat{\rho}_1$ and $\hat{\rho}_2$.

Entanglement is also defined for a mixed state density matrix by generalizing the above concept. We understood previously that if there is a classical probability distribution on the states of a system with density matrix $\hat{\rho}^{(n)}$ being appropriate with probability p_n , then the effective density matrix of the ensemble is:

$$\hat{\rho} = \sum_n p_n \hat{\rho}^{(n)}. \quad (9.1.125)$$

Thus, a linear combination of density matrices with positive coefficients that sum to 1 can be interpreted as a “classical mixture”, meaning equivalent in terms of summaries to a classical probability distribution on the state of the system. (Such a linear combination is called a convex linear combination.) Any density matrix can be written as a classical mixture of pure states, because the diagonal form of $\hat{\rho}$ is automatically so. The density matrix of a two component quantum system is said to be separable if it is possible to write that density matrix as a convex linear combination of pure states which are themselves separable. Otherwise, that density matrix is called entangled. Unfortunately, it is a very difficult computational problem to determine whether a general density matrix on a large Hilbert space is entangled. There is no known simple criterion to check.

There is an analog to the factorization property (9.1.122) possible for density matrices, but it is stronger than separability. The subsystems of a bipartite quantum system are said to be uncorrelated if for all operators of the form $\hat{A} \otimes \hat{B}$:

$$\langle\hat{A} \otimes \hat{B}\rangle = \langle\hat{A}\rangle_1 \langle\hat{B}\rangle_2. \quad (9.1.126)$$

Automatically it follows that by considering $\hat{A} = |n_1\rangle\langle m_1|$, $\hat{B} = |n'_2\rangle\langle m'_2|$:

$$\langle m_1 m'_2 | \hat{\rho} | n_1 n'_2 \rangle = \langle m_1 | \hat{\rho}_1 | n_1 \rangle \langle m'_2 | \hat{\rho}_2 | n'_2 \rangle \quad (9.1.127)$$

$$\implies \hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2. \quad (9.1.128)$$

The converse follows by an equally short calculation. Thus the subsystems are uncorrelated if and only if the combined system density matrix factorizes as $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$.

Much like interactions between subsystems create correlations in classical statistical mechanics, interactions between subsystems create correlations and entanglement in quantum mechanics. This is because the von Neumann equation only applies to an isolated whole system, not to an interacting subsystem. Consider a bipartite quantum system. Let $\hat{H}_1$ be the Hamiltonian operator of the first subsystem when it is free and $\hat{H}_2$ be the Hamiltonian operator of the second subsystem when it is free. Then, let $\hat{H}_{\text{int}}$ be the interaction term in the Hamiltonian operator between the two subsystems. So, the full Hamiltonian operator $\hat{H}$ of the

bipartite system is:

$$\hat{H} = \hat{H}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_2 + \hat{H}_{\text{int}}. \quad (9.1.129)$$

The full density matrix $\hat{\rho}$ evolves according to the von Neumann equation. Let us see how $\hat{\rho}_1$, the density matrix of the first subsystem, evolves. By definition:

$$\frac{d\hat{\rho}_1}{dt} = \frac{d}{dt} \text{Tr}_2(\hat{\rho}) = \sum_n \langle n_2 | \frac{d\hat{\rho}}{dt} | n_2 \rangle = \sum_n \frac{1}{i\hbar} \langle n_2 | (\hat{H}\hat{\rho} - \hat{\rho}\hat{H}) | n_2 \rangle \quad (9.1.130)$$

$$= \frac{1}{i\hbar} \sum_n \langle n_2 | ((\hat{H}_1 \otimes \mathbb{1})\hat{\rho} + (\mathbb{1} \otimes \hat{H}_2)\hat{\rho} + \hat{H}_{\text{int}}\hat{\rho} - \hat{\rho}(\hat{H}_1 \otimes \mathbb{1}) - \hat{\rho}(\mathbb{1} \otimes \hat{H}_2) - \hat{\rho}\hat{H}_{\text{int}}) | n_2 \rangle. \quad (9.1.131)$$

By inserting complete sets of states, these terms can be simplified individually to give:

$$\sum_n \langle n_2 | (\hat{H}_1 \otimes \mathbb{1}) \hat{\rho} | n_2 \rangle = \hat{H}_1 \hat{\rho}_1 \quad (9.1.132)$$

$$\sum_n \langle n_2 | \hat{\rho} (\hat{H}_1 \otimes \mathbb{1}) | n_2 \rangle = \hat{\rho}_1 \hat{H}_1 \quad (9.1.133)$$

$$\sum_n \langle n_2 | (\mathbb{1} \otimes \hat{H}_2) \hat{\rho} | n_2 \rangle = \sum_{mm'nn'} |m_1\rangle \langle n_2 | \hat{H}_2 | n'_2 \rangle \langle m_1 n'_2 | \hat{\rho} | m'_1 n_2 \rangle \langle m'_1 | \quad (9.1.134)$$

$$\sum_n \langle n_2 | \hat{\rho} (\mathbb{1} \otimes \hat{H}_2) | n_2 \rangle = \sum_n \langle n_2 | (\mathbb{1} \otimes \hat{H}_2) \hat{\rho} | n_2 \rangle. \quad (9.1.135)$$

Thus, after simplification:

$$\frac{d\hat{\rho}_1}{dt} + \frac{1}{i\hbar} [\hat{\rho}_1, \hat{H}_1] + \frac{1}{i\hbar} \text{Tr}_2([\hat{\rho}, \hat{H}_{\text{int}}]) = 0. \quad (9.1.136)$$

So, the density matrix $\hat{\rho}_1$ of the subsystem does not have an autonomous equation of motion. It is not possible in the case of interaction to determine the exact time evolution of $\hat{\rho}_1$ without knowing the full state $\hat{\rho}$ of the combined system (it is sometimes possible to come up with some useful approximations under special conditions). The forcing operator $\frac{1}{i\hbar} \text{Tr}_2([\hat{\rho}, \hat{H}_{\text{int}}])$ is essentially an arbitrary self-adjoint operator that preserves the trace and nonnegativity of $\hat{\rho}_1$. Because of this, it is not in general possible to find an operator $\hat{V}(t, t_0)$ so that $\hat{\rho}_1(t) = \hat{V}(t, t_0) \hat{\rho}(t_0) \hat{V}^\dagger(t, t_0)$ and consequently, even if $\hat{\rho}(t_0)$ is a pure state it is not in general possible to identify a time dependent state vector so that $\hat{\rho}_1(t)$ can be written as a pure state in terms of that vector. Thus, the presence of interactions causes pure states to become mixed states. From the subsystem perspective, this means that interactions cause the subsystems to become entangled. A note to be careful: partial traces only have the cyclicity property on operators entirely in the Hilbert space being traced over. By that I mean, although $\text{Tr}(\hat{\rho} \hat{H}_{\text{int}}) = \text{Tr}(\hat{H}_{\text{int}} \hat{\rho})$ is true, it is also true that $\text{Tr}_2(\hat{\rho} \hat{H}_{\text{int}}) \neq \text{Tr}_2(\hat{H}_{\text{int}} \hat{\rho})$, which can be confirmed by a short calculation putting these expressions in explicit bases.

9.1.4 Canonical Structure of Density Matrices

In state vector quantum mechanics we found it is possible to reconstruct the state vector up to an overall phase from operator summaries, thus making the state vector observable up to that phase. Similarly and more generally, when using a density matrix in quantum mechanics, the entire density matrix can unambiguously be reconstructed from operator summaries. Thus quantum tomography applies to quantum mechanics in general. Consider a quantum system on a Hilbert space with orthonormal basis $|n\rangle$ and define the operators $\hat{S}_{mn}$ and $\hat{A}_{mn}$ by:

$$\hat{S}_{mn} = \frac{|m\rangle\langle n| + |n\rangle\langle m|}{2}, \quad \hat{A}_{mn} = \frac{|m\rangle\langle n| - |n\rangle\langle m|}{2i}. \quad (9.1.137)$$

Then, $\hat{\rho}$ is explicitly given by:

$$\langle \hat{S}_{mn} \rangle + i \langle \hat{A}_{mn} \rangle = \text{Tr}(|m\rangle\langle n| \hat{\rho}) = \langle n | \hat{\rho} | m \rangle \quad (9.1.138)$$

$$\implies \hat{\rho} = \sum_{mn} (\langle \hat{S}_{mn} \rangle + i \langle \hat{A}_{mn} \rangle) |n\rangle\langle m|. \quad (9.1.139)$$

The density matrix approach makes it extremely clear why the overall phase of the wavefunction/state vector is meaningless. The true state of a quantum system is a density matrix, and in the case that density matrix is a pure state it can be written in the form $\hat{\rho} = |\Psi\rangle\langle\Psi|$ thus allowing one to identify $|\Psi\rangle$ as the effective state. However, there is no unique way to decompose a pure state in this way as if and only if $|\Psi'\rangle = e^{i\varphi} |\Psi\rangle$ for some

phase φ then $\hat{\rho} = |\Psi\rangle\langle\Psi| = |\Psi'\rangle\langle\Psi'|$. Thus, the overall phase ambiguity of the wavefunction derives purely from the ambiguity of this decomposition. **The density matrix itself is entirely physical, uniquely defined, and determinable by quantum tomography.**

In this section we reorganized our entire operator formalism into the density matrix approach and found that it naturally reproduced the mathematical structure of quantum mechanics while remaining faithful as a representation to the structures introduced in section 1.3, unlike the Poisson representation. This representation is called the Schrödinger representation. However, it is possible to describe all of quantum mechanics perfectly normally within the Poisson representation and a classical Hamiltonian, as long as it is formulated on the correct phase space. This should not be at all surprising to you as we established in chapter 1 that any system of differential equations can be described by a Hamiltonian on a sufficiently large phase space. In the state vector description of quantum mechanics, the Hamiltonian we know is given by:

$$\mathcal{H} = \langle\hat{H}\rangle = \langle\Psi|\hat{H}|\Psi\rangle \quad (9.1.140)$$

where in an arbitrary orthonormal basis $|n\rangle$ the components $\Psi_n = \langle n|\Psi\rangle$ have the Poisson brackets:

$$\{\Psi_n, \Psi_m\} = 0, \quad \{\Psi_n, \Psi_m^*\} = \frac{1}{i\hbar}\delta_{nm}. \quad (9.1.141)$$

We can rewrite the Hamiltonian in terms of the density matrix $\hat{\rho} = |\Psi\rangle\langle\Psi|$ as:

$$\mathcal{H} = \langle\hat{H}\rangle = \text{Tr}(\hat{\rho}\hat{H}) \quad (9.1.142)$$

and compute the Poisson brackets of the components $\rho_{mn} = \langle m|\hat{\rho}|n\rangle = \Psi_m\Psi_n^*$ using the product rule:

$$\{\rho_{mn}, \rho_{m'n'}\} = \{\Psi_m\Psi_n^*, \Psi_{m'}\Psi_{n'}^*\} = \Psi_m\Psi_{n'}^*\{\Psi_n^*, \Psi_{m'}\} + \Psi_{m'}\Psi_n^*\{\Psi_m, \Psi_{n'}^*\} \quad (9.1.143)$$

$$= -\frac{1}{i\hbar}\rho_{mn'}\delta_{m'n} + \frac{1}{i\hbar}\rho_{m'n}\delta_{mn'}. \quad (9.1.144)$$

From this Poisson bracket, the von Neumann immediately follows from the standard Hamilton's equations:

$$\frac{d\hat{\rho}}{dt} = \{\hat{\rho}, \mathcal{H}\} = \sum_{mn} |m\rangle\langle m|\{\hat{\rho}, \mathcal{H}\}|n\rangle\langle n| = \sum_{mn} \left\{ \rho_{mn}, \sum_{m'n'} \rho_{m'n'} \langle n'|\hat{H}|m'\rangle \right\} \langle n| \quad (9.1.145)$$

$$= \sum_{mm'nn'} |m\rangle\langle n'|\hat{H}|m'\rangle\langle n|\{\rho_{mn}, \rho_{m'n'}\} = \sum_{mm'nn'} |m\rangle\langle n'|\hat{H}|m'\rangle\langle n| \left(-\frac{1}{i\hbar}\rho_{mn'}\delta_{m'n} + \frac{1}{i\hbar}\rho_{m'n}\delta_{mn'} \right) \quad (9.1.146)$$

$$= \frac{1}{i\hbar}\hat{H}\hat{\rho} - \frac{1}{i\hbar}\hat{\rho}\hat{H}. \quad (9.1.147)$$

Thus, even though we derived the form of the Hamiltonian and Poisson brackets for a pure state they give the correct results for a general density matrix.

The density matrix Poisson bracket can be written equivalently in terms of the operator summaries of generic operators. Let $\hat{A}$ and $\hat{B}$ be two operators on the Hilbert space. Then:

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\} = \sum_{mm'nn'} \langle n|\hat{A}|m\rangle\langle n'|\hat{B}|m'\rangle\{\rho_{mn}, \rho_{m'n'}\} \quad (9.1.148)$$

$$= \sum_{mm'nn'} \langle n|\hat{A}|m\rangle\langle n'|\hat{B}|m'\rangle \left(-\frac{1}{i\hbar}\rho_{mn'}\delta_{m'n} + \frac{1}{i\hbar}\rho_{m'n}\delta_{mn'} \right) \quad (9.1.149)$$

$$= \frac{1}{i\hbar}\text{Tr}([\hat{A}, \hat{B}]\hat{\rho}) = \langle\frac{1}{i\hbar}[\hat{A}, \hat{B}]\rangle. \quad (9.1.150)$$

Thus, Dirac's theorem is replicated for density matrices. This Poisson bracket determines the full density matrix Poisson bracket by simply considering $\hat{A} = |m\rangle\langle n|$ and $\hat{B} = |m'\rangle\langle n'|$.

Summary 9.1: Mathematical Formulation of Quantum Mechanics

In quantum mechanics, the state of the system is represented by a trace 1, self-adjoint, nonnegative operator $\hat{\rho}(t)$ on a Hilbert space $\mathbb{H}$ known as the density matrix.

All of the properties of the state of the system are contained in the operator summary map $\langle\cdot\rangle$ which

for a generic operator $\hat{A}$ on $\mathbb{H}$ is defined by:

$$\langle \hat{A} \rangle = \text{Tr}(\hat{\rho}\hat{A}). \quad (9.1.151)$$

Real valued properties are the summaries of self-adjoint operators. This includes the Hamiltonian $\mathcal{H} = \langle \hat{H} \rangle$ where the self-adjoint operator $\hat{H}$ is called the Hamiltonian operator.

The Poisson bracket of the density matrix is captured by Dirac's theorem:

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\} = \langle \frac{1}{i\hbar} [\hat{A}, \hat{B}] \rangle \quad (9.1.152)$$

for arbitrary $\hat{A}, \hat{B}$.

The resulting equation of motion for the density matrix is the von Neumann equation:

$$\frac{d\hat{\rho}}{dt} = \{\hat{\rho}, \mathcal{H}\} \implies \frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar} [\hat{\rho}, \hat{H}] = 0. \quad (9.1.153)$$

The time evolution of the density matrix is solved by:

$$\hat{\rho}(t) = \hat{U}(t, t_0) \hat{\rho}(t_0) \hat{U}^\dagger(t, t_0) \quad (9.1.154)$$

where the time evolution operator $\hat{U}(t, t_0)$ is given by:

$$\hat{U}(t, t_0) = \mathbb{1}, \quad i\hbar \frac{d\hat{U}(t, t_0)}{dt} = \hat{H}(t) \hat{U}(t, t_0) \implies \hat{U}(t, t_0) = \mathcal{T} : e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt'}. \quad (9.1.155)$$

When two quantum subsystems on Hilbert spaces $\mathbb{H}_1$ and $\mathbb{H}_2$ are brought together to interact, the Hilbert space of the combined system is $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$. The full system is described by a density matrix on $\mathbb{H}$. It is possible to identify an effective density matrix for either subsystem by using the partial trace over the other subsystem:

$$\hat{\rho}_1 = \text{Tr}_2(\hat{\rho}), \quad \hat{\rho}_2 = \text{Tr}_1(\hat{\rho}). \quad (9.1.156)$$

Quantum mechanics as formulated above is done on an arbitrary Hilbert space. Very often, the Hilbert space of interest for us is of a particular form. Specifically, it is often the Hilbert space of square integrable functions of some real valued coordinates Q^a . Because the space of coordinate values is called configuration space, we call such a Hilbert space a **configuration Hilbert space**. There are several nice additional formulas that can be derived for quantum mechanics on a configuration Hilbert space that we will derive throughout this chapter.

Exercises

Problem 9.1: Spread Theorems for Density Matrices. For operators $\hat{A}, \hat{B}$ define the operator correlation in the state $\hat{\rho}$ between $\hat{A}$ and $\hat{B}$ exactly as in state vector quantum mechanics by:

$$\text{Cor}(\hat{A}, \hat{B}) = \frac{1}{2} \left(\langle (\hat{A}^\dagger - \langle \hat{A} \rangle \mathbb{1})(\hat{B} - \langle \hat{B} \rangle \mathbb{1}) \rangle + \langle (\hat{B} - \langle \hat{B} \rangle \mathbb{1})(\hat{A}^\dagger - \langle \hat{A} \rangle \mathbb{1}) \rangle \right).$$

as well define the operator spread of $\hat{\mathcal{O}}$ again by:

$$\text{Spr}(\hat{\mathcal{O}}) = \text{Cor}(\hat{\mathcal{O}}, \hat{\mathcal{O}}).$$

However, use the summary map defined by the density matrix:

$$\langle \hat{\mathcal{O}} \rangle = \text{Tr}(\hat{\rho}\hat{\mathcal{O}}).$$

- (a) Let $\hat{\mathcal{O}}$ be a normal operator. Let $\mathcal{O}_n$ be the different eigenvalues of $\hat{\mathcal{O}}$. Show based on the spectral theorem that $\hat{\mathcal{O}}$ can be written as:

$$\hat{\mathcal{O}} = \sum_n \mathcal{O}_n \hat{\pi}_n$$

where $\hat{\pi}_n$ projects into the subspace of $\mathbb{H}$ on which $\hat{\mathcal{O}}$ has eigenvalue $\mathcal{O}_n$. Show that these projectors satisfy:

$$\hat{\pi}_n \hat{\pi}_k = \delta_{nk} \hat{\pi}_k, \quad \hat{\pi}_n = \hat{\pi}_n^\dagger, \quad \sum_n \hat{\pi}_n = \mathbb{1}$$

with no implicit summation intended over repeated indices.

- (b) Let $\hat{\mathcal{O}}$ be a normal operator and the $\hat{\pi}_n$ be its eigenspace projectors as in the previous part. Show that the density matrix is in a state of 0 operator spread for $\hat{\mathcal{O}}$, meaning $\text{Spr}(\hat{\mathcal{O}}) = 0$, if and only if then there exists an n so that:

$$\hat{\rho} = \hat{\pi}_n \hat{\rho} \hat{\pi}_n.$$

- (c) By following our previous proof of the uncertainty theorem, show that its conclusion is completely unchanged when density matrices are used. That is, show that for any two operators $\hat{A}$ and $\hat{B}$:

$$\text{Spr}(\hat{A})\text{Spr}(\hat{B}) \geq \left| \frac{1}{2} \langle [\hat{A}^\dagger, \hat{B}] \rangle + \text{Cor}(\hat{A}, \hat{B}) \right|^2.$$

- (d) Show that the spectral spread theorem generalizes precisely to density matrices as well. That is, show that for any density matrix $\hat{\rho}$ and normal operator $\hat{\mathcal{O}}$, there is always an eigenvalue of $\hat{\mathcal{O}}$ within a distance of at most $\sqrt{\text{Spr}(\hat{\mathcal{O}})}$ from $\langle \hat{\mathcal{O}} \rangle$.

Problem 9.2: State Purification. Consider a density matrix $\hat{\rho}$ for a quantum system with Hilbert space $\mathbb{H}$.

- (a) Explain that there exist nonnegative coefficients p_n and normalized state vectors $|\Psi_n\rangle$ so that:

$$\hat{\rho} = \sum_n p_n |\Psi_n\rangle \langle \Psi_n|, \quad \sum_n p_n = 1.$$

Explain that if $\hat{\rho}$ is a mixed state then there are infinitely many decompositions of $\hat{\rho}$ of this form. These $|\Psi_n\rangle$ are not required to be orthogonal to each other.

- (b) Consider one particular decomposition of $\hat{\rho}$ in the form of the previous part. Consider a new Hilbert space $\mathbb{H}'$ of dimension at least as large as the number of terms in the decomposition of $\hat{\rho}$ and define the total Hilbert space $\mathbb{H}_{\text{total}} = \mathbb{H} \otimes \mathbb{H}'$. Let $|\Phi_n\rangle$ be orthonormal vectors in $\mathbb{H}'$ where the range of n is equal to the number of terms in the decomposition of $\hat{\rho}$. Consider the state vector:

$$|\Psi_{\text{total}}\rangle = \sum_n \sqrt{p_n} |\Psi_n\rangle \otimes |\Phi_n\rangle.$$

Show that the reduced density matrix on $\mathbb{H}$ derived from this state vector is precisely $\hat{\rho}$. Thus, conclude that every density matrix can be understood as the reduced state of a pure state on a Hilbert space of sufficiently large dimension. Explain that there are infinitely many ways to “purify” a density matrix in this way.

- (c) Show that the usual state vector definitions of operator summary, correlation, and spread for operators that act only in $\mathbb{H}$ with this state vector $|\Psi_{\text{total}}\rangle$ reduce to the density matrix definitions we have given for operator summary, correlation, and spread.

Problem 9.3: Action for Quantum Mechanics. Consider a density matrix $\hat{\rho}(t)$ and a unitary operator $\hat{U}(t)$ on a Hilbert space. (Do not assume this $\hat{U}(t)$ to be the time evolution operator just because we are using the letter U).

- (a) Define the velocity operator $\hat{V}(t)$ and the variation operator $\delta\hat{\theta}(t)$ by:

$$\hat{V}(t) = i\hbar \frac{d\hat{U}}{dt} \hat{U}^\dagger, \quad \delta\hat{\theta}(t) = i\hbar \delta\hat{U} \hat{U}^\dagger \quad (9.1.157)$$

where $\delta\hat{U}$ represents a general variation of $\hat{U}$ that preserves unitarity. Show that $\hat{V}$ and $\delta\hat{\theta}$ are self-adjoint and that there are no other constraints placed on them from the unitarity of $\hat{U}$.

- (b) Show that under variations of $\hat{U}$:

$$\delta\hat{V} = \frac{d}{dt} \delta\hat{\theta} + \frac{i}{\hbar} [\delta\hat{\theta}, \hat{V}]. \quad (9.1.158)$$

- (c) Consider (for Hamiltonian operator $\hat{H}(t)$) the action:

$$S[\hat{\rho}, \hat{U}] = \int_{t_0}^{t_f} \text{Tr}(\hat{\rho}(\hat{V} - \hat{H})) dt. \quad (9.1.159)$$

Show that the variation of this action under variations which preserve the initial and final values of $\hat{U}$

yields:

$$\delta S = \int_{t_0}^{t_f} \text{Tr} \left(\delta \hat{\rho} (\hat{V} - \hat{H}) - \delta \hat{\theta} \left(\frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar} [\hat{\rho}, \hat{V}] \right) \right) dt. \quad (9.1.160)$$

Thus, demonstrate the equations of motion produced by this action are precisely:

$$i\hbar \frac{d\hat{U}}{dt} = \hat{H}\hat{U}, \quad \frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar} [\hat{\rho}, \hat{H}] = 0. \quad (9.1.161)$$

The first shows that $\hat{U}$ does indeed become the time evolution operator and $\hat{\rho}$ satisfies the von Neumann equation as desired. Thus, this action is the action for quantum mechanics.

9.2 The Classical Limit

Quantum mechanics is our status quo best fundamental formalism for physics. However, very often classical physics is in excellent agreement with experiment. In this section we will understand thoroughly how classical physics emerges out of quantum mechanics under appropriate conditions. Quantum dynamics is fully specified by the Hamiltonian operator $\hat{H}$ appearing in the von Neumann equation whereas classical dynamics is fully specified by a classical Hamiltonian function $\mathcal{H}_{\text{cl}}$. Whatever $\hat{H}$ a quantum system has thus will imply a particular $\mathcal{H}_{\text{cl}}$ whenever that quantum system is well approximated by classical mechanics.

Consider a quantum system on a configuration Hilbert space with d coordinate operators $\hat{Q}^a$ and their conjugate momentum operators $\hat{P}_a$. Automatically these operators satisfy the canonical commutation relations in (9.1.9). By Dirac's theorem (9.1.152), their operator summaries are canonically conjugate variables in the classical sense:

$$\{\langle\hat{Q}^a\rangle, \langle\hat{Q}^b\rangle\} = 0, \quad \{\langle\hat{Q}^a\rangle, \langle\hat{P}_b\rangle\} = \delta_b^a, \quad \{\langle\hat{P}_a\rangle, \langle\hat{P}_b\rangle\} = 0. \quad (9.2.1)$$

Define $\bar{Q}^a = \langle\hat{Q}^a\rangle$ and $\bar{P}_a = \langle\hat{P}_a\rangle$ as shorthand for these quantities.

9.2.1 The Weyl Transform

In order to get a classical Hamiltonian function out of the Hamiltonian operator, we need some reasonable way of mapping an operator on Hilbert space to a function on classical phase space. We can find a reasonable such map by studying the matrix elements of the operator. From the Hamiltonian operator $\hat{H}(t)$, define the complex valued function $\zeta(t, Q, P)$ by the matrix element combination:

$$\zeta(t, Q, P) = \frac{\langle P | \hat{H}(t) | Q \rangle}{\langle P | Q \rangle}. \quad (9.2.2)$$

The fact that $\hat{H}$ is self-adjoint imposes conditions on ζ . In particular:

$$\zeta^*(t, Q, P) = \frac{\langle Q | \hat{H}^\dagger | P \rangle}{\langle Q | P \rangle} = \frac{1}{\langle Q | P \rangle} \langle Q | \int | P' \rangle \langle P' | Q' \rangle \langle Q' | \zeta(t, Q', P') d^d Q' d^d P' | P \rangle \quad (9.2.3)$$

$$= \int \frac{\langle Q | P' \rangle \langle P' | Q' \rangle \langle Q' | P \rangle}{\langle Q | P \rangle} \zeta(t, Q', P') d^d Q' d^d P' \quad (9.2.4)$$

$$= \int e^{-\frac{i}{\hbar}(Q^a - Q'^a)(P_a - P'_a)} \zeta(t, Q', P') \frac{d^d Q' d^d P'}{(2\pi\hbar)^d}. \quad (9.2.5)$$

Thus ζ and ζ^* have a very complicated relationship with each other. We can gradually disentangle this relationship by Fourier transforming. Consider the Fourier transform of both sides with respect to P :

$$\int e^{-i\lambda^a P_a} \zeta^*(t, Q, P) d^d P = \int e^{\frac{i}{\hbar}(Q^a - Q'^a)P'_a} e^{-\frac{i}{\hbar}(\hbar\lambda^b + Q'^b - Q'^b)P_b} \zeta(t, Q', P') \frac{d^d Q' d^d P'}{(2\pi\hbar)^d} d^d P \quad (9.2.6)$$

$$= \int e^{\frac{i}{\hbar}(Q^a - Q'^a)P'_a} \delta(Q' - Q - \hbar\lambda) \zeta(t, Q', P') d^d Q' d^d P' \quad (9.2.7)$$

$$= \int e^{-i\lambda^a P'_a} \zeta(t, Q + \hbar\lambda, P') d^d P'. \quad (9.2.8)$$

Now the two sides look much more similar. We can make them look even more similar by shifting the value of Q^a to $Q^a - \frac{\hbar\lambda^a}{2}$:

$$\int e^{-i\lambda^a P'_a} \zeta^* \left(t, Q - \frac{\hbar\lambda}{2}, P' \right) d^d P' = \int e^{-i\lambda^a P'_a} \zeta \left(t, Q + \frac{\hbar\lambda}{2}, P' \right) d^d P'. \quad (9.2.9)$$

Inverse Fourier transform this with respect to λ back into P :

$$\int e^{i\lambda^a (P_a - P'_a)} \zeta^* \left(t, Q - \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d} = \int e^{i\lambda^a (P_a - P'_a)} \zeta \left(t, Q + \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d} \quad (9.2.10)$$

$$\implies \left(\int e^{-i\lambda^a (P_a - P'_a)} \zeta \left(t, Q - \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d} \right)^* = \int e^{i\lambda^a (P_a - P'_a)} \zeta \left(t, Q + \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d}. \quad (9.2.11)$$

If we now rename the integration variable λ^a on the left-hand side to $-\lambda^a$, we find:

$$\left(\int e^{i\lambda^a (P_a - P'_a)} \zeta \left(t, Q + \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d} \right)^* = \int e^{i\lambda^a (P_a - P'_a)} \zeta \left(t, Q + \frac{\hbar\lambda}{2}, P' \right) \frac{d^d \lambda d^d P'}{(2\pi)^d}. \quad (9.2.12)$$

Therefore, the self-adjointness of $\hat{H}$ ensures that this complicated integral expression involving ζ is a real-valued function (as it is equal to its own complex conjugate). Define then the function $H(t, Q, P)$ by this combination:

$$H(t, Q, P) = \int e^{i\lambda^a(P_a - P'_a)} \zeta\left(t, Q + \frac{\hbar\lambda}{2}, P'\right) \frac{d^d\lambda d^dP'}{(2\pi)^d} \implies H^*(t, Q, P) = H(t, Q, P). \quad (9.2.13)$$

By using the definition of ζ in terms of $\hat{H}$, we can give H a simpler and more direct definition in terms of $\hat{H}$:

$$H(t, Q, P) = \int e^{i\lambda^a(P_a - P'_a)} \frac{\langle P' | \hat{H} | Q + \frac{\hbar\lambda}{2} \rangle}{\langle P' | Q + \frac{\hbar\lambda}{2} \rangle} \frac{d^d\lambda d^dP'}{(2\pi)^d} \quad (9.2.14)$$

$$= (2\pi\hbar)^{\frac{d}{2}} \int e^{i\lambda^a P_a + \frac{i}{\hbar}(Q^a - \frac{\hbar\lambda^a}{2})P'_a} \langle P' | \hat{H} | Q + \frac{\hbar\lambda}{2} \rangle \frac{d^d\lambda d^dP'}{(2\pi)^d} \quad (9.2.15)$$

$$= (2\pi\hbar)^d \int e^{i\lambda^a P_a} \langle Q - \frac{\hbar\lambda}{2} | P' \rangle \langle P' | \hat{H} | Q + \frac{\hbar\lambda}{2} \rangle \frac{d^d\lambda d^dP'}{(2\pi)^d} \quad (9.2.16)$$

$$= \int e^{i\lambda^a P_a} \langle Q - \frac{\hbar\lambda}{2} | \hat{H} | Q + \frac{\hbar\lambda}{2} \rangle \hbar^d d^d\lambda. \quad (9.2.17)$$

Finally changing to the new integration variable $q^a = \hbar\lambda$, we have:

$$H(t, Q, P) = \int e^{\frac{i}{\hbar}q^a P_a} \left\langle Q - \frac{q}{2} \left| \hat{H}(t) \right| Q + \frac{q}{2} \right\rangle d^d q. \quad (9.2.18)$$

We can recover $\hat{H}$ from H by again Fourier transforming with respect to P :

$$\int e^{-\frac{i}{\hbar}q^a P_a} H(t, Q, P) d^d P = (2\pi\hbar)^d \left\langle Q - \frac{q}{2} \left| \hat{H} \right| Q + \frac{q}{2} \right\rangle. \quad (9.2.19)$$

Now replace Q with $\frac{Q+Q'}{2}$ and q with $Q - Q'$:

$$\int e^{\frac{i}{\hbar}P_a(Q'^a - Q^a)} H\left(t, \frac{Q+Q'}{2}, P\right) d^d P = (2\pi\hbar)^d \langle Q' | \hat{H} | Q \rangle. \quad (9.2.20)$$

Finally multiplying $|Q'\rangle\langle Q|$ onto both sides and integrating over both Q and Q' , using that the $|Q\rangle$ form a complete set of states, we have:

$$\hat{H} = \int e^{\frac{i}{\hbar}P_a(Q'^a - Q^a)} H\left(t, \frac{Q+Q'}{2}, P\right) |Q'\rangle\langle Q| d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d}. \quad (9.2.21)$$

So, the relationship between $\hat{H}$ and H is invertible. This is a very nice discovery! We now see that for any operator on Hilbert space (in this case we used $\hat{H}$), we can define a function on phase space associated to it by (9.2.18). The original operator can be recovered from that function by (9.2.21). In the case that operator is self-adjoint, the associated function is real-valued (the converse holds as well, from the inverse formula). This map relating functions on classical phase space and operators on quantum Hilbert space is known as the **Weyl transform**. We write $\hat{\mathcal{W}}$ to mean the Weyl transform that takes a function on classical phase space and returns an operator on Hilbert space and $\mathcal{W}^{-1}$ to mean the inverse Weyl transform:

$$\hat{H} = \hat{\mathcal{W}}(H), \quad H = \mathcal{W}^{-1}(\hat{H}). \quad (9.2.22)$$

The function H given by the inverse Weyl transform of $\hat{H}$ is called the **Wigner function** associated to $\hat{H}$. The Weyl transform has several nice properties we will uncover over the rest of the section. It should be stressed that we have **NOT** shown that $H(t, Q, P)$ is the classical Hamiltonian. In fact, we will show that such a claim is generally wrong. The classical Hamiltonian is related to $H(t, Q, P)$ but that relationship is unambiguously unequal.

As written in (9.2.21), the Weyl transform does not seem symmetric in how it treats the coordinates and their conjugate momenta. However, we can make it manifestly symmetric between them with a bit of effort. To begin, rename the integration variable Q' to $Q - \hbar\lambda$ (with λ the new integration variable):

$$\hat{H} = \int e^{-\frac{i}{\hbar}\lambda^a P_a} H\left(t, Q - \frac{\hbar\lambda}{2}, P\right) |Q - \hbar\lambda\rangle\langle Q| d^d\lambda \frac{d^d Q d^d P}{(2\pi)^d}. \quad (9.2.23)$$

We can rewrite $|Q - \hbar\lambda\rangle$ more simply using:

$$|Q - \hbar\lambda\rangle = \int |P\rangle\langle P|Q - \hbar\lambda\rangle d^d P = \int |P\rangle e^{i\lambda^a P_a} \frac{e^{-\frac{i}{\hbar} Q^a P_a}}{(2\pi\hbar)^{\frac{d}{2}}} d^d P = \int e^{i\lambda^a P_a} |P\rangle\langle P|Q\rangle d^d P = e^{i\lambda^a \hat{P}_a} |Q\rangle \quad (9.2.24)$$

$$\implies \hat{H} = \int e^{i\lambda^a \hat{P}_a} e^{-i\lambda^b P_b} H\left(t, Q - \frac{\hbar\lambda}{2}, P\right) |Q\rangle\langle Q| d^d \lambda \frac{d^d Q d^d P}{(2\pi)^d}. \quad (9.2.25)$$

We can rewrite $|Q\rangle\langle Q|$ nicely by noting:

$$\delta(\hat{Q} - Q) = \int \delta(\hat{Q} - Q)|Q'\rangle\langle Q'|d^d Q' = \int \delta(Q' - Q)|Q'\rangle\langle Q'|d^d Q' = |Q\rangle\langle Q| \quad (9.2.26)$$

$$\implies \hat{H} = \int e^{i\lambda^a \hat{P}_a} e^{-i\lambda^b P_b} \delta(\hat{Q} - Q) H\left(t, Q - \frac{\hbar\lambda}{2}, P\right) d^d \lambda \frac{d^d Q d^d P}{(2\pi)^d}. \quad (9.2.27)$$

We can turn this Dirac delta into another exponential by using the fundamental Fourier integral:

$$\delta(\hat{Q} - Q) = \int \delta(Q' - Q)|Q'\rangle\langle Q'|d^d Q' = \int \frac{e^{ik_a(Q'^a - Q^a)}}{(2\pi)^d} |Q'\rangle\langle Q'|d^d Q' d^d k = \int \frac{e^{ik_a(\hat{Q}^a - Q^a)}}{(2\pi)^d} d^d k \quad (9.2.28)$$

$$\implies \hat{H} = \int e^{i\lambda^a \hat{P}_a} e^{ik_b \hat{Q}^b} e^{-ik_c Q^c - i\lambda^c P_c} H\left(t, Q - \frac{\hbar\lambda}{2}, P\right) \frac{d^d \lambda d^d k d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.29)$$

The two operator exponentials cannot be combined the way that numerical exponentials can be because $\hat{Q}^a$ and $\hat{P}_a$ do not commute. However, using the Baker-Campbell-Hausdorff formula, we can combine them in a more complicated way. In problem 8.20, we showed that for operators $\hat{A}$ and $\hat{B}$ satisfying $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$:

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]}. \quad (9.2.30)$$

Of interest to us is $\hat{A} = i\lambda^a \hat{P}_a$ and $\hat{B} = ik_b \hat{Q}^b$. Automatically, using the canonical commutation relation between $\hat{Q}^a$ and $\hat{P}_b$, we have that $[\hat{A}, \hat{B}] = i\hbar\lambda^a k_a \mathbb{1}$, which because it is proportional to the identity operator commutes with $\hat{A}$ and $\hat{B}$. Therefore:

$$e^{i\lambda^a \hat{P}_a} e^{ik_b \hat{Q}^b} = e^{ik_a \hat{Q}^a + i\lambda^a \hat{P}_a} e^{\frac{i\hbar}{2}\lambda^b k_b} \quad (9.2.31)$$

$$\implies \hat{H} = \int e^{ik_a \hat{Q}^a + i\lambda^a \hat{P}_a} e^{-ik_b(Q^b - \frac{\hbar\lambda^b}{2}) - i\lambda^b P_b} H\left(t, Q - \frac{\hbar\lambda}{2}, P\right) \frac{d^d \lambda d^d k d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.32)$$

For the final step, simply shift the integration variable Q to $Q + \frac{\hbar\lambda}{2}$:

$$\boxed{\hat{H} = \int e^{ik_a(\hat{Q}^a - Q^a) + i\lambda^a(\hat{P}_a - P_a)} H(t, Q, P) \frac{d^d \lambda d^d k d^d Q d^d P}{(2\pi)^{2d}}.} \quad (9.2.33)$$

This formula is now manifestly symmetric in its treatment of the coordinates and momenta.

The formula (9.2.33) can help us understand precisely what the Weyl transform is really doing to the function H . First, it Fourier transforms the full phase space dependence of H from (Q, P) to (k, λ) then it inverse Fourier transforms back from (k, λ) into the operators $(\hat{Q}, \hat{P})$ in a way symmetric between $\hat{Q}$ and $\hat{P}$. Thus, it essentially replaces Q and P with $\hat{Q}$ and $\hat{P}$ in an appropriately symmetric way. Let us now compute explicitly what I mean by “appropriately symmetric”. Let (q, p) be a point in classical phase space. By shifting the definitions of Q and P in (9.2.33) we can rewrite it as:

$$\hat{H} = \int e^{ik_a(\hat{Q}^a - q^a) + i\lambda^a(\hat{P}_a - p_a)} e^{-ik_b Q^b - i\lambda^b P_b} H(t, q + Q, p + P) \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.34)$$

Next, Taylor expand the operator exponential:

$$e^{ik_a(\hat{Q}^a - q^a) + i\lambda^a(\hat{P}_a - p_a)} = \sum_{N=0}^{\infty} \frac{i^N}{N!} \left(k_a(\hat{Q}^a - q^a) + \lambda^a(\hat{P}_a - p_a) \right)^N. \quad (9.2.35)$$

If we expand out the N^{th} power operator polynomial here, it will contain once each every possible order of factors $k_a(\hat{Q}^a - q^a)$ and $\lambda^a(\hat{P}_a - p_a)$ so that the total number of factors of both is N . Recall the definition of

the symmetrized product of operators from (8.2.103). Then, the operator binomial theorem is:

$$(\hat{A} + \hat{B})^N = \sum_{n=0}^N \frac{N!}{n!(N-n)!} \text{Sym}(\hat{A}, \dots, \hat{A}(n \text{ copies}), \hat{B}, \dots, \hat{B}(N-n \text{ copies})). \quad (9.2.36)$$

Using this in the exponential series:

$$e^{ik_a(\hat{Q}^a - q^a) + i\lambda^a(\hat{P}_a - p_a)} = \sum_{N=0}^{\infty} \sum_{n=0}^N \frac{i^N}{N!} \frac{N!}{n!(N-n)!} \text{Sym}(k_a(\hat{Q}^a - q^a)(n \text{ copies}), \lambda^b(\hat{P}_b - p_b)(N-n \text{ copies})) \quad (9.2.37)$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{i^{m+n}}{m!n!} k_{a_1} \dots k_{a_m} \lambda^{b_1} \dots \lambda^{b_n} \text{Sym}((\hat{Q}^{a_1} - q^{a_1}), \dots, (\hat{Q}^{a_m} - q^{a_m}), (\hat{P}_{b_1} - p_{b_1}), \dots, (\hat{P}_{b_n} - p_{b_n})). \quad (9.2.38)$$

For brevity, define the operators:

$$\hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n} = \text{Sym}((\hat{Q}^{a_1} - q^{a_1}), \dots, (\hat{Q}^{a_m} - q^{a_m}), (\hat{P}_{b_1} - p_{b_1}), \dots, (\hat{P}_{b_n} - p_{b_n})). \quad (9.2.39)$$

Importantly, these operators do not depend on any of our integration variables, so we can freely move them around the integral. Returning to the integral, we have:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{i^{m+n}}{m!n!} \hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n} \int k_{a_1} \dots k_{a_m} \lambda^{b_1} \dots \lambda^{b_n} e^{-ik_c Q^c - i\lambda^c P_c} H(t, q + Q, p + P) \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.40)$$

Each factor of k_a can be rewritten as coming from a Q^a derivative of the exponential. Similarly, each factor of λ^a can be rewritten as coming from a P_a derivative of the exponential. Thus:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{m!n!} \hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n} \int H(t, q + Q, p + P) \frac{\partial}{\partial Q^{a_1}} \dots \frac{\partial}{\partial Q^{a_m}} \frac{\partial}{\partial P_{b_1}} \dots \frac{\partial}{\partial P_{b_n}} e^{-ik_c Q^c - i\lambda^c P_c} \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}} \quad (9.2.41)$$

We can now integrate all of these derivatives by parts all derivatives off of the exponential and onto H . Doing so we will acquire no surface terms because the regulator (exponential damping) used in the definition of the Fourier integral kills them. Therefore:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n}}{m!n!} \int e^{-ik_c Q^c - i\lambda^c P_c} \frac{\partial}{\partial Q^{a_1}} \dots \frac{\partial}{\partial Q^{a_m}} \frac{\partial}{\partial P_{b_1}} \dots \frac{\partial}{\partial P_{b_n}} H(t, q + Q, p + P) \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.42)$$

Because $H(t, q + Q, p + P)$ depends only on Q through $q + Q$, differentiating it with respect to Q is the same as differentiating with respect to q . Similarly, differentiating it with respect to P is the same as differentiating it with respect to p and so:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n}}{m!n!} \frac{\partial}{\partial q^{a_1}} \dots \frac{\partial}{\partial q^{a_m}} \frac{\partial}{\partial p_{b_1}} \dots \frac{\partial}{\partial p_{b_n}} \int e^{-ik_c Q^c - i\lambda^c P_c} H(t, q + Q, p + P) \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.43)$$

Now the k and λ integrals can be done easily using the fundamental Fourier integral:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\hat{M}^{a_1 \dots a_m}_{b_1 \dots b_n}}{m!n!} \frac{\partial}{\partial q^{a_1}} \dots \frac{\partial}{\partial q^{a_m}} \frac{\partial}{\partial p_{b_1}} \dots \frac{\partial}{\partial p_{b_n}} \int (2\pi)^{2d} \delta(Q) \delta(P) H(t, q + Q, p + P) \frac{d^d k d^d \lambda d^d Q d^d P}{(2\pi)^{2d}}. \quad (9.2.44)$$

The Q and P integrals are now automatic, giving us ultimately:

$$\hat{H} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{m!n!} \frac{\partial^{m+n} H(t, q, p)}{\partial q^{a_1} \dots \partial q^{a_m} \partial p_{b_1} \dots \partial p_{b_n}} \text{Sym}(\hat{Q}^{a_1} - q^{a_1}, \dots, \hat{Q}^{a_m} - q^{a_m}, \hat{P}_{b_1} - p_{b_1}, \dots, \hat{P}_{b_n} - p_{b_n}). \quad (9.2.45)$$

The original point (q, p) was arbitrary and so the right hand side is independent of the choice of (q, p) even though it is not manifest. The right hand side here is just the Taylor series for the function $H(t, q, p)$ when

one wishes to formally evaluate it at $(\hat{Q}, \hat{P})$ where the prescription for how to resolve any ordering ambiguities is to fully symmetrize the operator products. This is the precise meaning of “appropriately symmetric”. Thus formally we write:

$$\hat{H}(t) = \text{Sym}(H(t, \hat{Q}, \hat{P})) \quad (9.2.46)$$

where the precise meaning of the right hand side here is defined by (9.2.45).

9.2.2 Classicality Conditions

The variables $\bar{Q}^a = \langle \hat{Q}^a \rangle$ and $\bar{P}_a = \langle \hat{P}_a \rangle$ are the classical degrees of freedom which should satisfy appropriate classical equations of motion (Hamilton’s equations from some Hamiltonian $\mathcal{H}_{\text{cl}}(t, \bar{Q}, \bar{P})$) in the classical limit. Using Ehrenfest’s theorem we know that their exact quantum equations of motion are:

$$\frac{d\langle \hat{Q}^a \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{Q}^a, \hat{H}] \rangle, \quad \frac{d\langle \hat{P}_a \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{P}_a, \hat{H}] \rangle. \quad (9.2.47)$$

Using the Weyl transform, we can make this look even more suggestive. Using (9.2.21) and recalling our ability to integrate by parts, we find for the first of these:

$$\frac{1}{i\hbar} [\hat{Q}^a, \hat{H}] = \frac{1}{i\hbar} \int e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} H\left(t, \frac{Q + Q'}{2}, P\right) (\hat{Q}^a |Q'\rangle \langle Q| - |Q'\rangle \langle Q| \hat{Q}^a) d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.48)$$

$$= \frac{1}{i\hbar} \int H\left(t, \frac{Q + Q'}{2}, P\right) (Q'^a - Q^a) e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} |Q'\rangle \langle Q| d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.49)$$

$$= - \int H\left(t, \frac{Q + Q'}{2}, P\right) \frac{\partial}{\partial P_a} e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} |Q'\rangle \langle Q| d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.50)$$

$$= \int e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} \frac{\partial H}{\partial P_a} \left(t, \frac{Q + Q'}{2}, P\right) |Q'\rangle \langle Q| d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.51)$$

$$= \hat{\mathcal{W}} \left(\frac{\partial H}{\partial P_a} \right). \quad (9.2.52)$$

To evaluate the second, it is useful to recall (9.1.8), from which we have (by taking the adjoint):

$$\langle Q | \hat{P}_a = -i\hbar \frac{\partial \langle Q |}{\partial Q^a} \implies \hat{P}_a |Q\rangle = i\hbar \frac{\partial |Q\rangle}{\partial Q^a}. \quad (9.2.53)$$

Then, again using (9.2.21):

$$\frac{1}{i\hbar} [\hat{P}_a, \hat{H}] = \frac{1}{i\hbar} \int e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} H\left(t, \frac{Q + Q'}{2}, P\right) \left(i\hbar \frac{\partial |Q'\rangle}{\partial Q'^a} \langle Q| + i\hbar |Q'\rangle \frac{\partial \langle Q|}{\partial Q^a} \right) d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.54)$$

$$= - \int |Q'\rangle \langle Q| \left(\frac{\partial}{\partial Q'^a} + \frac{\partial}{\partial Q^a} \right) \left(e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} H\left(t, \frac{Q + Q'}{2}, P\right) \right) d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.55)$$

$$= - \int |Q'\rangle \langle Q| e^{\frac{i}{\hbar} P_b(Q'^b - Q^b)} \frac{\partial H(t, q, P)}{\partial q^a} \Big|_{q=\frac{Q+Q'}{2}} d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.56)$$

$$= -\hat{\mathcal{W}} \left(\frac{\partial H}{\partial Q^a} \right). \quad (9.2.57)$$

Because of these nice results, it is instructive to use them to define the operator derivative:

$$\frac{\partial \hat{H}}{\partial \hat{Q}^a} \stackrel{\text{def}}{=} \hat{\mathcal{W}} \left(\frac{\partial}{\partial Q^a} \mathcal{W}^{-1}(\hat{H}) \right), \quad \frac{\partial \hat{H}}{\partial \hat{P}_a} \stackrel{\text{def}}{=} \hat{\mathcal{W}} \left(\frac{\partial}{\partial P_a} \mathcal{W}^{-1}(\hat{H}) \right). \quad (9.2.58)$$

Then, Ehrenfest’s theorem for $\langle \hat{Q}^a \rangle$ and $\langle \hat{P}_a \rangle$ gives the exact quantum equations:

$$\frac{d\langle \hat{Q}^a \rangle}{dt} = \left\langle \frac{\partial \hat{H}}{\partial \hat{P}_a} \right\rangle, \quad \frac{d\langle \hat{P}_a \rangle}{dt} = - \left\langle \frac{\partial \hat{H}}{\partial \hat{Q}^a} \right\rangle. \quad (9.2.59)$$

These are obviously visually similar to Hamilton’s equations of motion, however we still need to think about in what circumstances classical mechanics should be approximately valid to truly make the connection.

In order for $\bar{Q}^a$ and $\bar{P}_a$ to satisfy classical equations of motion in terms of a Hamiltonian $\mathcal{H}_{\text{cl}}(t, \bar{Q}, \bar{P})$, they must (in the classical limit) decouple from all of the other degrees of freedom present in the density matrix and only interact with each other. One way we can package all of these other degrees of freedom is in

the various moments of the density matrix (meaning the operator summaries of symmetrized products of $\hat{Q}$ and $\hat{P}$). The full quantum theory is always described by the full Hamiltonian $\mathcal{H}_{\text{qm}} = \text{Tr}(\hat{\rho}\hat{H})$ and so to have this decoupling we must have in the classical limit $\mathcal{H}_{\text{qm}} = \mathcal{H}_{\text{cl}} + \text{small corrections}$. Using (9.2.45) with the choice $(q, p) = (\bar{Q}, \bar{P})$, we have:

$$\mathcal{H}_{\text{qm}} = \sum_{\substack{m=0 \\ n=0}}^{\infty, \infty} \frac{1}{m!n!} \frac{\partial^{m+n} H(t, \bar{Q}, \bar{P})}{\partial \bar{Q}^{a_1} \dots \partial \bar{Q}^{a_m} \partial \bar{P}_{b_1} \dots \partial \bar{P}_{b_n}} \langle \text{Sym}(\hat{Q}^{a_1} - \bar{Q}^{a_1}, \dots, \hat{Q}^{a_m} - \bar{Q}^{a_m}, \hat{P}_{b_1} - \bar{P}_{b_1}, \dots, \hat{P}_{b_n} - \bar{P}_{b_n}) \rangle \quad (9.2.60)$$

$$= H(t, \bar{Q}, \bar{P}) + \frac{1}{2} \frac{\partial^2 H}{\partial \bar{Q}^a \partial \bar{Q}^b} \text{Cor}(\hat{Q}^a, \hat{Q}^b) + \frac{\partial^2 H}{\partial \bar{Q}^a \partial \bar{P}_b} \text{Cor}(\hat{Q}^a, \hat{P}_b) + \frac{1}{2} \frac{\partial^2 H}{\partial \bar{P}_a \partial \bar{P}_b} \text{Cor}(\hat{P}_a, \hat{P}_b) + \text{Higher Order Terms.} \quad (9.2.61)$$

The choice $(q, p) = (\bar{Q}, \bar{P})$ is the only choice so that the $m = 1, n = 0$ and $m = 0, n = 1$ terms vanish and so that the higher order terms all become moments evaluated about the classical variables $\bar{Q}, \bar{P}$. Thus, we can see that the series terms correspond to summaries of increasingly higher powers of deviations of the density matrix from its central summary position and momentum values and so when the density matrix is essentially localized (with respect to our experimental resolution) in both position and momentum, the higher order terms in this series will be suppressed.

For the rest of this and the next subsection, it is notationally simplest to consider a one dimensional configuration space $d = 1$. None of the logic we give needs to be changed for $d > 1$, but the indices become annoying to manage, and so for readability we will take $d = 1$ for now. Let w_Q be our experimental resolution with which we can distinguish coordinates and w_P be the experimental resolution with which we can distinguish momenta. A density matrix is approximately classical when its central moments are small compared to the experimental resolution:

$$\text{Approximate Classicality} \rightarrow \frac{\langle \text{Sym}(\hat{Q} - \bar{Q}(m \text{ copies}), \hat{P} - \bar{P}(n \text{ copies})) \rangle}{w_Q^m w_P^n} \ll 1. \quad (9.2.62)$$

This is because if the density matrix is such that the operator spread of an operator $\hat{O}$ is much smaller than our experimental resolution for that operator's summary $\langle \hat{O} \rangle$, then the behavior of that operator on the density matrix is well approximated by simply $\langle \hat{O} \rangle \mathbb{1}$. Therefore, if our experimental resolution for our coordinates and momenta are large compared to their spreads, the coordinate and momenta operators can effectively be identified with their summary values.

The (m, n) order variation $\Delta^{(m, n)} G(q, p)$ of a quantity G at (q, p) is defined by the differential variation in G over the region of standard experimental resolution:

$$\Delta^{(m, n)} G(q, p) = \frac{\partial^{m+n} G(q, p)}{\partial q^m \partial p^n} w_Q^m w_P^n. \quad (9.2.63)$$

Then, $\mathcal{H}_{\text{qm}}$ can be written exactly as:

$$\mathcal{H}_{\text{qm}} = \sum_{\substack{m=0 \\ n=0}}^{\infty, \infty} \frac{1}{m!n!} \Delta^{(m, n)} H(t, \bar{Q}, \bar{P}) \frac{\langle \text{Sym}(\hat{Q} - \bar{Q}(m \text{ copies}), \hat{P} - \bar{P}(n \text{ copies})) \rangle}{w_Q^m w_P^n}. \quad (9.2.64)$$

So, if the density matrix is approximately classical and the function H has small variations over the window of experimental resolution, then the value of $\mathcal{H}_{\text{qm}}$ is approximately given by the low order terms in this series. Because of the classicality conditions, approximate classicality only extends to quantities of interest satisfying the hierarchy of scales in which the distance in classical phase space one must travel to vary them significantly is much larger than the experimental resolution which is in turn much larger than the spread of the density matrix. The first term in the series is purely $H(t, \bar{Q}, \bar{P})$ and thus has the correct classical degrees of freedom. All of the higher order terms depend on increased numbers of degrees of freedom. So, in the classical limit this first term should dominate. This domination is required in order for the necessary decoupling of $\bar{Q}$ and $\bar{P}$ from the other degrees of freedom in the density matrix to occur, as only that first term depends exclusively on $\bar{Q}$ and $\bar{P}$. Thus, in the classical limit, we have $\mathcal{H}_{\text{qm}} = H(t, \bar{Q}, \bar{P}) + \text{small corrections}$. We argued previously that in the classical limit $\mathcal{H}_{\text{qm}} = \mathcal{H}_{\text{cl}}(t, \bar{Q}, \bar{P}) + \text{small corrections}$. Thus, the imprecise relationship between H and $\mathcal{H}_{\text{cl}}$ is that:

$$\boxed{H(t, \bar{Q}, \bar{P}) = \mathcal{H}_{\text{cl}}(t, \bar{Q}, \bar{P}) + \text{small corrections}} \quad (9.2.65)$$

where the precise relationship we will develop by studying exactly what is meant by “small corrections”.

It is impossible to exactly realize the classical limit because the density matrix cannot be simultaneously exactly localized in both coordinate space and momentum space. This is analogous to the fact that it is impossible to exactly realize the nonrelativistic limit for any system in which there is motion as at any nonzero velocity there are relativistic corrections present, however small in consideration of experimental resolution. The inability to localize the density matrix simultaneously in coordinate and momentum space is captured by the uncertainty theorem:

$$\text{Spr}(\hat{Q})\text{Spr}(\hat{P}) \geq \frac{\hbar^2}{4}. \quad (9.2.66)$$

Through use of the uncertainty theorem and (9.2.62), we find that approximate classicality requires:

$$\frac{\hbar^2}{4w_P^2} \ll \text{Spr}(\hat{Q}) \ll w_Q^2, \quad \frac{\hbar^2}{4w_Q^2} \ll \text{Spr}(\hat{P}) \ll w_P^2, \quad w_Q w_P \gg \frac{\hbar}{2} \quad (9.2.67)$$

exactly along the lines of (8.5.168), (8.5.169), (8.5.171). Thus, $\hbar$ formally acts as a parameter which controls how small the simultaneous spreads can be made, in the way that $\frac{1}{c}$ in the nonrelativistic limit formally acts as a parameter which controls velocity corrections. Just as c is always the same finite value and the nonrelativistic theory is an approximate effective theory at low velocities, $\hbar$ is always the same finite value and the “classical theory” in which $\hat{Q}$ and $\hat{P}$ form a closed system of equations is an appropriate approximate effective theory when the above scaling hierarchy is satisfied. Because of this, formally $\hbar \rightarrow 0$ is necessary (but not sufficient) for the classical limit in the same way that $\frac{1}{c} \rightarrow 0$ is necessary for the nonrelativistic limit. $\hbar \rightarrow 0$ is required to be able to simultaneously localize the density matrix in position and momentum space. However, we must then also perform that localization.

In problem 8.14 we defined the dilation generator:

$$\hat{G} = \frac{(\hat{Q} - q)(\hat{P} - p) + (\hat{P} - p)(\hat{Q} - q)}{2} \quad (9.2.68)$$

and the dilation transformation:

$$\hat{D}(\varepsilon) = e^{-\frac{i}{\hbar}\varepsilon\hat{G}}. \quad (9.2.69)$$

From these, we showed:

$$\hat{D}^\dagger \hat{Q} \hat{D} = q + e^\varepsilon (\hat{Q} - q), \quad \hat{D}^\dagger \hat{P} \hat{D} = p + e^{-\varepsilon} (\hat{P} - p). \quad (9.2.70)$$

We would like to localize the density matrix about $\bar{Q}$ in position space and $\bar{P}$ in position space and so we will use dilation with center $(q, p) = (\bar{Q}, \bar{P})$. Then, with this choice, the density matrix spread as a function of ε becomes:

$$\text{Spr}_\varepsilon(\hat{Q}) = e^{2\varepsilon} \text{Spr}_0(\hat{Q}), \quad \text{Spr}_\varepsilon(\hat{P}) = e^{-2\varepsilon} \text{Spr}_0(\hat{P}) \quad (9.2.71)$$

where Spr_ε is computed using the dilated density matrix:

$$\hat{\rho}(\varepsilon) = \hat{D}(\varepsilon) \hat{\rho}_0 \hat{D}^\dagger(\varepsilon) \quad (9.2.72)$$

and $\hat{\rho}_0$ is the base density matrix of the system. In order to localize the density matrix in position space we thus need to take $\varepsilon \rightarrow -\infty$. Define $s = e^\varepsilon$ so that instead we need $s \rightarrow 0$. Then, the moments of the density matrix depend on s as:

$$\langle \text{Sym}(\hat{Q} - \bar{Q}(m \text{ copies}), \hat{P} - \bar{P}(n \text{ copies})) \rangle_\varepsilon = s^{m-n} \langle \text{Sym}(\hat{Q} - \bar{Q}(m \text{ copies}), \hat{P} - \bar{P}(n \text{ copies})) \rangle_0. \quad (9.2.73)$$

Localizing the density matrix in position space will antilocalize it in momentum space unless we first take $\hbar \rightarrow 0$, because their spreads are inversely dependent on ε . To implement this correctly we need to be slightly careful. We would like to keep the expected momentum $\bar{P}$ of the density matrix fixed as it should survive in the classical limit. We can strip off this expected momentum and leave behind a density matrix of expected momentum 0 by recalling the momentum translation operator as defined in (8.5.61) and expressed simply in (8.5.91):

$$e^{\frac{i}{\hbar}p\hat{Q}}|P\rangle = |P+p\rangle \quad (9.2.74)$$

Automatically:

$$e^{\frac{i}{\hbar}p\hat{Q}} \hat{P} e^{-\frac{i}{\hbar}p\hat{Q}} = \int_{-\infty}^{\infty} P e^{\frac{i}{\hbar}p\hat{Q}} |P\rangle \langle P| e^{-\frac{i}{\hbar}p\hat{Q}} dP = \int_{-\infty}^{\infty} P |P+p\rangle \langle P+p| dP = \int_{-\infty}^{\infty} (P-p) |P\rangle \langle P| dP = \hat{P} - p1. \quad (9.2.75)$$

So, if we define the shifted density matrix $\hat{\sigma}$ by:

$$\hat{\sigma} = e^{-\frac{i}{\hbar} \bar{P} \hat{Q}} \hat{\rho}_0 e^{\frac{i}{\hbar} \bar{P} \hat{Q}} \quad (9.2.76)$$

then we have:

$$\langle \hat{P} \rangle_{\sigma} = \text{Tr}(\hat{\sigma} \hat{P}) = \text{Tr} \left(\hat{\rho}_0 e^{\frac{i}{\hbar} \bar{P} \hat{Q}} \hat{P} e^{-\frac{i}{\hbar} \bar{P} \hat{Q}} \right) = \text{Tr}(\hat{\rho}_0 (\hat{P} - \bar{P} \mathbb{1})) = \bar{P} - \bar{P} = 0. \quad (9.2.77)$$

The momentum operator contains a factor of $\hbar$ in its definition and so it is useful to define the $\hat{K}$ operator so that for a wavefunction $|\Psi\rangle$:

$$\hat{K}|\Psi\rangle = \frac{\hat{P}}{\hbar}|\Psi\rangle = -i \int_{-\infty}^{\infty} \frac{\partial \Psi}{\partial Q} |Q\rangle dQ \quad (9.2.78)$$

In terms of these ingredients, $\mathcal{H}_{\text{qm}}$ computed using our dilated density matrix becomes:

$$\mathcal{H}_{\text{qm}} = \langle \hat{H} \rangle_{\varepsilon} = \sum_{\substack{m=0 \\ n=0}}^{\infty, \infty} \frac{\hbar^n s^{m-n}}{m!n!} \frac{\partial^{m+n} H(t, \bar{Q}, \bar{P})}{\partial \bar{Q}^m \partial \bar{P}^n} \langle \text{Sym}(\hat{Q} - \bar{Q} (m \text{ copies}), \hat{K} (n \text{ copies})) \rangle_{\sigma}. \quad (9.2.79)$$

Because this last summary is computed using σ , we need not worry about the scaling of momentum spoiling the value of $\bar{P}$, as it has safely been separated out from that summary and rescaling of 0 by anything remains 0.

The function $H(t, \bar{Q}, \bar{P})$ is an at this time completely unknown function, and so is fully allowed to depend on $\hbar$ as well. So, we write its expansion in terms of $\hbar$ as:

$$H(t, \bar{Q}, \bar{P}) = \sum_{k=0}^{\infty} \hbar^k H^{(k)}(t, \bar{Q}, \bar{P}) \quad (9.2.80)$$

in terms of the $\hbar$ independent pieces $H^{(k)}(t, \bar{Q}, \bar{P})$. Returning this expansion to $\mathcal{H}_{\text{qm}}$ we have:

$$\mathcal{H}_{\text{qm}} = \sum_{\substack{m=0 \\ n=0 \\ k=0}}^{\infty, \infty, \infty} \frac{\hbar^{n+k} s^{m-n}}{m!n!} \frac{\partial^{m+n} H^{(k)}(t, \bar{Q}, \bar{P})}{\partial \bar{Q}^m \partial \bar{P}^n} \langle \text{Sym}(\hat{Q} - \bar{Q} (m \text{ copies}), \hat{K} (n \text{ copies})) \rangle_{\sigma}. \quad (9.2.81)$$

To take the classical limit now we must first take $\hbar \rightarrow 0$ so that it becomes possible to simultaneously localize the density matrix in both coordinates and momenta (again, this is conceptually just like taking $c \rightarrow \infty$ in the nonrelativistic limit):

$$\lim_{\hbar \rightarrow 0^+} \mathcal{H}_{\text{qm}} = \sum_{m=0}^{\infty} \frac{s^m}{m!} \frac{\partial^m H^{(0)}(t, \bar{Q}, \bar{P})}{\partial \bar{Q}^m} \langle (\hat{Q} - \bar{Q})^m \rangle_{\sigma}. \quad (9.2.82)$$

Finally, the $s \rightarrow 0$ limit completes the localization to give the full classical limit:

$$\boxed{\mathcal{H}_{\text{cl}}(t, \bar{Q}, \bar{P}) = \lim_{s \rightarrow 0^+} \lim_{\hbar \rightarrow 0^+} \mathcal{H}_{\text{qm}} = H^{(0)}(t, \bar{Q}, \bar{P})}. \quad (9.2.83)$$

This is the precise statement of (9.2.65), which we could now write as:

$$\boxed{H(t, Q, P) = \mathcal{H}_{\text{cl}}(t, Q, P) + \sum_{n=1}^{\infty} \hbar^n H^{(n)}(t, Q, P)} \quad (9.2.84)$$

with the understanding that the classical limit does nothing to fix $H^{(n)}$ for $n > 0$. The corrections are justified as being called small in the classical limit because formally the classical limit takes $\hbar \rightarrow 0^+$. All of this same logic can be repeated for other quantities of interest besides the Hamiltonian. Therefore, the **the classical limit fixes the $\hbar$ independent piece of each operator's Wigner function to be the corresponding classical function. But, the classical limit says nothing about the $\hbar$ dependent pieces of an operator's Wigner function.**

A scheme for taking a classical theory (and thus an $\mathcal{H}_{\text{cl}}(t, Q, P)$) and assigning it a set of $\hbar$ -corrections $H^{(n)}$ to arrive at a canonical choice of quantum theory (meaning a specific Hamiltonian operator $\hat{H}$) is called a **quantization scheme**. We will see shortly, that **there is no such thing as canonical quantization**. Specifically, what we mean is there does not exist a quantization scheme which is self-consistent under canonical transformations. The underlying cause of this is that a canonical transformations of the Q and P coordinates mixes different orders of $\hbar$ corrections with each other and because classical and quantum mechanics are not equivalent as representations, this mixing cannot possibly preserve the scheme. The

meaning of the fact that canonical quantization does **NOT** exist is that you should *always* think about the quantum theory as more fundamental. A quantum theory defines an unambiguous corresponding classical theory by the classical limit but a classical theory does **NOT** define an unambiguous corresponding quantum theory. There are generally infinitely many different quantum theories possessing the same classical limit. Classical mechanics alone is not enough to learn everything (this should not be surprising; we need quantum mechanics for a reason).

9.2.3 Groenewold's theorem

The specific result that canonical quantization does not exist is called Groenewold's theorem, which we will now prove. The method of proof will be by contradiction. Suppose we have quantum theory on a configuration Hilbert space and suppose further that there exists a map from generators in classical phase space into generators in the quantum theory which is preserved by canonical transformations. A generator in the classical theory is a function $G(Q, P)$ on the classical phase space. A generator in the quantum theory is the operator summary $\langle \hat{G} \rangle$ of some operator $\hat{G}$. Thus, such a map would be characterized by a map from classical functions into operators, which we write as $\hat{R}$ (R standing for "representation"). That is, such a map would have:

$$\hat{G} = \hat{R}(G). \quad (9.2.85)$$

The unit constant function 1 on classical phase space is necessarily mapped to the identity operator $\mathbb{1}$ so that $\langle \hat{R}(1) \rangle = 1$ always:

$$\hat{R}(1) = \mathbb{1}. \quad (9.2.86)$$

Because $\langle \hat{Q} \rangle$ and $\langle \hat{P} \rangle$ are the classical conjugate canonical variables, we must have:

$$\hat{R}(Q) = \hat{Q}, \quad \hat{R}(P) = \hat{P}. \quad (9.2.87)$$

In order for generic extensive quantities in the classical theory to remain extensive in the quantum theory, $\hat{R}$ must be linear:

$$\hat{R}(aF(Q, P) + bG(Q, P)) = a\hat{R}(F) + b\hat{R}(G) \quad (9.2.88)$$

for constants a, b and functions F, G . In order for a real-valued classical quantity to be mapped to a real-valued quantum quantity, $\langle \hat{R}(G) \rangle$ must be real for real-valued G , and so $\hat{R}(G)$ must be self-adjoint:

$$G = G^* \implies \hat{R}(G) = (\hat{R}(G))^\dagger. \quad (9.2.89)$$

So far these conditions are all satisfied by the Weyl transform. It is the final condition that will spell death for canonical quantization. In order for the map $\hat{R}$ to be preserved under canonical transformation, we must have that whether $\hat{R}$ is applied before or after performing a canonical transformation the same result is achieved. Consider the canonical transformation generated in classical mechanics by G . The corresponding transformation in quantum mechanics is thus generated by $\langle \hat{R}(G) \rangle$ and so in order to preserve $\hat{R}$, we must have that the change in any generator F or its quantum version $\langle \hat{R}(F) \rangle$ coincide. That change is, as always, implemented by the Poisson bracket:

$$\{\langle \hat{R}(F) \rangle, \langle \hat{R}(G) \rangle\}_{\text{qm}} = \langle \hat{R}(\{F, G\}_{\text{cl}}) \rangle. \quad (9.2.90)$$

The left hand side is how the change in $\langle \hat{R}(F) \rangle$ as would be computed purely in quantum mechanics while the right hand side is how the change in $\langle \hat{R}(F) \rangle$ as would be computed by first changing it in classical mechanics and then applying the map. For the map $\hat{R}$ to be preserved by G , these two must agree. This must hold for all F, G in order for the map to be preserved under generic canonical transformations.

We now proceed with direct computation to show that this last property leads to contradictions. First note that using Dirac's theorem we can express it more simply as:

$$\frac{1}{i\hbar} \langle [\hat{R}(F), \hat{R}(G)] \rangle = \langle \hat{R}(\{F, G\}_{\text{cl}}) \rangle \quad (9.2.91)$$

which because this must hold in a generic state $\hat{\rho}$, means:

$$[\hat{R}(F), \hat{R}(G)] = i\hbar \hat{R}(\{F, G\}_{\text{cl}}). \quad (9.2.92)$$

Consider $\hat{R}(Q^2)$. By computing the classical Poisson brackets:

$$\{Q^2, Q\}_{\text{cl}} = 0, \quad \{Q^2, P\}_{\text{cl}} = 2Q \quad (9.2.93)$$

we have then:

$$[\hat{R}(Q^2), \hat{Q}] = 0, \quad [\hat{R}(Q^2), \hat{P}] = 2i\hbar\hat{Q}. \quad (9.2.94)$$

These can be rewritten as:

$$[\hat{R}(Q^2) - \hat{Q}^2, \hat{Q}] = 0, \quad [\hat{R}(Q^2) - \hat{Q}^2, \hat{P}] = 0 \quad (9.2.95)$$

and thus $\hat{R}(Q^2) - \hat{Q}^2$ must not be a function of $\hat{Q}$ or $\hat{P}$; all that is left is for it to be proportional to the identity operator. So, for some constant a :

$$\hat{R}(Q^2) = \hat{Q}^2 + a\mathbb{1}. \quad (9.2.96)$$

Consider now $\hat{R}(QP)$. By computing the classical Poisson brackets:

$$\{QP, Q\}_{\text{cl}} = -Q, \quad \{QP, P\}_{\text{cl}} = P \quad (9.2.97)$$

we have then:

$$[\hat{R}(QP), \hat{Q}] = -i\hbar\hat{Q}, \quad [\hat{R}(QP), \hat{P}] = i\hbar\hat{P}. \quad (9.2.98)$$

These can be rewritten as:

$$[\hat{R}(QP) - \frac{\hat{Q}\hat{P} + \hat{P}\hat{Q}}{2}, \hat{Q}] = 0, \quad [\hat{R}(QP) - \frac{\hat{Q}\hat{P} + \hat{P}\hat{Q}}{2}, \hat{P}] = 0. \quad (9.2.99)$$

Thus, for some constant b :

$$\hat{R}(QP) = \frac{\hat{Q}\hat{P} + \hat{P}\hat{Q}}{2} + b\mathbb{1}. \quad (9.2.100)$$

Consider now $\hat{R}(P^2)$. By computing the classical Poisson brackets:

$$\{P^2, Q\}_{\text{cl}} = -2P, \quad \{P^2, P\}_{\text{cl}} = 0 \quad (9.2.101)$$

we have then:

$$[\hat{R}(P^2), \hat{Q}] = -2i\hbar\hat{P}, \quad [\hat{R}(P^2), \hat{P}] = 0. \quad (9.2.102)$$

These can be rewritten as:

$$[\hat{R}(P^2) - \hat{P}^2, \hat{Q}] = 0, \quad [\hat{R}(P^2) - \hat{P}^2, \hat{P}] = 0. \quad (9.2.103)$$

Thus, for some constant c :

$$\hat{R}(P^2) = \hat{P}^2 + c\mathbb{1}. \quad (9.2.104)$$

We can now determine the constants a, b, c by looking at the Poisson brackets of Q^2 , QP , P^2 with each other. By computing the classical Poisson brackets:

$$\{Q^2, QP\}_{\text{cl}} = 2Q^2, \quad \{Q^2, P^2\}_{\text{cl}} = 4QP, \quad \{QP, P^2\}_{\text{cl}} = 2P^2 \quad (9.2.105)$$

we have then:

$$[\hat{R}(Q^2), \hat{R}(QP)] = 2i\hbar\hat{R}(Q^2), \quad [\hat{R}(Q^2), \hat{R}(P^2)] = 4i\hbar\hat{R}(QP), \quad [\hat{R}(QP), \hat{R}(P^2)] = 2i\hbar\hat{R}(P^2). \quad (9.2.106)$$

Simplifying these using our found expressions for $\hat{R}(Q^2)$, $\hat{R}(QP)$, $\hat{R}(P^2)$ gives simply:

$$a = b = c = 0. \quad (9.2.107)$$

So, ultimately, we must have:

$$\hat{R}(Q^2) = \hat{Q}^2, \quad \hat{R}(QP) = \frac{\hat{Q}\hat{P} + \hat{P}\hat{Q}}{2}, \quad \hat{R}(P^2) = \hat{P}^2. \quad (9.2.108)$$

Now that we have exhausted quadratic polynomials, let us move onto to computing how $\hat{R}$ must affect cubic polynomials. Begin with Q^3 . The Classical Poisson bracket with lower order polynomials requires:

$$\{Q^3, Q\}_{\text{cl}} = 0, \quad \{Q^3, P\}_{\text{cl}} = 3Q^2, \quad \{Q^3, Q^2\}_{\text{cl}} = 0, \quad \{Q^3, QP\}_{\text{cl}} = 3Q^3, \quad \{Q^3, P^2\}_{\text{cl}} = 6Q^2P \quad (9.2.109)$$

The first two of these as commutators require (using $\hat{R}(Q^2) = \hat{Q}^2$):

$$[\hat{R}(Q^3), \hat{Q}] = 0, \quad [\hat{R}(Q^3), \hat{P}] = 3i\hbar\hat{Q}^2 \quad (9.2.110)$$

$$\implies [\hat{R}(Q^3) - \hat{Q}^3, \hat{Q}] = 0, \quad [\hat{R}(Q^3) - \hat{Q}^3, \hat{P}] = 0 \quad (9.2.111)$$

$$\implies \hat{R}(Q^3) = \hat{Q}^3 + d\mathbb{1} \quad (9.2.112)$$

for some constant d . The third of these is automatically satisfied for all d , however the fourth allows the computation of d :

$$[\hat{R}(Q^3), \frac{\hat{Q}\hat{P} + \hat{P}\hat{Q}}{2}] = \hat{R}(Q^3) \quad (9.2.113)$$

which is only true if $d = 0$. So:

$$\hat{R}(Q^3) = \hat{Q}^3. \quad (9.2.114)$$

Using this result, the fifth and final Poisson bracket then gives a convenient way of computing $\hat{R}(Q^2P)$:

$$\hat{R}(Q^2P) = \frac{1}{6i\hbar}[\hat{Q}^3, \hat{P}^2] \quad (9.2.115)$$

$$\implies \hat{R}(Q^2P) = \frac{\hat{Q}^2\hat{P} + \hat{P}\hat{Q}^2}{2}. \quad (9.2.116)$$

We can now study the Poisson bracket conditions on $\hat{R}(Q^2P)$. By direct computation:

$$\begin{aligned} \{Q^2P, Q\}_{\text{cl}} &= -Q^2, & \{Q^2P, P\}_{\text{cl}} &= 2QP, \\ \{Q^2P, Q^2\}_{\text{cl}} &= -2Q^3, & \{Q^2P, QP\}_{\text{cl}} &= Q^2P, & \{Q^2P, P^2\}_{\text{cl}} &= 4QP^2. \end{aligned} \quad (9.2.117)$$

The first three of these are automatically satisfied by (9.2.116). However, the fourth written as a commutator requires:

$$\frac{1}{i\hbar}[\hat{R}(Q^2P), \hat{R}(QP)] = \hat{R}(Q^2P). \quad (9.2.118)$$

Using our previous results the left hand side is given by:

$$\frac{1}{i\hbar}[\hat{R}(Q^2P), \hat{R}(QP)] = \hat{Q}\hat{P}\hat{Q} \quad (9.2.119)$$

however the right hand side is given by (9.2.116). Because $\hat{Q}$ and $\hat{P}$ do not commute, these two expressions do not agree. Therefore, there is no way to define $\hat{R}(Q^2P)$ consistent with the preceding conditions. And so, the canonical quantization map $\hat{R}$ does not exist. This is Groenewold's theorem.

Because the map $\hat{R}$ does not exist, if some generic scheme is used to map a classical theory into a quantum theory in one system of coordinates, then it is possible to perform a canonical transformation of the classical coordinates so that when the same scheme is applied the resulting quantum theory will be inequivalent to the first one. Thus, every generic quantization scheme is defined relative to a preferred coordinate system. Physics has no preferred coordinate system; in both classical and quantum mechanics we can perform canonical transformations to change the specifics of our description without changing at all what we are describing. However, there is no map from classical to quantum mechanics invariant under such transformations. Don't try to use one! You will be violating the fact that physics is the same in all coordinate systems if you do. Groenewold's theorem concretely proves that the Poisson representation (using the classical Poisson bracket for the phase space variables) is an unfaithful representation of the operator formalism put forward in section 1.3. This is in contrast to the Schrödinger representation used in quantum mechanics, which is manifestly faithful as it just adds an overall multiplicative factor to the operators.

IMPORTANT: It is very interesting to note that there were no problems with $\hat{R}$ when we considered only generators that were at most quadratic polynomials in Q and P . Such quadratic polynomials generate linear canonical transformation and so inadvertently we have proven that linear canonical transformations in classical and quantum mechanics are perfectly well mapped onto each other with no issues. This will be important later when we discuss symmetries in quantum field theory as very often the fields in quantum field theory will only have symmetries in which they transform linearly.

9.2.4 Quantum Mechanics in Classical Phase Space

While there is no map consistent with canonical transformations that maps classical mechanics into quantum mechanics, there plainly is a map consistent with canonical transformations that maps quantum mechanics into classical mechanics: the classical limit. By (9.2.83), from a self-adjoint operator $\hat{G}$ on Hilbert space, we can define a corresponding classical function G_{cl} as:

$$G_{\text{cl}}(Q, P) = \lim_{\hbar \rightarrow 0^+} \mathcal{W}^{-1}(\hat{G}) = \mathcal{C}(\hat{G}) \quad (9.2.120)$$

where we use this to define the classical limit map $\mathcal{C}$. Similarly but conversely to the previous subsection, in order for this map to be preserved by canonical transformations, we need, for operators $\hat{F}$ and $\hat{G}$:

$$\{\mathcal{C}(\hat{F}), \mathcal{C}(\hat{G})\}_{\text{cl}} = \mathcal{C}\left(\frac{1}{i\hbar}[\hat{F}, \hat{G}]\right). \quad (9.2.121)$$

Shortly, we will confirm that this is in fact the case.

In order to show this, and also for some other nice results, let us study how the Weyl transform interacts with multiplication. Consider operators $\hat{F}$ and $\hat{G}$. Each of these can be written as the Weyl transform of a Wigner function $(F(Q, P), G(Q, P))$. However, the Weyl transform of a product of Wigner functions is not the product of their Weyl transforms. That is:

$$\hat{F} = \hat{\mathcal{W}}(F), \quad \hat{G} = \hat{\mathcal{W}}(G), \quad \hat{F}\hat{G} \neq \hat{\mathcal{W}}(FG). \quad (9.2.122)$$

Instead, the effective product that is induced on Wigner functions by the Weyl transform is called the star product:

$$F \star G = \mathcal{W}^{-1}(\hat{\mathcal{W}}(F)\hat{\mathcal{W}}(G)). \quad (9.2.123)$$

To actually compute the star product, we can use (9.2.18) and (9.2.21). Applying these gives, in fully glory:

$$\begin{aligned} F \star G &= \int e^{\frac{i}{\hbar}(q^a P_a + P'_a(Q'^a - \tilde{Q}'^a) + P''_a(Q''^a - \tilde{Q}''^a))} F\left(\frac{Q' + \tilde{Q}'}{2}, P'\right) G\left(\frac{Q'' + \tilde{Q}''}{2}, P''\right) \\ &\quad \cdot \langle Q - q/2 | Q' \rangle \langle \tilde{Q}' | Q'' \rangle \langle \tilde{Q}'' | Q + q/2 \rangle d^d q d^d Q' d^d Q'' \frac{d^d \tilde{Q}' d^d P'}{(2\pi\hbar)^d} \frac{d^d \tilde{Q}'' d^d P''}{(2\pi\hbar)^d} \end{aligned} \quad (9.2.124)$$

$$\begin{aligned} &= \int e^{\frac{i}{\hbar}(q^a P_a + P'_a(Q^a - q^a/2 - Q''^a) + P''_a(Q''^a - Q^a - q^a/2))} \\ &\quad \cdot F\left(\frac{Q - q/2 + Q''}{2}, P'\right) G\left(\frac{Q'' + Q + q/2}{2}, P''\right) \frac{d^d q d^d P'}{(2\pi\hbar)^d} \frac{d^d Q'' d^d P''}{(2\pi\hbar)^d} \end{aligned} \quad (9.2.125)$$

after simplifying the Q state inner products into Dirac deltas and using those deltas to reduce the integrals. Now change from the integration variable Q'' to a new variable $\tilde{q}$ defined so that the Q argument of F becomes $Q + \tilde{q}$. Then:

$$F \star G = \int e^{\frac{i}{\hbar}(q^a P_a - P'_a(2\tilde{q}^a + q^a) + 2P''_a\tilde{q}^a)} F(Q + \tilde{q}, P') G\left(Q + \tilde{q} + \frac{q}{2}, P''\right) \frac{d^d q d^d P'}{(2\pi\hbar)^d} \frac{d^d \tilde{q} d^d P''}{(\pi\hbar)^d}. \quad (9.2.126)$$

Similarly changing from the integration variable q to a new variable $\tilde{q}'$ so that the Q argument of G becomes $Q + \tilde{q}'$ gives:

$$F \star G = \int e^{\frac{2i}{\hbar}(\tilde{q}'^a(P_a - P'_a) + \tilde{q}^a(P''_a - P_a))} F(Q + \tilde{q}, P') G(Q + \tilde{q}', P'') \frac{d^d \tilde{q} d^d P'}{(\pi\hbar)^d} \frac{d^d \tilde{q}' d^d P''}{(\pi\hbar)^d}. \quad (9.2.127)$$

We can now just rename $\tilde{q}$ to q and $\tilde{q}'$ to q' . For our last change of variables, change the integration variables P' and P'' into p and p' by $P' = P + p$ and $P'' = P + p'$:

$$F \star G = \int e^{\frac{2i}{\hbar}(q^a p'_a - q'^a p_a)} F(Q + q, P + p) G(Q + q', P + p') \frac{d^d q d^d p}{(\pi\hbar)^d} \frac{d^d q' d^d p'}{(\pi\hbar)^d}. \quad (9.2.128)$$

This is the proper integral expression for the star product and is as simple as it can be made without any abuse of notation. However, it is extremely convenient to do some abuse of notation going further to find a simpler and still correct (if applied correctly) formula for the star product.

By using the operator exponential of the derivative operator, we can write (formally):

$$F(Q + q, P + p) = e^{q^a \overleftarrow{\partial}_{Q^a} + p_a \overrightarrow{\partial}_{P_a}} F(Q, P) \quad (9.2.129)$$

and analogously so for $G(Q + q', P + p')$ where the meaning of the exponential is as always made concrete by its series representation. It is useful to define the “left-derivative” as a derivative that acts only on expressions to its left, in contrast with the usual derivative which by standard convention acts on expressions to its right. When working with the left-derivative, we will also carefully note when we mean a right-derivative. In either case, the direction a derivative is supposed to act is marked by the direction of the arrow we draw above it:

$$F(Q, P) \overleftarrow{\partial}_{Q^a} G(Q, P) = \frac{\partial F}{\partial Q^a} G, \quad F(Q, P) \overrightarrow{\partial}_{Q^a} G(Q, P) = F \frac{\partial G}{\partial Q^a}. \quad (9.2.130)$$

Then, we can rewrite (9.2.128) as:

$$F \star G = \int F(Q, P) e^{q^a \frac{\overleftarrow{\partial}}{\partial Q^a} + p_a \frac{\overleftarrow{\partial}}{\partial P_a}} e^{\frac{2i}{\hbar} (q^b p'_b - q'^b p_b)} e^{q^c \frac{\overrightarrow{\partial}}{\partial Q^c} + p_c \frac{\overrightarrow{\partial}}{\partial P_c}} G(Q, P) \frac{d^d q d^d p}{(\pi \hbar)^d} \frac{d^d q' d^d p'}{(\pi \hbar)^d}. \quad (9.2.131)$$

With regard to the q, q', p, p' integrals, the Q and P derivatives can be treated as if they were constants (this can be made more proper by writing this in terms of the Fourier transforms of F and G , in which case these derivatives literally become replaced by constants as the Fourier transform parameters). Performing the q and p integration (with this understanding of how to treat derivatives inspired by the Fourier transform) using the fundamental Fourier integral gives:

$$F \star G = \int F(Q, P) \delta \left(p' - \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial Q} \right) \delta \left(q' + \frac{i\hbar}{2} \frac{\overleftarrow{\partial}}{\partial P} \right) e^{q'^a \frac{\overrightarrow{\partial}}{\partial Q^a} + p'_a \frac{\overrightarrow{\partial}}{\partial P_a}} G(Q, P) d^d q' d^d p'. \quad (9.2.132)$$

Completing then the final integration (and thankfully leaving behind the worst of this notation):

$$F \star G = F e^{\frac{i\hbar}{2} \left(\frac{\overleftarrow{\partial}}{\partial Q^a} \frac{\overrightarrow{\partial}}{\partial P_a} - \frac{\overleftarrow{\partial}}{\partial P_a} \frac{\overrightarrow{\partial}}{\partial Q^a} \right)} G. \quad (9.2.133)$$

The operator which is exponentiated here is simply the classical Poisson bracket! Therefore, define the notation:

$$\{\leftarrow, \rightarrow\}_{\text{cl}} \stackrel{\text{def}}{=} \frac{\overleftarrow{\partial}}{\partial Q^a} \frac{\overrightarrow{\partial}}{\partial P_a} - \frac{\overleftarrow{\partial}}{\partial P_a} \frac{\overrightarrow{\partial}}{\partial Q^a} \quad (9.2.134)$$

$$\implies F \{\leftarrow, \rightarrow\}_{\text{cl}} G = \{F, G\}_{\text{cl}}. \quad (9.2.135)$$

With this, the star product can be written simply as:

$$F \star G = F e^{\frac{i\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}}} G. \quad (9.2.136)$$

Note that for real F and G , this expression is not necessarily real. This should not be surprising as for self-adjoint $\hat{F}$ and $\hat{G}$, $\hat{F}\hat{G}$ is not necessarily self-adjoint. The fact that the classical Poisson bracket is antisymmetric implies that:

$$G \star F = G e^{\frac{i\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}}} F = F e^{-\frac{i\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}}} G \quad (9.2.137)$$

as at each order in the series swapping F and G gives a minus sign for each power of the Poisson bracket.

By Dirac's theorem, the quantum Poisson bracket of operator summaries simply reduces to the operator summary of $\frac{1}{i\hbar}$ times their commutator. Thus, it is an interesting question of what does the commutator of operators do to Wigner functions? From the star product, it quickly follows that:

$$\mathcal{W}^{-1} \left(\frac{1}{i\hbar} [\hat{F}, \hat{G}] \right) = \frac{1}{i\hbar} (F \star G - G \star F) = F \frac{e^{\frac{i\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}}} - e^{-\frac{i\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}}}}{i\hbar} G = F \frac{2}{\hbar} \sin \left(\frac{\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}} \right) G. \quad (9.2.138)$$

This motivates the definition of the **Moyal bracket**:

$$\{F, G\} \stackrel{\text{def}}{=} F \frac{2}{\hbar} \sin \left(\frac{\hbar}{2} \{\leftarrow, \rightarrow\}_{\text{cl}} \right) G \quad (9.2.139)$$

so that:

$$\frac{1}{i\hbar} [\hat{F}, \hat{G}] = \hat{\mathcal{W}} \left(\{ \mathcal{W}^{-1}(\hat{F}), \mathcal{W}^{-1}(\hat{G}) \} \right). \quad (9.2.140)$$

Thus, the Weyl transform and the induced Moyal bracket on the Wigner functions provides a completely invertible representation of all of the quantum operators in terms of functions on the classical phase space. There is no contradiction here with Groenewold's theorem, because the Moyal bracket is **NOT** the classical Poisson bracket.

From the Moyal bracket, it is very easy to see how the classical Poisson bracket emerges in the classical limit. Simply series expanding the Moyal bracket in powers of $\hbar$ and defining $F^{(0)}$ and $G^{(0)}$ by the $\hbar \rightarrow 0^+$ limits of F and G :

$$\{F, G\} = F \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \left(\frac{\hbar}{2} \right)^{2n} \{\leftarrow, \rightarrow\}_{\text{cl}}^{2n+1} G = \{F^{(0)}, G^{(0)}\}_{\text{cl}} + \mathcal{O}(\hbar). \quad (9.2.141)$$

The great comedy of this is that evidently classical mechanics is the $\sin x \approx x$ approximation of quantum

mechanics. From (9.2.140) it immediately follows that:

$$\lim_{\hbar \rightarrow 0^+} \mathcal{W}^{-1} \left(\frac{1}{i\hbar} [\hat{F}, \hat{G}] \right) = \lim_{\hbar \rightarrow 0^+} \{ \mathcal{W}^{-1}(\hat{F}), \mathcal{W}^{-1}(\hat{G}) \} \quad (9.2.142)$$

$$\implies \mathcal{C} \left(\frac{1}{i\hbar} [\hat{F}, \hat{G}] \right) = \{ \lim_{\hbar \rightarrow 0^+} \mathcal{W}^{-1}(\hat{F}), \lim_{\hbar \rightarrow 0^+} \mathcal{W}^{-1}(\hat{G}) \}_{\text{cl}} \quad (9.2.143)$$

$$\implies \mathcal{C} \left(\frac{1}{i\hbar} [\hat{F}, \hat{G}] \right) = \{ \mathcal{C}(\hat{F}), \mathcal{C}(\hat{G}) \}_{\text{cl}} \quad (9.2.144)$$

thus fully establishing (9.2.121) as promised.

The existence of the Moyal bracket is perhaps initially surprising given a very old result of ours, namely theorem 1.2, in which we showed that the classical Poisson bracket is the only possible bracket of phase space functions satisfying bilinearity, antisymmetry, the Jacobi identity, and the Leibniz property. The operator commutator certainly satisfies all four of these properties, so shouldn't the Moyal bracket? But then, shouldn't the Moyal bracket be the classical Poisson bracket? There is actually no issue, because while yes the Moyal bracket does satisfy all four of these properties, it satisfies one of them *slightly* differently than we intended in section 1.4 and so avoids the logic of theorem 1.2. The subtlety is that in section 1.4 we assumed that the bracket we were developing would satisfy the Leibniz property with respect to ordinary multiplication. If that is required (in addition to the other three properties), the only possibility is the classical Poisson bracket. However, the Moyal bracket satisfies the Leibniz property not with respect to ordinary multiplication, but with respect to the star product instead:

$$\{ \{ F, GH \} \} = \{ \{ F, G \} \} \star H + G \star \{ \{ F, H \} \}. \quad (9.2.145)$$

This property follows automatically from the Leibniz property of operator commutators:

$$[\hat{F}, \hat{G}\hat{H}] = [\hat{F}, \hat{G}]\hat{H} + \hat{G}[\hat{F}, \hat{H}]. \quad (9.2.146)$$

Using the Moyal bracket, star product, and Weyl transform it is possible to express all of the equations of quantum mechanics purely in terms of Wigner functions, with no operators to be seen. This formulation is typically called “quantum mechanics in (classical) phase space”. To begin this formulation, let us compute the trace of an operator product in terms of Wigner functions (using (9.2.21)):

$$\text{Tr}(\hat{F}\hat{G}) = \int \langle Q | \hat{F}\hat{G} | Q \rangle d^d Q \quad (9.2.147)$$

$$= \int e^{\frac{i}{\hbar}(P_a(Q'^a - \tilde{Q}'^a) + P'_a(Q''^a - \tilde{Q}''^a))} F \left(\frac{Q' + \tilde{Q}'}{2}, P \right) G \left(\frac{Q'' + \tilde{Q}''}{2}, P' \right) \cdot \langle Q | Q' \rangle \langle \tilde{Q}' | Q'' \rangle \langle \tilde{Q}'' | Q \rangle d^d Q d^d Q' d^d Q'' \frac{d^d \tilde{Q}' d^d P}{(2\pi\hbar)^d} \frac{d^d \tilde{Q}'' d^d P'}{(2\pi\hbar)^d} \quad (9.2.148)$$

$$= \int e^{\frac{i}{\hbar}(P'_a - P_a)(Q''^a - Q^a)} F \left(\frac{Q + Q''}{2}, P \right) G \left(\frac{Q'' + Q}{2}, P' \right) \frac{d^d Q d^d P}{(2\pi\hbar)^d} \frac{d^d Q'' d^d P'}{(2\pi\hbar)^d}. \quad (9.2.149)$$

Shift the integration variable Q'' to $Q'' + Q$:

$$\text{Tr}(\hat{F}\hat{G}) = \int e^{\frac{i}{\hbar}(P'_a - P_a)Q''^a} F \left(Q + \frac{Q''}{2}, P \right) G \left(Q + \frac{Q''}{2}, P' \right) \frac{d^d Q d^d P}{(2\pi\hbar)^d} \frac{d^d Q'' d^d P'}{(2\pi\hbar)^d}. \quad (9.2.150)$$

Then, shift the integration variable Q to $Q - Q''/2$:

$$\text{Tr}(\hat{F}\hat{G}) = \int e^{\frac{i}{\hbar}(P'_a - P_a)Q''^a} F(Q, P) G(Q, P') \frac{d^d Q d^d P}{(2\pi\hbar)^d} \frac{d^d Q'' d^d P'}{(2\pi\hbar)^d} \quad (9.2.151)$$

$$= \int (2\pi\hbar)^d \delta(P - P') F(Q, P) G(Q, P') \frac{d^d Q d^d P}{(2\pi\hbar)^d} \frac{d^d P'}{(2\pi\hbar)^d}. \quad (9.2.152)$$

Simplifying this last equation we arrive at the extremely convenient fact:

$$\text{Tr}(\hat{F}\hat{G}) = \int F(Q, P) G(Q, P) \frac{d^d Q d^d P}{(2\pi\hbar)^d}. \quad (9.2.153)$$

This convenient fact does not generalize to a product of three operators, because of the distinction between the star product and the ordinary product.

Let $\rho(t, Q, P)$ be the Wigner function associated to the density matrix $\hat{\rho}(t)$. Typically we will call

$\rho(t, Q, P)$ the Wigner density. Using (9.2.153) with $\hat{F} = \mathbb{1}$ and $\hat{G} = \hat{\rho}$, we have that the normalization condition on ρ becomes:

$$\text{Tr}(\hat{\rho}) = 1 \implies \int \rho(t, q, P) \frac{d^d Q d^d P}{(2\pi\hbar)^d} = 1. \quad (9.2.154)$$

The fact that $\hat{\rho}$ is self-adjoint ensures that $\rho(t, Q, P)$ is real-valued. You would be reasonable to hope that since $\hat{\rho}$ is a nonnegative operator we could conclude that $\rho(t, Q, P)$ is a nonnegative function. I am sorry to disappoint you. There is no guarantee that $\rho(t, Q, P)$ is nonnegative (in fact in almost all settings it will be negative in some region of phase space). We will understand conceptually why this had to be true in a few sections. Instead, the nonnegativity of $\hat{\rho}$ simply ensures that for any wavefunction $\psi(Q)$ (using (9.2.21)):

$$\langle \psi | \hat{\rho} | \psi \rangle = \int e^{\frac{i}{\hbar} P_a(Q'^a - Q^a)} \rho\left(t, \frac{Q + Q'}{2}, P\right) \psi^*(Q') \psi(Q) d^d Q' \frac{d^d Q d^d P}{(2\pi\hbar)^d} \geq 0 \quad (9.2.155)$$

which is not a particularly easy to use property. This property however does ensure that $\rho(t, Q, P)$ is only negative in a very restricted and contained way.

The quantities of interest in quantum mechanics are operator summaries $\langle \hat{F} \rangle = \text{Tr}(\hat{\rho} \hat{F})$. Using (9.2.153) these operator summaries can be expressed very nicely as:

$$\langle \hat{F} \rangle = \text{Tr}(\hat{\rho} \hat{F}) = \int \rho(t, Q, P) F(t, Q, P) \frac{d^d Q d^d P}{(2\pi\hbar)^d}. \quad (9.2.156)$$

In classical statistical mechanics, the dynamical variable is the phase space density $f(t, Q, P)$ which is a real-valued, nonnegative function which integrates to 1; the quantities of interest are statistical expectations computed using that density as the probability distribution on phase space. The Wigner density is similar to the phase space density in how it is working here. It is a real-valued function which integrates to 1 and which can only be negative in a limited way, and the quantities of interest are integrals of the same form as a statistical expectation. Continuing with this restricted analogy, we define the Moyalization or “M-expectation” of a Wigner function by:

$$\mathbb{M}(F) = \int \rho(t, Q, P) F(t, Q, P) \frac{d^d Q d^d P}{(2\pi\hbar)^d} \quad (9.2.157)$$

$$\implies \boxed{\langle \hat{F} \rangle = \mathbb{M}(F)}. \quad (9.2.158)$$

This Moyalization is not a genuine expectation in the sense of probability theory because the Wigner density is not a valid probability density (because it is not nonnegative). From (9.2.140) it immediately follows that:

$$\boxed{\{\mathbb{M}(F), \mathbb{M}(G)\} = \mathbb{M}(\{F, G\})}. \quad (9.2.159)$$

This formula establishes precisely that the Moyal bracket is the correct bracket to use for Wigner functions under a continuous transformation in quantum mechanics.

The analogy of the Wigner density to the classical phase space density is not accidental. Suppose we have an uncertain density matrix and so have some probability distribution on it. By equation (9.1.97), the statistical expectation of operator summaries is still described by standard density matrix formulas purely in terms of the statistical expectation of the density matrix. Let $\hat{\rho}$ be the statistical expectation of the density matrix and let $\rho(t, Q, P)$ be its associated Wigner density. It follows then that for generic $\hat{F}$:

$$\mathbb{E}(\langle \hat{F} \rangle) = \mathbb{M}(F) \quad (9.2.160)$$

where the Moyalization is computed with respect to $\rho(t, Q, P)$ and F is the Wigner function associated to $\hat{F}$. In the classical limit, $\langle \hat{F} \rangle$ will approach some classical quantity of interest F_{cl} . In the case that $\rho(t, Q, P)$ was simultaneously localized in position and momentum space in the classical limit, the resulting right hand side would just be F_{cl} evaluated at the classical coordinates and momenta. However, in the case that in the classical limit $\rho(t, Q, P)$ is some nontrivial distribution $\rho^{(0)}(t, Q, P)$ then the classical limit of this formula gives:

$$\mathbb{E}(F_{\text{cl}}) = \int \rho^{(0)}(t, Q, P) F^{(0)}(t, Q, P) d\mathbb{P} \quad (9.2.161)$$

where $d\mathbb{P}$ is the same phase space measure introduced in chapter 5. This is precisely the classical expectation formula from classical statistical mechanics, and so we can see that the classical phase space density $f(t, Q, P)$

is the classical limit of $\rho(t, Q, P)$:

$$f(t, Q, P) = \lim_{\hbar \rightarrow 0^+} \rho(t, Q, P). \quad (9.2.162)$$

This explains why $\hbar$ was introduced in the definition of the phase space measure of classical statistical mechanics (I put it in there precisely so that this above equation would hold without any extra normalization factor).

The classical phase space density satisfies the Liouville equation. The Wigner density satisfies a similar but appropriately more complicated equation of motion. From the von Neumann equation with H the Wigner function associated to $\hat{H}$ and using (9.2.140):

$$\mathcal{W}^{-1} \left(\frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar} [\hat{\rho}, \hat{H}] \right) = 0 \quad (9.2.163)$$

$$\Rightarrow \boxed{\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0.} \quad (9.2.164)$$

This final equation, the equation of motion for the Wigner density, is the Liouville-Moyal equation.

While there is no such thing as canonical quantization as a generic map for turning classical theories into quantum ones, the Moyal bracket can implement a highly restricted notion of mapping a classical theory to a quantum theory. Suppose we have studied a system classically and found that it has some symmetry algebra, meaning that there is some set of classical quantities T_{cl}^a which transform the system in some way and which are symmetries of the theory. In classical mechanics these generators will satisfy some algebra:

$$\{T_{\text{cl}}^a, T_{\text{cl}}^b\}_{\text{cl}} = f^{ab}_c T_{\text{cl}}^c \quad (9.2.165)$$

with some structure constants f^{ab}_c . Typically the symmetries of interest are motivated by geometric considerations, and so we expect that whatever the quantum version of the system fundamentally is, it has the same symmetries. Then, there must be operators $\hat{T}^a$ on the Hilbert space so that:

$$[\hat{T}^a, \hat{T}^b] = i\hbar f^{ab}_c \hat{T}^c \quad (9.2.166)$$

by theorem 8.5. Let T^a be the Wigner functions associated to the $\hat{T}^a$. These means we need:

$$\{\{T^a, T^b\}\} = f^{ab}_c T^c. \quad (9.2.167)$$

For the classical limit, we need:

$$T^a = T_{\text{cl}}^a + \sum_{n=1}^{\infty} \hbar^n T^{(n)a}. \quad (9.2.168)$$

The combination of (9.2.167) and (9.2.168) provide a set of conditions on the $\hbar$ corrections of each T^a . Depending on the precise algebra of interest, these conditions may be trivially satisfied by the classical T_{cl}^a , they may provide loose but nontrivial constraints on $T^{(n)a}$, they may fully determine the $T^{(n)a}$, or they may have no solution at all (in which case, one cannot extend the classical symmetry unchanged to the quantum theory). This is the limited extent in which classical mechanics plus some information about what symmetries we demand be maintained can provide some restrictions on the quantum theory.

Exercises

Problem 9.4: The WKB Approximation in general. Consider a quantum system in a pure state on configuration Hilbert space. Define the real-valued fields $\rho(t, Q), S(t, Q)$ by:

$$\Psi(t, Q) = e^{\frac{i}{\hbar} S(t, Q)} \sqrt{\rho(t, Q)}.$$

- (a) Show, from the Poisson brackets satisfied by Ψ and Ψ^* that ρ and S satisfy the Poisson brackets:

$$\{\rho(Q), \rho(Q')\} = 0, \quad \{\rho(Q), S(Q')\} = \delta(Q - Q'), \quad \{S(Q), S(Q')\} = 0.$$

Thus, conclude that ρ and S are canonically conjugate fields (S is the conjugate momentum field to ρ).

- (b) Show that in terms of ρ , S , and H (Wigner function associated to the Hamiltonian operator $\hat{H}$), the quantum Hamiltonian becomes exactly:

$$\mathcal{H} = \int e^{i(\lambda^a P_a - \frac{1}{\hbar}(S(t, Q + \frac{\hbar\lambda}{2}) - S(t, Q - \frac{\hbar\lambda}{2})))} \sqrt{\rho\left(t, Q + \frac{\hbar\lambda}{2}\right) \rho\left(t, Q - \frac{\hbar\lambda}{2}\right)} H(t, Q, P) d^d \lambda \frac{d^d Q d^d P}{(2\pi)^d}.$$

Explain how this formula may be systematically expanded in powers of $\hbar$ to develop a semiclassical

approximation to quantum mechanics. (Sadly, this expansion often is poorly behaved beyond low orders.)

- (c) Show that in the $\hbar \rightarrow 0^+$ the above Hamiltonian becomes:

$$\mathcal{H} = \int \rho(t, Q) \mathcal{H}_{\text{cl}} \left(t, Q, \frac{\partial S}{\partial Q} \right) d^d Q.$$

Show that the equations of motion from this Hamiltonian are precisely:

$$\frac{\partial S}{\partial t} + \mathcal{H}_{\text{cl}} \left(t, Q, \frac{\partial S}{\partial Q} \right) = 0, \quad \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial Q^a} \left(\rho \frac{\partial \mathcal{H}_{\text{cl}}(t, Q, P)}{\partial P_a} \Big|_{P=\frac{\partial S}{\partial Q}} \right) = 0.$$

Explain that these are exactly the Hamilton-Jacobi equation for S and a continuity equation for ρ in which the flow velocity is the classical velocity field.

9.3 The Measurement Problem

This section is based on [76], [1], and conversations with John P. Ralston. As presented so far, in quantum mechanics the state of the system is a well-defined physically real quantity known as the density matrix which evolves deterministically according to the von Neumann equation and which has well-defined properties given by operator summaries. This seems to be in stark contrast to the usual presentation of quantum mechanics, in which the Born rule and probability are abound. In this section we will explain how the Born rule and effective probability are derived concepts in quantum mechanics that originate from the statistical mechanics of interacting systems. Neumaier [76] calls this the **Thermal Interpretation of Quantum Mechanics** and is the most thoroughly descriptive source I know of on this way of thinking (the name thermal coming from the statistical mechanical origin of the peculiarities of quantum measurement). I also call this way of thinking the Unitary Interpretation of Quantum Mechanics, because the key point in my eyes is that quantum mechanical dynamics is always deterministically unitary, even during measurement. I have encountered several physicists who think this way, and there is historical precedent for this perspective throughout the entire century of quantum mechanics' history. For example, in 1929 Mott [75] showed that once a charged particle has ionized a single atom in a bubble chamber, it will only ionize further particles in a nearly straight line, thus leading to the apparent point-particle-like trajectories in such a chamber using purely deterministic wave-mechanics and in 2021 Schonfeld [103] showed how the fact Born rule distribution of the first such ionization event can be derived from statistical mechanics.

Consider a microscopic quantum system of interest for observation which we will call the System (S). Because it is microscopic, we cannot access its properties directly. Instead, in order to measure anything about it we need to have it interact with some macroscopic measurement device we call the Detector (D) so that some property of the System becomes correlated with a macroscopic property of the Detector. Then, because that property is macroscopic, it is available to us to be directly observed. The detector will include not only the meter that we read off but many many more environmental degrees of freedom (in say the double-slit experiment, the detector is the entire physical apparatus of the experiment including the air and the space the waves travel through while the meter is just the screen or any equipment capable of measuring at the slits). The combined Hilbert space of the System+Detector system we call $\mathbb{H} = \mathbb{H}_S \otimes \mathbb{H}_D$. In any single experimental trial, at time $t = 0$ before the System and Detector have interacted, the System and Detector are completely uncorrelated and so:

$$\hat{\rho}_0 = \hat{\rho}_S \otimes \hat{\rho}_D. \quad (9.3.1)$$

The System and Detector will interact through some total Hamiltonian operator $\hat{H}$ so that $\hat{\rho}(t)$ of the combined system satisfies the von Neumann equation:

$$\frac{d\hat{\rho}}{dt} + \frac{1}{i\hbar}[\hat{\rho}, \hat{H}] = 0, \quad \hat{\rho}(0) = \hat{\rho}_0. \quad (9.3.2)$$

During the interaction the combined system is isolated and so $\hat{H}$ has no explicit time dependence. Consequently, the time evolution is solved by:

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t), \quad \hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}. \quad (9.3.3)$$

With $|n_S\rangle$ an orthonormal basis of states of $\mathbb{H}_S$ and $|n_D\rangle$ an orthonormal basis of states of $\mathbb{H}_D$, we can define the operators $\hat{U}_{mn}(t)$ which are operators on $\mathbb{H}_D$ by:

$$\hat{U}_{mn}(t) = \sum_{m'n'} |m'_D\rangle \langle m_S m'_D| \hat{U}(t) |n_S n'_D\rangle \langle n'_D|. \quad (9.3.4)$$

Automatically then:

$$\hat{U}(t) = \sum_{mn} |m_S\rangle \langle n_S| \otimes \hat{U}_{mn}(t). \quad (9.3.5)$$

There will be some generator on the Detector's phase space which we are capable of measuring, and so there is some associated operator $\hat{A}$ on the Detector's Hilbert space so that experimentally we have access to $\langle \hat{A} \rangle_D$ (where the D indicates the operator summary is taken using the Detector's density matrix). Automatically, the corresponding operator $\hat{X}$ on the full Hilbert space is:

$$\hat{X} = \mathbb{1}_S \otimes \hat{A}. \quad (9.3.6)$$

Then the property given by $\hat{X}$ on the space of the combined system is:

$$\langle \hat{X} \rangle(t) = \text{Tr}(\hat{\rho}(t)\hat{X}) = \text{Tr}(\hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t)\hat{X}) = \text{Tr}(\hat{\rho}_0\hat{U}^\dagger(t)\hat{X}\hat{U}(t)) \quad (9.3.7)$$

$$= \sum_{mm'nn'} \text{Tr} \left(\hat{\rho}_0(|n'_S\rangle\langle m'_S| \otimes \hat{U}_{m'n'}^\dagger(t)) (\mathbb{1}_S \otimes \hat{A}) (|m_S\rangle\langle n_S| \otimes \hat{U}_{mn}(t)) \right) \quad (9.3.8)$$

$$= \sum_{mm'nn'} \text{Tr} \left(\hat{\rho}_0 \langle m'_S | m_S \rangle |n'_S\rangle\langle n_S| \otimes (\hat{U}_{m'n'}^\dagger(t) \hat{A} \hat{U}_{mn}(t)) \right) \quad (9.3.9)$$

$$= \sum_{lmn} \text{Tr} \left((\hat{\rho}_S \otimes \hat{\rho}_D) (|m_S\rangle\langle n_S| \otimes (\hat{U}_{lm}^\dagger(t) \hat{A} \hat{U}_{ln}(t))) \right) \quad (9.3.10)$$

$$= \sum_{lmm'nn'} \langle m'_S n'_D | (\hat{\rho}_S |m_S\rangle\langle n_S|) \otimes (\hat{\rho}_D \hat{U}_{lm}^\dagger(t) \hat{A} \hat{U}_{ln}(t)) |m'_S n'_D\rangle \quad (9.3.11)$$

$$= \sum_{lmnn'} \langle n_S | \hat{\rho}_S |m_S\rangle \langle n'_D | \hat{\rho}_D \hat{U}_{lm}^\dagger(t) \hat{A} \hat{U}_{ln}(t) |n'_D\rangle \quad (9.3.12)$$

$$= \text{Tr}_S \left(\hat{\rho}_S \sum_{klmn} |m_S\rangle\langle k_D | \hat{\rho}_D \hat{U}_{lm}^\dagger(t) \hat{A} \hat{U}_{ln}(t) |k_D\rangle\langle n_S| \right). \quad (9.3.13)$$

If we now define the operator $\hat{A}_S(t)$ by:

$$\hat{A}_S(t) = \sum_{lmn} |m_S\rangle \text{Tr}_D(\hat{\rho}_D \hat{U}_{lm}^\dagger(t) \hat{A} \hat{U}_{ln}(t)) \langle n_S| \quad (9.3.14)$$

then we have:

$$\langle \hat{X} \rangle(t) = \langle \hat{A} \rangle_D(t) = \langle \hat{A}_S(t) \rangle_S. \quad (9.3.15)$$

Therefore, if we measure the value of $\langle \hat{A} \rangle_D(t)$ by looking at the Detector, we are equivalently observing the value of $\langle \hat{A}_S(t) \rangle_S$ and thus able to learn something about the state of the System. In a well designed experiment, $\hat{A}_S$ will closely resemble some particular operator $\hat{s}$ of interest in S.

We must note something extremely important about the definition of $\hat{A}_S(t)$; it depends on $\hat{\rho}_D$! Because we are able to measure the property $\langle \hat{A} \rangle_D$ directly, it must be macroscopic. Thus, the Detector itself must be macroscopic and so consist of a large number of microscopic degrees of freedom. Because the Detector is macroscopic, we are unable to control its microscopic state exactly and so we must treat the detector's state using statistical mechanics. Consequently, in different experimental trials with the same macroscopic experimental setup the microscopic state of the Detector will be different. The full initial microscopic state of the Detector is contained in $\hat{\rho}_D$ and thus we must treat $\hat{\rho}_D$ as a random variable distributed according to statistical mechanics in whatever distribution appropriately describes our experimental setup procedure.

Because for different experimental trials $\hat{\rho}_D$ is in fact different, the resulting property $\langle \hat{A}_S \rangle_S$ is different in different experimental trials, with distribution determined by the distribution of $\hat{\rho}_D$ and the precise coupling between the System and Detector. Thus, even when the system of interest is prepared in the exact same microscopic state in each experimental trial and even though quantum mechanics itself is fundamentally deterministic, because we are only able to access that state through a macroscopic interaction, the results of our experiments are apparently random. This apparent randomness is exactly as in statistical mechanics. The only remaining questions are then what distribution may be expected for $\langle \hat{A}_S \rangle_S$ in an idealized measurement scheme and how can we set the interaction between S and D so that $\langle \hat{A}_S \rangle_S$ closely resembles some fixed quantity of interest $\langle \hat{s} \rangle_S$ we would like to learn about the System.

In a measurement the System will interact with the Detector for some period of time according to a Hamiltonian operator $\hat{H}$ which we engineer to correlate some part of the final state of the Detector as strongly as possible with a property of the incoming System. In principle, at all times the Hamiltonian operator can as always be written in the form:

$$\hat{H} = \hat{H}_S \otimes \mathbb{1}_D + \mathbb{1}_S \otimes \hat{H}_D + \hat{H}_{\text{int}} \quad (9.3.16)$$

where $\hat{H}_S$ and $\hat{H}_D$ are the free Hamiltonian operators of the System and Detector respectively and $\hat{H}_{\text{int}}$ contains their interactions. The interaction term $\hat{H}_{\text{int}}$ is all that is under our control in designing the experimental apparatus. Before the System reaches the Detector, the interaction between the two is negligible and so the interaction term can be neglected. Once the System is sufficiently close to the Detector, we assume in an ideal measurement that the interaction between them is very strong (so the system can properly drive the Detector during that time). Thus, during the interaction we approximate:

$$\hat{H} \approx \hat{H}_{\text{int}} \quad (9.3.17)$$

Going forward in our analysis of the measurement interaction, we will simply neglect the contributions from

$\hat{H}_S, \hat{H}_D$.

Let us now try to determine the form of $\hat{H}$ most suited to an “ideal measurement”. In an ideal measurement of some real-valued generator $\langle \hat{s} \rangle_S$ of the System (and thus self-adjoint $\hat{s}$), we require that the behavior of the operator $\hat{s}$ on the System is perturbed as little as possible and that there is no finer structure than what is provided by $\hat{s}$ which is also disturbed as little as possible. To make this more precise it will be helpful to introduce a little notation. Let s_n be the eigenvalues of $\hat{s}$ and let $\hat{\pi}_n$ be its eigenspace projectors so that for all $|\Psi\rangle \in \mathbb{H}_S$:

$$\hat{\pi}_n |\Psi\rangle = |\Psi\rangle \iff \hat{s} |\Psi\rangle = s_n |\Psi\rangle. \quad (9.3.18)$$

Then automatically (with no summation over indices intended):

$$\hat{\pi}_m \hat{\pi}_n = \delta_{mn} \hat{\pi}_n, \quad \sum_n \hat{\pi}_n = \mathbb{1}_S, \quad \hat{s} = \sum_n s_n \hat{\pi}_n. \quad (9.3.19)$$

It will be convenient to have an explicit orthonormal eigenbasis for $\hat{s}$ on $\mathbb{H}_S$. Let $|n, a_S\rangle$ be an orthonormal basis of $\mathbb{H}_S$ with labels n, a where n labels the eigenvalue s_n of this vector under $\hat{s}$ and a is some label (with in general range dependent on n) that is necessary because the eigenvalue s_n may be degenerate:

$$\hat{s} |n, a_S\rangle = s_n |n, a_S\rangle, \quad \langle n, a_S | n', a'_S \rangle = \delta_{nn'} \delta_{aa'}. \quad (9.3.20)$$

Then, automatically:

$$\hat{\pi}_n = \sum_a |n, a_S\rangle \langle n, a_S|. \quad (9.3.21)$$

We can now precisely state our conditions on $\hat{H}$ to “ideally measure” $\langle \hat{s} \rangle_S$. Suppose that the System is initially in a state of 0 operator spread with respect to $\hat{s}$: $\text{Spr}_S(\hat{s}) = 0$. Then, for some n , $\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S$ and $\langle \hat{s} \rangle_S = s_n$. In order for $\langle \hat{s} \rangle_S$ to be disturbed as little as possible, we require that if the System is initially in a state of 0 operator spread with respect to $\hat{s}$ then it remains in a state of 0 operator spread with respect to $\hat{s}$, with the same value of $\langle \hat{s} \rangle_S = s_n$. Further, if the eigenspace projected into by $\hat{\pi}_n$ has dimension greater than 1, our experiment should not be able to resolve any of this degeneracy because if it could then it would not be $\langle \hat{s} \rangle_S$ that we are measuring, it would be some other generator $\langle \hat{s}' \rangle_S$ where $\hat{s}'$ is less degenerate than $\hat{s}$. Thus, if for some n , $\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S$, then not only should the System stay in a state of $\hat{s}$ -spread 0, it should stay in the *same* state of $\hat{s}$ -spread 0. Recalling that $\text{Tr}_D(\hat{\rho})$ is the reduced density matrix of the system at all times, this means that:

$$\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S \implies \frac{d}{dt} (\text{Tr}_D(\hat{\rho})) = 0. \quad (9.3.22)$$

By using (9.1.136) then, we have that:

$$\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S \implies \text{Tr}_D([\hat{\rho}, \hat{H}]) = 0. \quad (9.3.23)$$

To see specifically what this requires, it is useful to decompose $\hat{H}$ into a sum of tensor products along the lines of how we decomposed $\hat{U}$ into operators $\hat{U}_{mn}$. Define the operators $\hat{H}_{m'n'}$ by:

$$\hat{H}_{m'n'} = \sum_{mnab} |m, a_S\rangle \langle m, a_S m'_D | \hat{H} | n, b_S n'_D \rangle \langle n, b_S |. \quad (9.3.24)$$

In terms of these $\hat{H}_{m'n'}$, we can express $\hat{H}$ as:

$$\hat{H} = \sum_{mm'nn'ab} |m, a_S m'_D\rangle \langle m, a_S m'_D | \hat{H} | n, b_S n'_D \rangle \langle n, b_S n'_D | = \sum_{m'n'} \hat{H}_{m'n'} \otimes |m'_D\rangle \langle n'_D|. \quad (9.3.25)$$

Letting $\rho_{Dn'm'} = \langle n'_D | \hat{\rho}_D | m'_D \rangle$ be the matrix elements of $\hat{\rho}_D$, we can now compute:

$$\text{Tr}_D(\hat{\rho} \hat{H}) = \sum_{manbkm'n'} |m, a_S\rangle \langle m, a_S k_D | (\hat{\rho}_S \otimes \hat{\rho}_D) (\hat{H}_{m'n'} \otimes |m'_D\rangle \langle n'_D |) | n, b_S k_D \rangle \langle n b_S | \quad (9.3.26)$$

$$= \sum_{m'n'} \rho_{Dn'm'} \hat{\rho}_S \hat{H}_{m'n'}. \quad (9.3.27)$$

Similarly:

$$\text{Tr}_D(\hat{H} \hat{\rho}) = \sum_{m'n'} \rho_{Dn'm'} \hat{H}_{m'n'} \hat{\rho}_S. \quad (9.3.28)$$

Therefore (9.3.23) becomes:

$$\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S \implies \sum_{m'n'} \rho_{Dn'm'} [\hat{\rho}_S, \hat{H}_{m'n'}] = 0. \quad (9.3.29)$$

This must hold for all valid density matrices $\hat{\rho}_D$, and so this requires each term in the sum to vanish independently²:

$$\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S \implies [\hat{\rho}_S, \hat{H}_{m'n'}] = 0. \quad (9.3.30)$$

Consider a valid density matrix $\hat{\rho}_S$ which satisfies no particular conditions (is not necessarily a state of 0 $\hat{s}$ -spread). Then, we can define the valid density matrix $\hat{\rho}_S^{(n)}$ by:

$$\hat{\rho}_S^{(n)} = \frac{\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n}{\text{Tr}(\hat{\pi}_n \hat{\rho}_S)}. \quad (9.3.31)$$

The denominator ensures that $\hat{\rho}_S^{(n)}$ has trace 1 and the projectors ensure that $\hat{\rho}_S^{(n)}$ is a state of 0 $\hat{s}$ -spread in which $\langle \hat{s} \rangle_S = s_n$. Thus, for all $\hat{\rho}_S$, by (9.3.30) using $\hat{\rho}_S^{(n)}$ in place of $\hat{\rho}_S$ in that equation:

$$[\hat{\rho}_S^{(n)}, \hat{H}_{m'n'}] = 0 \quad (9.3.32)$$

$$\implies \hat{\pi}_n \hat{\rho}_S \hat{\pi}_n \hat{H}_{m'n'} = \hat{H}_{m'n'} \hat{\pi}_n \hat{\rho}_S \hat{\pi}_n. \quad (9.3.33)$$

This last condition now holds without restriction on $\hat{\rho}_S$.

Let us put this last condition in components and use (9.3.21):

$$\langle m, a_S | \hat{\pi}_k \hat{\rho}_S \hat{\pi}_k \hat{H}_{m'n'} | n, b_S \rangle = \langle m, a_S | \hat{H}_{m'n'} \hat{\pi}_k \hat{\rho}_S \hat{\pi}_k | n, b_S \rangle \quad (9.3.34)$$

$$\implies \sum_c \delta_{mk} \langle m, a_S | \hat{\rho}_S | k, c_S \rangle \langle k, c_S | \hat{H}_{m'n'} | n, b_S \rangle = \sum_c \delta_{nk} \langle m, a_S | \hat{H}_{m'n'} | k, c_S \rangle \langle k, c_S | \hat{\rho}_S | n, b_S \rangle. \quad (9.3.35)$$

We can now differentiate both sides with respect to the matrix element $\langle m, a_S | \hat{\rho}_S | k, c_S \rangle$ as those matrix elements may be freely specified³:

$$\implies \delta_{mk} \langle k, c_S | \hat{H}_{m'n'} | n, b_S \rangle = \sum_d \delta_{nk} \langle m, a_S | \hat{H}_{m'n'} | k, d_S \rangle \delta_{mk} \delta_{ad} \delta_{kn} \delta_{cb} \quad (9.3.36)$$

$$\implies \langle m, a_S | \hat{H}_{m'n'} | n, b_S \rangle = \delta_{mn} \delta_{ab} \langle n, c_S | \hat{H}_{m'n'} | n, c_S \rangle \quad (9.3.37)$$

where to get to this last line we summed the previous line over all m and then relabeled various indices. Note that the right hand side of the last expression looks like it depends on c , but the left hand side explicitly does not. Therefore, the right hand side does not either and so there exists numbers $h_{nm'n'}$ so that:

$$h_{nm'n'} = \langle n, c_S | \hat{H}_{m'n'} | n, c_S \rangle \quad (9.3.38)$$

$$\implies \langle m, a_S | \hat{H}_{m'n'} | n, b_S \rangle = \delta_{mn} \delta_{ab} h_{nm'n'}. \quad (9.3.39)$$

From this we explicitly have:

$$\hat{H}_{m'n'} = \sum_{mnab} |m, a_S\rangle \langle m, a_S | \hat{H}_{m'n'} | n, b_S\rangle \langle n, b_S| = \sum_{mnab} |m, a_S\rangle \delta_{mn} \delta_{ab} h_{nm'n'} \langle n, b_S| \quad (9.3.40)$$

$$\implies \hat{H}_{m'n'} = \sum_n h_{nm'n'} \hat{\pi}_n. \quad (9.3.41)$$

Define then the operators $\hat{h}_n$ on $\mathbb{H}_D$ by:

$$\hat{h}_n = \sum_{m'n'} |m'_D\rangle h_{nm'n'} \langle n'_D|. \quad (9.3.42)$$

Returning these to $\hat{H}$, we find:

$$\hat{H} = \sum_n \hat{\pi}_n \otimes \hat{h}_n. \quad (9.3.43)$$

Thus, this is the general form required of the Hamiltonian operator for when our System interacts with the Detector in an ideal measurement. Because $\hat{H}$ is necessarily self-adjoint, and the projectors $\hat{\pi}_n$ are all linearly independent and self-adjoint, it automatically follows that each $\hat{h}_n$ is self-adjoint. Often in discussions of

²A careful reader may worry that this isn't quite true, because a density matrix must still satisfy some basics conditions (self-adjointness, positivity, trace-1). However, a short component calculation reveals that if $\text{Tr}(\hat{\rho}\hat{O}) = 0$ for some operator $\hat{O}$ and all density matrices $\hat{\rho}$, then in fact $\hat{O} = 0$.

³This differentiation argument is legal by the same logic as the previous footnote.

measurement as a dynamical process, you may see the suggested interaction Hamiltonian $\hat{H} = \hat{s} \otimes \hat{d}$ for some operator $\hat{d}$ on $\mathbb{H}_D$. By rewriting $\hat{s} = \sum_n s_n \hat{\pi}_n$, you can see that $\hat{s} \otimes \hat{d}$ is actually of the form (9.3.43) with $\hat{h}_n = s_n \hat{d}$ and so this is a legal special case of our formula.

Using the form (9.3.43), we can explicitly compute the time evolution operator $\hat{U}(t)$. For a natural number N , note automatically that because $\hat{\pi}_m \hat{\pi}_n = \delta_{mn} \hat{\pi}_n$:

$$\hat{H}(\hat{\pi}_n \otimes \hat{h}_n^N) = \hat{\pi}_n \otimes \hat{h}_n^{N+1} \quad (9.3.44)$$

$$\implies \hat{H}^N(\hat{\pi}_n \otimes \mathbb{1}_D) = \hat{\pi}_n \otimes \hat{h}_n^N \quad (9.3.45)$$

by N fold application of that fact. Summing over all n reveals:

$$\hat{H}^N = \sum_n \hat{\pi}_n \otimes \hat{h}_n^N. \quad (9.3.46)$$

Thus, computing the exponential for $\hat{U}(t)$ we have:

$$\hat{U}(t) = \sum_n \hat{\pi}_n \otimes e^{-\frac{i}{\hbar} t \hat{h}_n}. \quad (9.3.47)$$

Using our expression for $\hat{U}(t)$, we can now repeat the calculation leading to (9.3.14) to find the appropriate expression for $\hat{A}_S$ in the case of an ideal measurement:

$$\langle \hat{X} \rangle(t) = \text{Tr}(\hat{\rho}_0 \hat{U}^\dagger \hat{X} \hat{U}) \quad (9.3.48)$$

$$= \sum_{mn} \text{Tr} \left((\hat{\rho}_S \otimes \hat{\rho}_D) \left(\hat{\pi}_m \otimes e^{\frac{i}{\hbar} t \hat{h}_m} \right) (\mathbb{1}_S \otimes \hat{A}) \left(\hat{\pi}_n \otimes e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \right) \quad (9.3.49)$$

$$= \sum_{mn} \text{Tr} \left((\hat{\rho}_S \hat{\pi}_m \hat{\pi}_n) \otimes \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_m} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \right) \quad (9.3.50)$$

$$= \sum_{mn} \delta_{mn} \text{Tr}_S(\hat{\rho}_S \hat{\pi}_n) \text{Tr}_D \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_m} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \quad (9.3.51)$$

$$= \sum_n \text{Tr}_S(\hat{\rho}_S \hat{\pi}_n) \text{Tr}_D \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right). \quad (9.3.52)$$

So, in an ideal measurement, we identify:

$$\hat{A}_S(t) = \sum_n \hat{\pi}_n \text{Tr}_D \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \quad (9.3.53)$$

which gives:

$$\langle \hat{X} \rangle(t) = \langle \hat{A}_S(t) \rangle_S \quad (9.3.54)$$

as desired.

The time dependent quantity $\langle \hat{X} \rangle(t)$ is **NOT** fully accessible in experiment, again due to the macroscopic nature of the Detector. The typical time scales on which quantum systems evolve are extremely microscopic compared to experimental resolution and so time-averaging and relaxation to equilibrium are inherent to how we as macroscopic beings access individual quantum systems. As well, we cannot access the exact real number value of the time-averaged relaxed version of $\langle \hat{X} \rangle$. Real data has finite precision; it is necessarily binned into bins of finite width. Each bin then defines an equivalence class of values of $\langle \hat{X} \rangle$ that are the considered the same with respect to the measurement. This is also inherent from the macroscopic nature of the Detector, because a bin essentially amounts to a “macrostate” with all of the different $\hat{\rho}_D$ that for a given $\hat{\rho}_S$ end up with $\langle \hat{X} \rangle$ in the same bin amounting to the very many “microstates” that we cannot distinguish between.

For each different trial in an experiment, $\hat{\rho}_D$ will be different due to the Detector having many microstates consistent with our macroscopic preparation. Because of this, we let ω label the microstate of the detector (in probability terms, be a point in the sample space) and $\hat{\rho}_D(\omega)$ be the resulting state of the detector giving that microstate (thus $\hat{\rho}_D(\omega)$ is a random variable in the standard sense of classical probability). The operator $\hat{A}_S$ depends on the detector through the time-dependent, ω dependent combinations $\text{Tr}_D \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right)$. After time-averaging/relaxation to equilibrium this quantity will approach *some* stable state which may depend on ω and n , because the original does. Thus, letting $\mathbb{T}$ indicate time averaging as usual, for some real numbers $A_n(\omega)$ we have:

$$\mathbb{T} \left(\text{Tr}_D \left(\hat{\rho}_D(\omega) e^{\frac{i}{\hbar} t \hat{h}_n} \hat{A} e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \right) = A_n(\omega). \quad (9.3.55)$$

The resulting time-averaged and relaxed value of $\langle \hat{X} \rangle$ is then also a random variable dependent on ω :

$$\mathbb{T}(\langle \hat{X} \rangle) = \sum_n \text{Tr}_S(\hat{\rho}_S \hat{\pi}_n) A_n(\omega). \quad (9.3.56)$$

When relating this time-relaxed value to the reading read out on a macroscopic detector, there is some sort of binning procedure which we represent mathematically by a function $\text{Bin}(\cdot)$ which takes a real number and spits out the corresponding bin value given to that real number. Thus, the final experimentally measured value X in a single trial is given by:

$$X(\omega) = \text{Bin}(\mathbb{T}(\langle \hat{X} \rangle)) = \text{Bin} \left(\sum_n \text{Tr}_S(\hat{\rho}_S \hat{\pi}_n) A_n(\omega) \right). \quad (9.3.57)$$

Because real data is discretely binned, the binning function cannot possibly be linear over the real numbers.

What properties does the binning function have? The binning function is determined by how the experiment is calibrated, and that calibration is necessary to manage the imperfectly prepared nature of each different experimental trial for $\hat{\rho}_D(\omega)$. There are two criteria used to calibrate the binning of a quantum experiment. Suppose the initial state of the System $\hat{\rho}_S$ is such that $\hat{s}$ has operator spread zero in that state: $\text{Spr}(\hat{s})_S = 0$. In such a state, $\hat{s}$ acts purely as $s_n \mathbb{1}$ and so unambiguously will be assigned the value s_n . Thus, in a perfectly calibrated measurement, the binning procedure would always assign the value s_n to the measurement of $\langle \hat{s} \rangle_S$:

$$\hat{\pi}_n \hat{\rho}_S \hat{\pi}_n = \hat{\rho}_S \implies X(\omega) = s_n \quad (9.3.58)$$

independent of ω . This criterion essentially defines the bins to which $X(\omega)$ may be assigned. Because each eigenspace projected onto by some $\hat{\pi}_n$ is intended to be distinguishable in our experiment (because that is what we mean by being able to measure $\langle \hat{s} \rangle_S$, and not the summary of some less refined operator), we must have a separate bin for each eigenspace. Because states within each eigenspace are intended to be indistinguishable (because that is what we mean by being able to measure $\langle \hat{s} \rangle_S$, and not the summary of some more refined operator), we must not have more than one bin for each eigenspace. Therefore, for a general $\hat{\rho}_S$, $X(\omega)$ will be assigned one of the values s_n .

Because $X(\omega)$ is intended to measure the value of $\langle \hat{s} \rangle_S$, the second criterion on a good binning procedure is that $X(\omega)$ is an unbiased estimator of $\langle \hat{s} \rangle_S$. That is, its statistical expectation should match $\langle \hat{s} \rangle_S$:

$$\mathbb{E}(X) = \langle \hat{s} \rangle_S. \quad (9.3.59)$$

Let p_n be the probability that X is sorted into the bin with value s_n for a given System state $\hat{\rho}_S$. Expanding both sides of this equation (using the definition of statistical expectation and the expression for $\hat{s}$ in (9.3.19), we have:

$$\sum_n s_n p_n = \sum_n s_n \text{Tr}(\hat{\rho}_S \hat{\pi}_n). \quad (9.3.60)$$

The eigenvalues s_n of $\hat{s}$ never entered the dynamics of the problem, only the eigenspace projectors $\hat{\pi}_n$. Therefore, as long as the s_n are sufficiently distinct from each other for the bins surrounded them to also remain distinct, the precise values of s_n are somewhat arbitrary. Essentially, a measurement of the summary of $\hat{s} = \sum_n s_n \hat{\pi}_n$ could equally well be called a measurement of the summary of $\hat{s}' = \sum_n s'_n \hat{\pi}_n$ if the s'_n values are still well separated. In that case, the associated random variable would be $X'(\omega)$ and assigned this alternate bin values. The eigenvalues s_n essentially amount to what we name the bins and are thus arbitrary. So, if this equation holds at a given set of values s_n , then it holds in a small neighborhood around that point. This allows us to differentiate this equation with respect to s_n and so identify that in a perfectly calibrated binning procedure, the binning must satisfy:

$$p_n = \text{Tr}(\hat{\rho}_S \hat{\pi}_n). \quad (9.3.61)$$

This is precisely the Born rule! So, we see that in an ideal measurement process where the measurement outcomes are binned so that a state of 0-spread is identified with a consistent value and so that the measurement outcome is an unbiased estimator of the true valued being measured, the Born rule is automatically emergent from the binning procedure.

The Born rule as written here is not the form most readily family to beginning quantum mechanics students, which is a special case of the above rule. Consider the special case that the eigenspace projected into by $\hat{\pi}_n$ has dimension 1. Then, we can identify a unit vector $|\phi\rangle$ so that $\hat{\pi}_n = |\phi\rangle\langle\phi|$. Further, consider the special case that $\hat{\rho}_S$ is a pure state. Then, we can identify a state vector $|\psi\rangle$ so that $\hat{\rho}_S = |\psi\rangle\langle\psi|$. Simplifying

the Born rule as above we find that in this exceptionally special case, the probability that the measured value lands in bin n becomes:

$$p_n = |\langle \phi | \psi \rangle|^2. \quad (9.3.62)$$

This is the form of the Born rule more familiar to those new to quantum mechanics. We have hopefully made it clear in this section that the magnitude squared inner product $|\langle \phi | \psi \rangle|^2$ for vectors $|\phi\rangle, |\psi\rangle$ a priori has no real interpretative meaning. It becomes a meaningful quantity only in the extremely special case of the more general Born rule probability $\text{Tr}(\hat{\rho}_S \hat{\pi}_n)$ which itself is only meaningful as a probability in the context of a perfectly calibrated ideal measurement interaction. On its own outside of this specific dynamical interaction context, $\text{Tr}(\hat{\rho}_S \hat{\pi}_n)$ is just a number.

Let us now look at the final state of the System after it has been measured. The time-dependent state $\hat{\rho}_S(t)$ is given as usual by the partial trace over everything else, in this case just the Detector:

$$\hat{\rho}_S(t) = \text{Tr}_D(\hat{\rho}(t)) = \text{Tr}_D(\hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t)). \quad (9.3.63)$$

Using the expression we found for $\hat{U}(t)$ in (9.3.47):

$$\langle m, a_S n'_D | \hat{U} = \sum_n \langle m, a_S n'_D | \left(\hat{\pi}_n \otimes e^{-\frac{i}{\hbar} t \hat{h}_n} \right) = \langle m, a_S | \otimes \left(\langle n'_D | e^{-\frac{i}{\hbar} t \hat{h}_n} \right). \quad (9.3.64)$$

Then:

$$\hat{\rho}_S(t) = \sum_{mnn'ab} |m, a_S\rangle \langle m, a_S n'_D | \hat{U} \hat{\rho}_d \hat{U}^\dagger |n, b_S n'_D\rangle \langle n, b_S| \quad (9.3.65)$$

$$= \sum_{mnn'ab} |m, a_S\rangle \left(\langle m, a_S | \otimes \langle n'_D | e^{-\frac{i}{\hbar} t \hat{h}_m} \right) \hat{\rho}_S \otimes \hat{\rho}_D \left(|n, b_S\rangle \otimes e^{\frac{i}{\hbar} t \hat{h}_n} |n'_D\rangle \right) \langle n, b_S| \quad (9.3.66)$$

$$= \sum_{mnn'ab} (|m, a_S\rangle \langle m, a_S | \hat{\rho}_S |n, b_S\rangle \langle n, b_S|) \langle n'_D | \hat{e}^{-\frac{i}{\hbar} t \hat{h}_m} \hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} |n'_D\rangle \quad (9.3.67)$$

$$= \sum_{mn} \hat{\pi}_m \hat{\rho}_S \hat{\pi}_n \text{Tr}_D \left(e^{-\frac{i}{\hbar} t \hat{h}_m} \hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \right). \quad (9.3.68)$$

Because $\hat{\rho}_D$ appearing on the right hand side is a random variable dependent on the experimental trial, the final state of the system on the left hand side is as well. In the long run and after time averaging the final system state will necessarily relax to some stationary state of the interaction. However, by design of the interaction we already know precisely what those stable states are. In individual experimental trials, the initial detector state will be effectively random, but it is possible to assign an averaged detector state $\hat{\rho}_D$ according to:

$$\hat{\rho}_D = \mathbb{E} \hat{\rho}_D. \quad (9.3.69)$$

Then, the average final state of the system is given by:

$$\mathbb{E} \hat{\rho}_S(t) = \sum_{mn} \hat{\pi}_m \hat{\rho}_S \hat{\pi}_n \text{Tr}_D \left(e^{-\frac{i}{\hbar} t \hat{h}_m} \hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \right). \quad (9.3.70)$$

In order for $\hat{h}_m$ and $\hat{h}_n$ for $m \neq n$ to drive the Detector toward different equilibria, they must be quite different operators. Consequently, for $m \neq n$, the operator $e^{\frac{i}{\hbar} t \hat{h}_n} e^{-\frac{i}{\hbar} t \hat{h}_m}$ oscillates very quickly in time. In individual preparations it is possible for the detector state to be supported on a part of the Hilbert space so that the combination $e^{-\frac{i}{\hbar} t \hat{h}_m}$ acts essentially trivially for some values of m, n . However, we assume that our average detector preparation is not biased toward the behavior of any particular such subspace and so under reasonable time averaging for a wide class of systems, this combination time-averages to 0. This is yet again the decoherence approximation. So, in the long run (using cyclicity of the trace) we have:

$$\mathbb{T} \left(\text{Tr}_D \left(e^{-\frac{i}{\hbar} t \hat{h}_m} \hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} \right) \right) = \delta_{mn} \mathbb{T} \left(\text{Tr}_D \left(\hat{\rho}_D e^{\frac{i}{\hbar} t \hat{h}_n} e^{-\frac{i}{\hbar} t \hat{h}_n} \right) \right) = \delta_{mn}. \quad (9.3.71)$$

Thus the ensemble-averaged time-averaged and relaxed final state $\hat{\rho}_S^{(f)}$ of the System is given by:

$$\hat{\rho}_S^{(f)} = \mathbb{T} \mathbb{E}(\hat{\rho}_S(t)) = \sum_{mn} \hat{\pi}_m \hat{\rho}_S \hat{\pi}_n \delta_{mn} \quad (9.3.72)$$

$$\implies \hat{\rho}_S^{(f)} = \sum_n \hat{\pi}_n \hat{\rho}_S \hat{\pi}_n. \quad (9.3.73)$$

This final sum can be given an alternate look by recalling the definition of $\hat{\rho}_S^{(n)}$ and the Born rule. In terms

of the $\hat{\rho}_S^{(n)}$ the final state of the System can be written as:

$$\hat{\rho}_S^{(f)} = \sum_n p_n \hat{\rho}_S^{(n)} \quad (9.3.74)$$

which is the same state as would be assigned to a statistical mixture of the $\hat{\rho}_S^{(n)}$ each with a probability p_n . Therefore, the statistical properties of an ensemble of ideal measurements are exactly consistent with assigning the final states $\hat{\rho}_S^{(n)}$ each with probability p_n to the system of interest. This is the origin of the collapse rule.

In essence, both of the basic features of quantum measurements typically described as mysterious, the Born rule and the collapse rule, can be understood totally naturally as emergent from a reasonable interacting model of a macroscopic detector with a microscopic system of interest. The arguments presented here are extremely generic, much like the arguments we gave for how thermodynamic equilibrium is reached by many systems in statistical mechanics. In statistical mechanics there have been many more detailed investigations into the precise way in which specific systems reach thermodynamic equilibrium. The same is true for quantum measurement; there is a meaningful body of literature dedicated to understanding the dynamical emergence of the properties of quantum measurements for particular systems. For more reading on this and closely related subjects, consult [1], [9], [11], [12], [76], [79].

Exercises

Problem 9.5: Neumaier Qubit. This question is based on [76]. Consider the measurement of a quantum system with a two dimensional Hilbert space $\mathbb{H}_S$. Let $|0\rangle$ and $|1\rangle$ form an orthonormal basis of $\mathbb{H}_S$. Let $\hat{A}_S(t)$ be the operator as constructed in (9.3.14) when this system interacts with our detector. The value $\langle \hat{A}_S(t) \rangle$ is intended to map to the physical location of a literal pointer arrow on a piece of equipment with $-\infty$ corresponding to the arrow moving all the way to the left and ∞ corresponding to the arrow moving all the way to the right. The detector is calibrated so that if $\hat{\rho}_S = |0\rangle\langle 0|$ then the pointer always moves to the left and so that if $\hat{\rho}_S = |1\rangle\langle 1|$ then the pointer always moves to the right.

- Let $a_{mn} = \mathbb{T}(\langle m | \hat{A}_S | n \rangle)$ be the time averaged equilibrium matrix elements of $\hat{A}_S(t)$. Show that the calibration conditions require: $a_{00} = -\infty$ and $a_{11} = \infty$. Explain that a_{12} and a_{00}/a_{11} depend on the experimental preparation and so may be different in each trial.
- Assume that the detector and interaction are calibrated so that a_{12}/a_{00} limits to 0 and so that what fraction of the sum $|a_{00}| + |a_{11}|$ is contributed to by each of $|a_{00}|$ and $|a_{11}|$ is uniform. That is, assume the random variable u defined by:

$$u = \frac{a_{00}}{a_{00} - a_{11}}$$

is uniformly distributed. Show that the pointer moves to the left with probability $\langle 0 | \hat{\rho}_S | 0 \rangle$ and that it moves to the right with probability $\langle 1 | \hat{\rho}_S | 1 \rangle$. Thus, explain that this detector calibration recovers the standard Born rule.

Problem 9.6: Low Rate Double Slit Experiment. In our previous analysis of the double slit experiment, we have always discussed a continuous interference pattern appearing on the screen. However, if the intensity of the incoming beam is sufficiently low, then the pattern that forms on the screen will form blob by blob and only after many particles in the beam have been sent will the full intensity pattern be visible. In this problem, we will explain these low rate results using our analysis of measurement in quantum mechanics. Suppose for simplicity in this question that the incoming particle happens to be a pure state and so has some wavefunction. Let vectors like $\vec{x}$ for this question specifically refer to vectors in the plane of the screen (and so they are 2-dimensional).

- Our screen is the detector, with the bins corresponding to our spatial resolution on the screen. In particular, suppose that the screen is divided into regions $\mathbb{M}_n$ with n labeling these different regions, so that if the incoming particle's wavefunction lies solely within a single $\mathbb{M}_n$ then precisely that pixel will light up upon detection. The property of the incoming wavefunction we wish to measure is central position, $\langle \vec{x} \rangle$. Explain that because of the finite resolution of the bins, the best we can actually measure is the coarse-grained position $\vec{x}_{\text{coarse}}$ defined by:

$$\vec{x}_{\text{coarse}} = \sum_n \langle \vec{x}_n \hat{\pi}_n \rangle$$

where $\vec{x}_n$ is the representative position assigned to $\mathbb{M}_n$ (say, the center of the pixel) and $\hat{\pi}_n$ is the

projector of the Hilbert space into the spatial region $\mathbb{M}_n$, or more precisely:

$$\hat{\pi}_n = \int_{\mathbb{M}_n} |\vec{x}\rangle \langle \vec{x}| d^2 \vec{x}.$$

A physical screen is a macroscopically large object connected to macroscopic electromagnetic equipment, and so easily satisfies the necessary condition for a detector to not have a precisely preparable microstate described in the section.

- (b) Show that in order for which pixel lights up to unbiasedly estimate the value of $\vec{x}_{\text{coarse}}$, we must have the probability p_n that pixel n fires be:

$$p_n = \int_{\mathbb{M}_n} |\psi(\vec{x})|^2 d^2 \vec{x}$$

where $\psi(\vec{x})$ is the wavefunction of the incoming particle just before it hits (begins interacting with) the screen.

- (c) Take the limit that the screen becomes arbitrarily precise. Show that $|\psi(\vec{x})|^2$ becomes the probability per unit area on the screen of that point on the screen lighting up for a single incoming particle, thus recovering the standard naive Born rule.

9.4 Misinterpretations of Quantum Mechanics

In the century since the beginning of quantum mechanics, there has been enormous confusion about what quantum mechanics even means. This confusion has led to several viewpoints, which we will discuss in this section. To begin, there are a few empirical facts which are unambiguously tested by experiment that everyone agrees on. Let us begin with the common ground.

Fact 1: Existence of an ensemble description

The statistical properties of an ensemble $\mathcal{E}$ of systems of interest prepared macroscopically identically are captured by a density matrix $\hat{\rho}_{\mathcal{E}}$ (which is a self-adjoint, nonnegative, trace-1 operator on the Hilbert space $\mathbb{H}$ of an element of the ensemble). These properties are *statistical* in the sense that $\hat{\rho}_{\mathcal{E}}$ does not in general predict the specific outcome of individual experimental trials or the properties of any particular system within the ensemble; $\hat{\rho}_{\mathcal{E}}$ predicts only distributions of results for possible experiments. If the element systems of the ensemble are isolated, then the density matrix evolves in time according to the von Neumann equation:

$$\frac{d\hat{\rho}_{\mathcal{E}}}{dt} + \frac{1}{i\hbar}[\hat{\rho}_{\mathcal{E}}, \hat{H}] = 0 \quad (9.4.1)$$

where $\hat{H}$ is the self-adjoint Hamiltonian operator on $\mathbb{H}$ for the element systems.

Fact 2: Operator-Generator correspondence

A given real-valued generator s of interest of an element of $\mathcal{E}$ which is intended to be “measured” in an appropriate “ideal” measurement is associated with a self-adjoint operator $\hat{s}$. Let s_n be the eigenvalues and $\hat{\pi}_n$ be the eigenspace projectors of $\hat{s}$:

$$\hat{s} = \sum_n s_n \hat{\pi}_n, \quad \hat{\pi}_n \hat{\pi}_m = \delta_{nm} \hat{\pi}_n, \quad \sum_n \hat{\pi}_n = \mathbb{1}_S. \quad (9.4.2)$$

s will be measured by coupling the System S to a Detector D through an interaction. In each trial, the detector will register a real value which is able to be observed and recorded by people.

Fact 3: Certain outcomes

If the ensemble $\mathcal{E}$ is such that there exists a value of n so that $\hat{\pi}_n \hat{\rho}_{\mathcal{E}} \hat{\pi}_n = \hat{\rho}_{\mathcal{E}}$, then s certainly takes the value s_n .

Fact 4: The Born Rule

For a general ensemble $\mathcal{E}$, in each trial the detector will read one of the $\{s_n\}$ as its value. Within the full ensemble $\mathcal{E}$, the distribution of which s_n is selected is given by the Born rule:

$$\text{Prob}(s = s_n) = p_n = \text{Tr}(\pi_n \hat{\rho}_{\mathcal{E}}). \quad (9.4.3)$$

Fact 5: Collapse Rule

After measuring an ensemble of instances of the system with the Detector, it is possible to form the subensemble $\mathcal{E}_n$ of instances which gave the value s_n under measurement. The statistical properties of that subensemble for future measurements are captured by the density matrix:

$$\hat{\rho}_{\mathcal{E}_n} = \frac{1}{p_n} \hat{\pi}_n \hat{\rho}_{\mathcal{E}} \hat{\pi}_n. \quad (9.4.4)$$

These facts are empirical in the sense that they are good tools for predicting the correct outcomes of many experiments. Whether these facts are fundamental properties of the universe or results derived from more fundamental physics that happen to be appropriate for the relevant experiments has historically been an interpretative question (with time, advances in measurement technology have made it clear that these cannot be exact facts). All five factors of what everyone agrees on are silent about the properties of an individual experimental trial (an individual system instance within the ensemble $\mathcal{E}$). Once a description of what happens in an individual experimental trial is desired, differences of opinion appear. Any interpretation of quantum mechanics has to be consistent with these five factors. The most conservative possible interpretation of quantum mechanics is the so-called minimal interpretation (also called the statistical interpretation), which is advocated for by Ballentine [3]. In the minimal interpretation, one is only allowed to make statements derivable from Facts 1-5. Therefore, you are not allowed to say anything about individual experimental trials. It is not legal in the minimal interpretation to talk about the energy of a particle; instead one must talk about the average energy of an ensemble of particles. The minimal interpretation has the advantage of

protecting one from saying anything plainly wrong by being too bold, but has the conjugate disadvantage of being unable to answer many of the questions we really care about. We live in *one* Universe, and there are many experiments that cannot be repeated by humans (good luck recreating the big bang), and if close adherence to the minimal interpretation is followed, it means we are not legally allowed to say anything about the quantum mechanical aspects of such experiments. The minimal interpretation essentially takes an agnostic approach to the physics of measurement by refusing to attempt to describe what happens in the measurement of an individual quantum system.

In the Thermal Interpretation, Fact 1 is allowed to be stated even about individual experimental trials, Fact 2 is justified by the form of the Hamiltonian in (9.3.43) implying a set of $\hat{\pi}_n$ and the s_n being essentially arbitrary bin labels, Facts 3 and 4 are determined by the conditions put on detector calibration to be minimally disturbing and unbiased, and Fact 5 is automatic because the final state of the System is unbiasedly estimated by assigning the final density matrix $\hat{\rho}_S^{(n)}$ with probability p_n . Thus, the Thermal Interpretation is consistent with all of the basic experimental facts of quantum mechanics. In the rest of this section we will discuss some alternate views of quantum mechanics which are also consistent with these factors.

9.4.1 Copenhagen Interpretation

Those unfamiliar with the territory of interpreting quantum mechanics may confuse the minimal interpretation with the Copenhagen interpretation. The Copenhagen interpretation, or classroom interpretation, is the one you are most likely to encounter in low-level popular science media. It was advocated for historically primarily by Niels Bohr and Werner Heisenberg, the principal scientist in the Nazi nuclear program. Whereas the minimal interpretation is very conservative by refusing to attempt to answer questions about individual systems, the Copenhagen interpretation is extremely bold because it explicitly asserts that such questions *cannot* be answered even in principle. Since the Copenhagen interpretation rejects the existence of answers to several questions about quantum mechanics, it has often been called the “shut-up and calculate” approach. There are a few interrelated assumptions defining the Copenhagen interpretation. The Copenhagen interpretation asserts Facts 1-5 as exact fundamental physical truths and additionally assumes:

Individuality: Fact 1 can be applied to individual experimental runs.

Indeterminacy: Quantum mechanics is fundamentally probabilistic with absolutely no possible underlying mechanism for how to explain the Born rule.

Naive collapse: When a quantum system is not being measured, it evolves according to the von Neumann (or Schrödinger, in the case of a state vector) equation and that when it is measured, that unitary time evolution ceases and the measurement causes the measured system’s state to “collapse” instantly to the appropriate eigenstate of the operator associated to the measurement described in Fact 5.

Limited Reality: A property of a quantum system exists and is physical only when it is being measured. When not measured, it is undefined.

The Copenhagen interpretation agrees with the Thermal interpretation in allowing the discussion of individual quantum systems (Individuality). Indeterminacy is a much bigger leap. Copenhagen treats the state (either state vector or density matrix) of the system being measured as the full set of data relevant in an experiment and then upon observation that the same preparation of such data leads to a distribution of experimental outcomes asserts that it is because of fundamental indeterminacy. You should know by now my thoughts on this, given that I argued against the scientific sensibility of indeterminacy in section 5.1.4 and provided an explicit model for how this distribution of experimental results can be explained with unitary time evolution in the previous section. The Indeterminacy assumption is philosophically and experimentally unwarranted and fundamentally at odds with every other known thing in the domain of science. Because the Copenhagen interpretation cannot predict the results of measurements even in principle, it is often called an incomplete theory (such as by Einstein). This is in contrast to the Thermal interpretation in which each experimental trial is deterministic but not macroscopically predictable due to the practical issue of not being able to consistently prepare the microstate of the detector.

Naive collapse has several fundamental problems. Because the Copenhagen interpretation refuses to describe collapse as a dynamical process given by some equation of motion, it is instantaneous at the time of

measurement. This assumes an exact moment of measurement can be identified and requires a notion of simultaneity. Relativity is fundamentally at odds with an invariant concept of simultaneity. An equal time slice in one reference frame is not an equal time slice in another boosted reference frame. Therefore, in naive collapse whether the measurement has even happened is not an observer independent statement. Because in the Copenhagen interpretation the state is believed to be instantly changed to an eigenstate of the operator associated to the measurement and whether the measurement has happened is not observer independent, in the Copenhagen interpretation the state of the system is not observer independent. Thus it cannot be considered a real physical property (in this interpretation).

Another way to see that the Copenhagen interpretation inherently rejects the state of a system as real is through the nonlocal nature of instant collapse. The density matrix of a quantum system describes the whole state of the system, and so for a spatially extended system contains data at spatially separated points. If the position operator (or a close approximate) is measured in the Copenhagen interpretation, the state will instantly collapse to an eigenstate of that operator and thus completely localize in space, changing the state instantly at spatially separated points. If the state is physical, this violates relativistic causality. Thus, the Copenhagen interpretation rejects the very notion that the physical state of a system is *physically real*. The philosophical absurdity of this position should be clear to anyone who comprehends the scientific method.

This denial of reality in Copenhagen is clarified by the final point Limited Reality. In the Copenhagen interpretation, the results of measurements that are actually performed are considered as real. Systems are not considered real when they are not being measured. This thinking is the origin of common popular science descriptions of quantum mechanics. In such a description you might hear the wave-particle duality described as beginning with the wavefunction being a fictitious mathematical tool (obviously the wavefunction can't be real, because it has an imaginary part⁴). Then, when the wavefunction is measured the wave will instantly become a perfect little point particle somewhere (which you should know is not even mathematically sane, based on our work in Part I). When that wave collapses to a little point particle it suddenly becomes physically real. If it were never measured, it wouldn't have been real. If my grandma had wheels, she would be a bicycle.

A resulting property of the Copenhagen interpretation is *complementarity*. Because the Copenhagen interpretation assumes a physical property of a system is real only at the time that property is measured and because by Fact 2 measurement results in resolving the operator associated to a property of interest into its eigenspaces, the mathematical fact that noncommuting operators cannot be simultaneously diagonalized results in the Copenhagen interpretation to it being impossible to simultaneously assign physically real values to two properties of a quantum system if the operators associated to those two properties do not commute. This is why you will hear those attempting to make quantum mechanics sound mysterious say that in quantum mechanics it is impossible to know the position and momentum of a particle at the same time. This metaphysical weirdness has nothing to do with quantum mechanics; it has solely to do with the Copenhagen interpretation. The central position $\langle \hat{x} \rangle$ and total linear momentum $\langle \hat{p} \rangle$ of a single particle quantum system are perfectly well-defined functions of time at all times with no weirdness. The same experimental setup one would use to measure $\langle \hat{x} \rangle$ by an ideal measurement does not serve as an ideal measurement of $\langle \hat{p} \rangle$, which is not at all mysterious. To measure different properties, one needs appropriately differently designed experiments.

Because the Copenhagen interpretation was very early to the historical game, its perspective was heavily used in assigning the standard names given to quantum mechanical objects. This has resulted in countless aspiring physicists baking in many of the concepts of the Copenhagen interpretation deep into their quantum mechanical thinking, even when completely unnecessary. Many physicists have been taught to think of $|\psi(t, \vec{x})|^2$ as the spatial probability density for finding a single quantum particle (because they always think of $|\langle \psi | \phi \rangle|^2$ as a Born rule probability), to think of $\langle \hat{H} \rangle$ as the (statistical) average energy of a quantum system (because books call in the expectation of $\hat{H}$), to think of a measurement as measuring an operator (even though the operators in quantum mechanics are not even dynamical variables), to think that quantum systems are always in eigenstates of whatever observables you care about (because of interpreting the eigenstate outcomes of the Born rule extremely literally), and so on with many basic unnecessary misconceptions.

Aside from the basic philosophical issues we have already mentioned with the Copenhagen interpretation, it further contains within itself a fundamental flaw: the Copenhagen interpretation does not define what a measurement is. By refusing to give a dynamical interactive picture for what constitutes a measurement, the Copenhagen interpretation admits that it at best provides an incomplete description of physics. Copenhagen

⁴This parenthetical is entirely sarcastic. This deranged “proof-by-same-word” logic of incorrectly interpreting what the real in real-numbers means is entirely without merit. Anyone capable of passing an undergraduate math class should be able to understand that.

simply says that we know when a measurement is performed in a lab because we do the measuring. But, it cannot answer basic scientific questions. Do atoms measure each other? There is a classic joke whose origin I haven't found that goes something like: does an amoeba measure a quantum system by getting too close to it, or does the amoeba have to get a PhD and a spectrometer first? Copenhagen can't say.

The Copenhagen interpretation is based on a familiar error. In the history of classical mechanics, it was commonly said that friction couldn't be explained by Hamiltonian/Action/Lagrangian mechanics. The core of the argument was that if you write down the term friction adds to the equation of motion of a particle, you can show that there is no term you could possibly add to the action which depends only on the degrees of freedom of the particle that results in adding that term to the equation of motion. The critical incorrect assumption here is that the correct way to add friction is to only consider the degrees of freedom of the particle. However, we have long since known that in fact friction and other dissipative effects originate precisely because of ignoring additional degrees of freedom. By adding terms to the action which include the requisite degrees of freedom to dissipate energy into, friction can unambiguously be treated with a variational principle. A half century later, in statistical mechanics there were many who would say that a Hamiltonian system cannot approach thermodynamic equilibrium, because the entropy of the phase space density of a Hamiltonian system is conserved. This is again the same error, in which time-averaging and the interaction of the system in question with an environment of external variables is ignored.

Another half century later, the same mistake was made again. The Copenhagen interpretation is born from the observation that the final states in Fact 5 depend nonlinearly on the initial state while the von Neumann equation is purely linear. There is no Hamiltonian operator that could result in the density matrix evolving nonlinearly, therefore (Copenhagen concludes) the fact that the Fact 5 states are empirically good after measurement must mean that measurement cannot be described by ordinary linear unitary quantum time evolution. Just like the friction example, this is wrong. Measurement is a dynamical interactive process, and so during measurement the System's density matrix does not satisfy the von Neumann equation, the combined System + Detector density matrix satisfies the von Neumann equation. The Copenhagen thinking ignores the Detector degrees of freedom. There is no reason to believe that the System's density matrix evolves linearly when it is a subsystem of an interacting system. In fact, we can explicitly construct physical examples in which it does not. The nonlinear relationship between the initial and final states of the System is fully able to be explained by linear unitary time evolution on the full System+Detector system. The ridiculous conclusions achieved by the Copenhagen interpretation are born from it beginning on line one with ridiculous assumptions incongruous with the basic physical and mathematical facts of measurement. Garbage in, garbage out.

It is worth noting that the greatest physicist of the quantum era (and quite possibly of all time), Einstein, never believed and in fact actively opposed the Copenhagen interpretation. It is further worth noting that Schrödinger, who actually found the equation of motion of quantum mechanics, also never believed the Copenhagen interpretation. Here is one of many things he had to say about it in his lifetime [104]:

With very few exceptions (such as Einstein and Laue) all the rest of the theoretical physicists were unadulterated asses and I was the only sane person left. The one great dilemma that ails us day and night is the wave-particle dilemma. In the last decade I have written quite a lot about it and have almost tired of doing so: just in my case the effect is null because most of my friendly nearer colleagues have formed the opinion that I am, naturally enough, in love with my great success in life via wave mechanics reaped at the time I still had all my wits at my command and therefore, so they say, I insist upon the view that "all is waves". Old-age dotage closes my eyes towards the marvelous discovery of "complementarity". So unable is the good average theoretical physicist to believe any sound person could refuse to accept the Copenhagen oracle.

Finally, it is important to understand that typical physics graduate students today have a much deeper math education than any of the founders of the Copenhagen interpretation. Heisenberg barely knew basic linear algebra. What mathematics Bohr and Heisenberg could or could not imagine is irrelevant to modern science. The Copenhagen interpretation entered history as the default description of quantum mechanics not because it was convincing, nor powerful, nor even the simplest explanation of observation, but because its progenitors were very powerful people. Because Facts 1-5, viewed as empirical observations have no interpretative content, the various ridiculous aspects of Copenhagen historically had no experimental impact. The Copenhagen interpretation does not enable you to explain any observations beyond what Facts 1-5 already explain. Consequently, the Copenhagen interpretation has no practical advantages over the minimal interpretation but it does have a mountain of philosophical disadvantages. It is a backward, confused historical

aberration which we have long outgrown the need for.

9.4.2 Post-Schrödinger Dynamics

Post-Schrödinger dynamics is not a specific interpretation, but more so a class of similar-in-concept interpretations. The historically most prominent representative of this class is called the de Broglie-Bohm interpretation. Post-Schrödinger interpretations allow Fact 1 to be applied to individual experimental runs and then try to derive, as much as possible, Facts 2-5 as emergent empirical facts rather than fundamental features of reality. So far, this is exactly what the Thermal/Unitary interpretation does. The only difference between the Thermal interpretation and post-Schrödinger interpretations is how these facts are intended to be derived. In the Thermal interpretation, these facts are derived by using ordinary unitary von Neumann/Schrödinger time evolution on the combined System+Detector system. Post-Schrödinger interpretations do not typically model the Detector directly; instead, they modify the von Neumann/Schrödinger equation for the System by adding to it some small extra terms that are intended to cause the dynamical derivation of the final states in Fact 5 and/or they add extra degrees of freedom still attached to the System that are supposed to be the variables we actually see in measurement. Post-Schrödinger interpretations thus intend to fundamentally replace/correct quantum mechanics with a new dynamical theory that is approximately quantum mechanics when measurements are not happening. It is very difficult to do this in a way consistent with experiment, because many quantum experiments are extremely precise and these new terms tend to cause at least some small changes in experimental consequences outside of simply Facts 1-5.

From the perspective of the Thermal interpretation, the extra terms and extra degrees of freedom of post-Schrödinger approaches are seen just as a clunky way of trying to derive facts fully explainable without modifications to the dynamical structure of quantum mechanics *if you actually include the full quantum system*. Thus, I view post-Schrödinger approaches as an understandable attempt, from a historical perspective, to figure what is going on in quantum mechanics though I believe their usefulness is nullified by the Thermal interpretation. Often one will hear post-Schrödinger approaches described as “hidden variable theories” as they (typically) add extra variables relevant to experiment beyond simply the density matrix or state vector. In the common lore of interpretations of quantum mechanics, it is often claimed that hidden variable theories cannot possibly explain the experimental facts of quantum mechanics. This incorrect lore is based on a common misunderstanding of Bell’s theorem, which we will discuss in the next section.

9.4.3 Many Worlds Interpretation

As the plain absurdity of the Copenhagen interpretation has become more socially acceptable to talk about and corrections to the lore around Bell’s theorem have not yet diffused into the general mass of physicsfolk, the Many Worlds interpretation has become the trendy way to think about quantum mechanics. In some ways, the many worlds interpretations is mathematically similar to the Thermal interpretation. The many worlds interpretation does model the full measurement process by System+Detector using the very same Hamiltonian operator as the Thermal interpretation. Using the same standard decoherence arguments as the Thermal interpretation, the many worlds interpretations shows dynamically that the final density matrix appropriate for a statistical ensemble of the System at the end of measurement is precisely:

$$\hat{\rho}_S^{(f)} = \sum_n p_n \hat{\rho}_S^{(n)}, \quad p_n = \text{Tr}(\hat{\pi}_n \hat{\rho}_S), \quad \hat{\rho}_S^{(n)} = \frac{1}{p_n} \hat{\pi}_n \hat{\rho}_S \hat{\pi}_n. \quad (9.4.5)$$

The real leap of the many worlds interpretation comes in how this formula is interpreted. This formula, as the density matrix of an ensemble of final system states, is *consistent* with a statistical distribution over the states $\hat{\rho}_S^{(n)}$ each with respective probability p_n . The many worlds interpretation takes this distribution literally and asserts that the ensemble is real. It claims that there are infinitely many copies of the universe and that in each copy whenever a measurement happens, exactly one of the results $\hat{\rho}_S^{(n)}$ is achieved, and that among all of the copies the fraction in which that specific result is achieved is p_n . The many worlds interpretation is thus essentially hyper-frequentist. The many worlds interpretation thus claims that there is no true randomness because all of the possibilities happen, we just simply don’t know which of the infinite number of universes in the ensemble we are in for a particular measurement until we read out the measurement results.

The calculation leading to (9.4.5) (produced in previous section) as the appropriate ensemble density matrix for the System after measurement is essentially entirely uncontroversial in modern quantum mechanics.

There is a second calculation that is used to motivate the many worlds interpretation. As presented here, that calculation is based on the calculation done in section 3.7 of [127], which in turn is based on several older papers cited in that section. Suppose that the final ensemble density matrix above is taken by hypothesis to be the appropriate density matrix to assign in the final state immediately before reading the experimental result of a single experimental trial. Then, consider N copies of the experiment running in parallel. The overall density matrix of these N copies then would be:

$$\hat{\rho}^{(N)} = \hat{\rho}_S^{(f)} \otimes \dots \otimes \hat{\rho}_S^{(f)} = \sum_{n_1 \dots n_N} p_{n_1} \dots p_{n_N} \hat{\rho}_S^{(n_1)} \otimes \dots \otimes \hat{\rho}_S^{(n_N)}. \quad (9.4.6)$$

Define the frequency operators $\hat{P}_n^{(N)}$ as operators which count precisely what fraction of times each outcome occurred when acting on states in definitive outcome eigenspaces. That is, if $|\psi_n\rangle$ is a vector in the Hilbert space of a single experiment which is purely in the eigenspace projected into by $\hat{\pi}_n$, then:

$$\hat{P}_n^{(N)}(|\psi_{n_1}\rangle \otimes \dots \otimes |\psi_{n_N}\rangle) = \frac{C(n_1, \dots, n_N; n)}{N} |\psi_{n_1}\rangle \otimes \dots \otimes |\psi_{n_N}\rangle \quad (9.4.7)$$

where $C(n_1, \dots, n_N; n)$ is the number of times n occurs among the list $n_1, \dots, n_N$. Then, we can compute:

$$\langle \hat{P}_n^{(N)} \rangle = \text{Tr}(\hat{\rho}_n^{(N)} \hat{\rho}^{(N)}) = \sum_{n_1, \dots, n_N} \frac{C(n_1, \dots, n_N; n)}{N} p_{n_1} \dots p_{n_N}. \quad (9.4.8)$$

For a fixed number $N_n = C(n_1, \dots, n_N; n)$ of occurrences of n , there are N choose N_n equivalent reorderings of the labels $n_1, \dots, n_N$. Therefore, with this factor, we can unambiguously fix the first N_n to be n and guarantee that the remaining $N - N_n$ are not n :

$$\langle \hat{P}_n^{(N)} \rangle = \sum_{N_n=0}^N \sum_{\substack{n_{N_n+1}, \dots, n_N \\ \text{None} = n}} \frac{N_n}{N} \binom{N}{N_n} p_n^{N_n} p_{N_n+1} \dots p_{n_N} = \sum_{N_n=0}^N \frac{N_n}{N} \binom{N}{N_n} p_n^{N_n} (1 - p_n)^{N - N_n} \quad (9.4.9)$$

$$= \frac{p_n}{N} \frac{\partial}{\partial p_n} \sum_{N_n=0}^N p_n^{N_n} q^{N - N_n} \Big|_{q=1-p_n} = \frac{p_n}{N} \frac{\partial}{\partial p_n} (p_n + q)^N \Big|_{q=1-p_n} = p_n. \quad (9.4.10)$$

Similarly:

$$\langle (\hat{P}_n^{(N)})^2 \rangle = \sum_{N_n=0}^N \sum_{\substack{n_{N_n+1}, \dots, n_N \\ \text{None} = n}} \frac{N_n^2}{N^2} \binom{N}{N_n} p_n^{N_n} p_{N_n+1} \dots p_{n_N} = \sum_{N_n=0}^N \frac{N_n^2}{N^2} \binom{N}{N_n} p_n^{N_n} (1 - p_n)^{N - N_n} \quad (9.4.11)$$

$$= \frac{p_n}{N^2} \frac{\partial}{\partial p_n} p_n \frac{\partial}{\partial p_n} \sum_{N_n=0}^N p_n^{N_n} q^{N - N_n} \Big|_{q=1-p_n} = \frac{p_n}{N^2} \frac{\partial}{\partial p_n} p_n \frac{\partial}{\partial p_n} (p_n + q)^N \Big|_{q=1-p_n} \quad (9.4.12)$$

$$= \frac{p_n(1 - p_n)}{N} + p_n^2. \quad (9.4.13)$$

Thus:

$$\langle \hat{P}_n^{(N)} \rangle = p_n, \quad \text{Spr}(\hat{P}_n^{(N)}) = \frac{p_n(1 - p_n)}{N}. \quad (9.4.14)$$

Imagining the $N \rightarrow \infty$ limit, we see that in that limit the state $\hat{\rho}^{(N)}$ tends toward having zero spread with respect to $\hat{P}_n^{(N)}$ and assigns it a summary value p_n . The many worlds thinking interprets this calculation as showing that the fraction of states in the ensemble of systems which land in the state $\hat{\rho}_S^{(n)}$ is precisely p_n , because that is (so it is claimed) what $\langle \hat{P}_n^{(N)} \rangle$ represents, since it counts occurrences in each individual eigenspace.

There are a two unjustified steps of reasoning in coming up with the many worlds interpretation. The first is that the density matrix $\hat{\rho}_S^{(f)}$ is assigned to *each* individual final state right before measurement when it is in fact the correct density matrix for the *ensemble* of final states. The decoherence argument necessary to derive $\hat{\rho}_S^{(f)}$ relies on a time-averaging, relaxation to equilibrium, and ensemble averaging. The time evolution that brings the System's state in this form is reliant on its coupling to the Detector (whose existence is suddenly ignored in the act of constructing the "many worlds" in $\hat{\rho}^{(N)}$). Thus, inadvertently the many worlds interpretation assumes the requisite ensemble on the first step of calculation. The second error in interpretation is the meaning assigned to $\hat{P}_n^{(N)}$. It is true (by construction) that when $\hat{P}_n^{(N)}$ acts on a state of the form in (9.4.7), it has the effect of simply multiplying by the count fraction N_n/N . However, it is a

separate leap to conclude that in some linear combination of such states, generally forming a state which is not an eigenstate of $\hat{P}_n^{(N)}$, the operator summary of $\hat{P}_n^{(N)}$ still represents anything like the fraction of counts of the experiment which will be assigned the final state $\hat{\rho}_S^{(n)}$. In fact, by hypothesis, the many worlds interpretation already assumes each final state is precisely assigned to be $\hat{\rho}_S^{(f)}$, not $\hat{\rho}_S^{(n)}$.

The many worlds interpretation's errors are born from a misunderstanding of the physical properties of a linear combination. It is not the only interpretation whose believers frequently misunderstand linearity, so remember the following points when thinking about other interpretations as well. The second error in the previous paragraph may (to someone not being careful) seem logically okay – if every element in a linear combination has a property then certainly the linear combination itself should have that property right? No. Absolutely not. That is not how linearity works. A linear combination of Dirac deltas at different points is a not a Dirac delta, so even though every state in such a linear combination has a position spread of 0, the linear combination does not. A vector pointing east in the plane is a linear combination of vectors pointing northeast and southeast, each of which have the property of changing the coordinate along the north-south axis, but their sum does not. In quantum electrodynamics, the electric field operator (defined in (8.10.41) and (8.10.44)) is a linear combination of creation and annihilation operators. Therefore, the electric field operator when acting on an N photon state results in a linear combination of states of $N - 1$ and $N + 1$ photons. Consequently, the classical electric field $\langle \hat{E} \rangle$ of every single N photon state is 0. However, a linear combination of states of different photon numbers gives a nonzero classical electric field. The literal existence of classical electromagnetism is proof that the logic of this second error is wrong.

At its core, the many worlds interpretation looks at the density matrix $\hat{\rho}_S^{(f)}$ and simply asserts that it is a genuine statistical mixture of the $\hat{\rho}_S^{(n)}$ with probabilities p_n . This is again a misunderstanding of how linearity works. The same final state ensemble density matrix $\hat{\rho}_S^{(f)}$ can be decomposed into a sum of the form (9.4.5) for multiple different sets of $\hat{\rho}_S^{(n)}$ and p_n ; that decomposition is ambiguous. Therefore any argument that attempts to derive the distribution p_n of outcomes $\hat{\rho}_S^{(n)}$ from the density matrix $\hat{\rho}_S^{(f)}$ is doomed to fail; it is wrong on principal. See the example given in the text of subsection 9.1.2. In order to actually justify the distribution of the ensemble density matrix, you must start from individual instances of the system and derive probabilities, as done in the Thermal Interpretation. The math is not reversible.

I find the many worlds interpretation not only logically unsatisfying but also philosophically vacuous. The silver bullet that the many worlds view uses to explain the empirical facts of quantum mechanics is the introduction of an infinite number of inaccessible other copies of the universe. The many worlds interpretation offers no even formal structure through which these other copies of the universe could ever even in principle be measured or interacted with, and therefore the claim of their existence is **NOT** a scientific hypothesis, as it is entirely unfalsifiable. The central claim of the many worlds interpretation is literally not science.

9.4.4 The Damned Cat

Ugh. Is it time to talk about Schrödinger's cat? I guess it is time to talk about Schrödinger's cat. If somehow you haven't heard about this poor cat, let me explain. Consider a cat in a sealed box which also contains some poison in a container with a release mechanism, a radioactive particle, and a detector capable of reading the radioactivity. The release mechanism is such that if the detector goes off, the poison is released, killing the cat (booooo). Initially the cat, viewed as a quantum system, is definitely in a subregion of its Hilbert space where it has the property of "alive". After the decay, the cat is definitely in a subregion of its Hilbert space where it has the property of "dead". While the box is closed and the particle is evolving, the particle's quantum state will generally be a linear combination of a state of particle number 1 and a state of particle number 0. It is supposed then that before the decay has happened, the cat is similarly in a linear combination of its before and after decay states. Thus, the cat is in a linear combination of states, the first term in the linear combination being a state which taken on its own is one in which the cat is definitely alive and the second being a state which taken on its own is one in which the cat is definitely dead. The thought experiment has the effect that a microscopic linear combination (of the radioactive particle) induces a macroscopic linear combination (of the cat's dead and alive states). The question is, what are the properties of this macroscopic linear combination?

Schrödinger originally considered this thought experiment to make fun of the Copenhagen interpretation. Within Copenhagen, the thought experiment reveals a basic question about what counts as measurement. Does the cat cause measurements? Does the detector cause measurements? Or, is it we who open the box

after a while who cause the measurement? If the cat, by being able to hear the detector click, is constantly measuring whether or not the decay has happened, then for some amount of time the cat is in the alive state until it hears a click and shortly after dies. If the cat does not constitute a measurer but the detector does, then the macroscopic linear combination of the cat between an alive state and dead state progressively forms and one has to wonder what it means for a cat to be in such a linear combination. At some point, the detector notices the decay and the cat dies. The final conceptualization of what counts as measurement is what Schrödinger was really trying to make fun of originally, which is to think that neither the cat nor the detector count as taking measurements. It is humans who count as performing the measurement when we open the box. Then, before we have opened the cat is in its macroscopic linear combination. When we open the box, either the detector will have gone off or not, and correspondingly the cat will suddenly collapse to either the alive state or the dead state. This position is so bizarre because it places humans in a special role in nature, which is antithetical to basic science (the Copernican principle). In a popular science magazine, you are likely to read the cat as being described as “both dead and alive” before the box is opened. The Copenhagen interpretation is not capable of resolving which of these three participants (the cat, the detector, or the humans) are doing the measuring, and so is again incomplete as a theory. In any of the three cases, when the box is opened the cat is seen to either be dead or alive and the probabilities computed from Facts 1-5 are the same. Copenhagen rejects reality except at the time of measurement, but in this case the time of measurement is not determined by Copenhagen, and so it is unclear what the interpretation counts as real.

In the many worlds interpretation, in the infinite ensemble of universes, the cat would generally be considered sufficiently macroscopic that at all times it counts as measuring the detector click and thus whether the decay has happened or not. The result is that at all times whether the box has been opened or not, the cat in each universe in the ensemble is or is not dead, with the distribution of proportions determined by the Born rule on the full ensemble of states. There is not much interesting here for the many worlds interpretation, and it does provide a much less silly answer than the Copenhagen interpretation.

In the thermal/unitary interpretation, the cat and the detector are both macroscopic. Whether or not the detector has gone off has a physically real answer. Once the detector has gone off the poison is released and the cat dies. We learn the answer to whether the cat is dead or alive once the box is opened but this does not mean anything like “before the box is opened the cat is dead and alive”. The cat goes from a state of definitely alive to definitely dead at an unpredictable time. That time is unpredictable because the time of the decay is unpredictable, and that time is unpredictable because of the coupling of the radioactive particle to infinitely many uncontrolled background degrees of freedom (the various fields that exist in our universe which weakly couple to basically everything at any nonzero temperature).

The objection one is likely to hear to the thermal interpretation’s accounting of events is about what does the macroscopic linear combination of dead and alive look like for the cat before the decay has happened? This question of course was also present in the Copenhagen interpretation, but because that interpretation rejects reality before the measurement, it doesn’t really have to answer it. The thermal interpretation does. Well, the whole concept of the cat being in a linear combination of a state in the alive part of the Hilbert and a state in the dead part of the Hilbert space meaning the cat is “both dead and alive” is again a complete misunderstanding of how linear combination works. There is absolutely no reason to believe that macroscopic properties (deadness/aliveness) are linear over the microscopic state of the system. For an easy physical example you can see with your eyes, consider the visible region of the electromagnetic spectrum. There is a certain band of the spectrum corresponding to red light; there is another band that corresponds to purple light. A state has the property “is red” if it is approximately purely in the spectrum band that is red (approximately within the resolution of the eye or other detector to see the components of colors outside of this band). A state has the property “is not red” if it has dominating components outside this band. Similarly, one can define the properties “is purple” and “is not purple” from its corresponding band. The color pink is a linear combination of both red light and purple light. Does this mean that pink is both red and also purple? Being a linear combination of two things, each with a property, does not mean that the combination has both or either property. Pink is not red and it is not purple. Back to the cat, for every state in the cat’s Hilbert space, it is possible to assign the property or alive, dead, or unclear to that state. The unclear condition exists because biologically what counts as alive is a little bit fuzzy (heart stopping versus brain death, for example) and we can basically ignore it for this question. Every state in the Hilbert space takes one of these three properties definitely. The properties are not linear over the linear structure of the Hilbert space, and so if one takes an arbitrary state from the alive region and combines it with an arbitrary state from the dead region, it will end up in some region, but completely unclear which. For another easy example, consider a two dimensional plane, divided into four quadrants. We can define a vector as type NE, NW, SE, SW, N, E, S,

W, or 0 (with letters corresponding to the cardinal directions) based on in the first four cases which quadrant it points from the origin into, in the fifth through eighth cases which pure cardinal direction it points along, and in the last case if it is the 0 vector. Thus every vector in the plane has the property of definitely fitting into exactly one of these nine categories. The property of which one it fits into is not linear over the vectors. Consider the vector $(3, 2)$ which is NE and the vector $(3, -3)$ which is SE; their linear combination is $(6, -1)$ which is SE. Alternatively, consider the vector $(3, 3)$ which is NE and the vector $(3, -1)$ which is SE; their linear combination is $(6, 2)$ which is NE. Therefore, from the properties assigned to the vectors (SE'lyness and NE'lyness) alone it is impossible to know what property to assign to their linear combination. Even worse, it would not even be an invariant property to assign $(6, 2)$ the property of “both NE and SE” as would be suggested by dead-and-alive logic; you can also write it as a linear combination of $(4, 1)$ and $(2, 1)$ which are both NE, no SE part to be found. This refutation is already possible in a 2 dimensional vector space. In the unimaginably high dimension Hilbert space of a cat, the complicated properties of aliveness and deadness have absolutely no reason to be asserted to be anything even related to linear over the microscopic state of the cat. That is neither how math nor how physics works⁵.

In short, the entire Schrödinger's cat discussion is basically irrelevant for actual physics. It is a funny jab at the ridiculousness of the Copenhagen interpretation but all of the weirdness described in the thought experiment is either an artifact of the absurdity of the interpretation used (in the case of Copenhagen) or of a misunderstanding of the nature of linear combination (in the case of claiming the cat is “both dead and alive”).

9.4.5 Bell-type Theorems and Their Consequences

Bell's theorem is one of the most frequently misreported results in all of physics. Those with a Wikipedia-level appreciation of the relevant physics are essentially certain to completely misunderstand it. Bell's theorem and various similar theorems at their core are mathematical statements. Bell-type theorems all consist of two parts. In the first, they give examples of quantum systems satisfying interesting equalities or inequalities. These relations are interesting because in the second part they show that no classical probability space could also satisfy them, where the operator summary is interpreted as a statistical expectation in that probability space. The effect of this is to show that quantum mechanics is not equivalent to classical probability theory. There is a layer of interpretation that is very often added to Bell-type theorems after this, and that layer is just wrong. The interpretive layer will claim that Bell's theorem disproves the possibility that the apparent randomness in quantum mechanics could be explained by a (local) hidden variable theory. This is certainly what Bell believed. However, this is wrong because the way the classical probability space is constructed in that thinking is not how one would construct the probability space in the relevant hidden variable theories. Let's explain the details. This section is based on [79].

We will treat only the most classic example of a Bell inequality, but the importance and logic of the result is the same regardless of the example. Consider a quantum system consisting of two interacting subsystems, each with a two dimensional Hilbert space (for example, each subsystem could be a spin-1/2 particle). Call the first system A (or often Alice, for cuteness) and the second system B (often Bob, similarly). Consider two different operators of interest in each system, $\hat{A}_0$ and $\hat{A}_1$ for Alice and $\hat{B}_0$ and $\hat{B}_1$ for Bob, defined by:

$$\hat{A}_0 = \sigma_z^{(A)} \otimes \mathbb{1}^{(B)}, \quad \hat{A}_1 = \sigma_x^{(A)} \otimes \mathbb{1}^{(B)}, \quad \hat{B}_0 = -\mathbb{1}^{(A)} \otimes \frac{\sigma_x^{(B)} + \sigma_z^{(B)}}{\sqrt{2}}, \quad \hat{B}_1 = \mathbb{1}^{(A)} \otimes \frac{\sigma_x^{(B)} - \sigma_z^{(B)}}{\sqrt{2}}. \quad (9.4.15)$$

Let $|+\rangle$ and $|-\rangle$ denote the eigenstates of σ_z with eigenvalues $+1$ and -1 , and consider the state vector:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|+_A - _B\rangle - |-_A + _B\rangle). \quad (9.4.16)$$

In this state, it follows that:

$$\langle \hat{A}_0 \rangle = 0, \quad \langle \hat{A}_1 \rangle = 0, \quad \langle \hat{B}_0 \rangle = 0, \quad \langle \hat{B}_1 \rangle = 0. \quad (9.4.17)$$

⁵But wait, I thought that all properties were linear over the microscopic state because the summary map is linear? No. The spread of a single operator is a property of the state of a system but is not linear over the density matrix. The entire density matrix is determined by the summary map, and therefore any property of a quantum system can be written as a function of the operator summaries, each of which is linear over the system state. But, one can consider nonlinear functions of these operator summaries, and the resulting property from that function is then nonlinear over the system state. Aliveness and NE'lyness are nonlinear functions of a variety of operator summaries.

As well, it follows that:

$$\langle \hat{A}_0 \hat{B}_0 \rangle = \langle \hat{A}_0 \hat{B}_1 \rangle = \langle \hat{A}_1 \hat{B}_0 \rangle = -\langle \hat{A}_1 \hat{B}_1 \rangle = \frac{1}{\sqrt{2}} \quad (9.4.18)$$

from which we have:

$$\langle \hat{A}_0 \hat{B}_0 \rangle + \langle \hat{A}_0 \hat{B}_1 \rangle + \langle \hat{A}_1 \hat{B}_0 \rangle - \langle \hat{A}_1 \hat{B}_1 \rangle = 2\sqrt{2}. \quad (9.4.19)$$

This identity, purely within the domain of our quantum system, is not very interesting. The above result is given import by considering a naively related system in probability theory.

Consider a probability space in which there are four random variables, a_0, a_1, b_0, b_1 , so that in each outcome of the probability space, each of these variables takes the value $+1$ or -1 . Plainly:

$$a_0 b_0 + a_0 b_1 + a_1 b_0 - a_1 b_1 = (a_0 + a_1) b_0 + (a_0 - a_1) b_1. \quad (9.4.20)$$

Because both a_0 and a_1 are either ± 1 , it must be that $a_0 = a_1$ or $a_0 = -a_1$. In the first case, the b_1 term on the right hand side above does not contribute and the expression has magnitude 2. In the second case, the b_0 term on the right hand side above does not contribute and the expression again has magnitude 2. Therefore, it is identically true that:

$$|a_0 b_0 + a_0 b_1 + a_1 b_0 - a_1 b_1| = 2. \quad (9.4.21)$$

There will be some probability that the expression inside the absolute value takes the value 2 and some probability it takes the value -2. But, because these are the only values it may take, its average cannot exceed 2 in magnitude. Therefore, for any distribution on these four variables:

$$|\mathbb{E}(a_0 b_0 + a_0 b_1 + a_1 b_0 - a_1 b_1)| \leq 2. \quad (9.4.22)$$

This identity considered purely in the domain of probability theory is also not very interesting. Let us now see how our two uninteresting ideas are often interpreted together.

Let us return to our quantum system and think about how it behaves under measurement without applying the thermal interpretation. We take the operators $\hat{A}_0, \hat{A}_1, \hat{B}_0, \hat{B}_1$ to all be of experimental interest. Each of these operators has eigenvalues $+1$ and -1 . We are going to prepare a large number of identical copies of our system and perform many measurements. Because $\hat{A}_0$ and $\hat{A}_1$ do not commute, in each trial we will only measure the property associated to one of them. Similarly so, in each trial we will only measure the property associated to either $\hat{B}_0$ or $\hat{B}_1$. That is, in our different trials we will have different settings on our measurement equipment appropriate for measuring different properties of the system. The A operators and B operators commute with members of the other set, and so in each trial we will select an A operator and a B operator and measure the properties associated to each of them. Let the properties associated to our operators be called a_0, a_1, b_0, b_1 . By the basic facts of measurement in section 9.4, in each experimental trial no matter which subset of a_0, a_1, b_0, b_1 are measured, each of the properties measured will take the value $+1$ or -1 . Experimentally, different trials will give different values for the measured variables and so there is some mechanism that induces a probability distribution on the results but we will be agnostic to what it is. We now add an interpretative element that is crucial in Bell's argument – we assume that in each experimental trial the properties a_0, a_1, b_0, b_1 are all physically real properties of our quantum system and the act of measuring that system reveals the true value of some of these variables (whichever pair of properties has been selected). We call this Bell-realism. Because $\hat{A}_0$ and $\hat{A}_1$ act only on system A and $\hat{B}_0$ and $\hat{B}_1$ act only on system B, they each only affect data in their respective system, and so the property associated to the product $\hat{A}_0 \hat{B}_0$ is simply $a_0 b_0$ (and similarly so for the other 3 combinations of products). We call this Bell-locality. Under the assumption of Bell-realism, in each experiment trial (which we now view as an outcome in probability space), there is a true value of a_0, a_1, b_0, b_1 and so we can assign a probability of occurrence in our experiment to each of the 16 possible combinations of values of the properties. Automatically then, (9.4.22) must hold. However, by the Born rule and Bell-locality, $\langle \hat{A}_0 \hat{B}_0 \rangle = \mathbb{E}(a_0 b_0)$ and similarly so for the other combinations of operators, and so we have by (9.4.19) that the left hand side of (9.4.22) must take the value $2\sqrt{2}$, violating the right hand side of (9.4.22). We have arrived at a contradiction. Therefore, either Bell-realism or Bell-locality must be incorrect. This is Bell's theorem.

You will notice that the above argument had absolutely nothing to do with hidden variables. Hidden variables are typically invoked in Bell-type discussions to explain why when the system of interest is prepared identically different measurement results are achieved. This argument goes by saying perhaps there are some unaccounted for degrees of freedom which determine the properties a_0, b_0, a_1, b_1 that have some probability distribution. This will induce a probability distribution on these variables and because no probability distribution is consistent with (9.4.19) one then concludes that local real hidden variables cannot correctly

account for the randomness of quantum mechanics. This argument is correct if Bell-realism and Bell-locality are true. But, the hidden variables are simply not needed to arrive at the challenge of Bell's result. Bell's theorem really states that quantum mechanics is not equivalent to the combination of probability theory, Bell-realism, Bell-locality. Some have interpreted Bell's theorem to prove that quantum mechanics is nonlocal, although you will notice that it is not at all clear that Bell-locality and locality in the sense we have always defined previously are the same thing.

There is a much simpler explanation of Bell's theorem – **Bell-realism is not true** (and is not the same thing as ordinary realism). Bell-realism takes the measurement outcomes a_0, b_0, a_1, b_1 to be real properties of the quantum system being measured. However, as demonstrated in section 9.3, the outcomes of individual experimental trials are actually properties of the experimental apparatus which in a well-designed experiment are correlated with the incoming state of the system being measured but not purely a reflection of it. Because $\hat{A}_0$ and $\hat{A}_1$ do not commute there is no way to prepare an interaction Hamiltonian operator $\hat{H}_{\text{int}}$ capable of ideally measuring $\hat{A}_0$ and $\hat{A}_1$ in the same experimental trial. Because a_0 and a_1 are defined through this measurement interaction, there is no way to define both a_0 and a_1 in a single trial. This is very different to Bell-realism. Bell-realism assumes that a_0 and a_1 each have an unknown true value and that the experiment measures one of them. In reality, the quantum system being measured has a real physical state and setting the experiment to measure a_0 or a_1 determines which one will be defined, while the other *does not even exist* in that setting; the defined variable then reveals some partial information about the actual state of the system of interest. So, it is no surprise it is impossible to design a joint probability distribution for a_0, a_1, b_0, b_1 able to describe the outcome of the experiment. The interacting mechanics of measurement never has more than two of those four variables even being well-defined in the same trial! The correct mathematical description of probability in quantum mechanics is that there is a probability space appropriate for each experimental setting (choice of things to measure, called a context).

The fundamental error of the common interpretation of Bell's theorem is that it ignores *contextuality* – the possible outcomes of experimental results in quantum mechanics are determined by the experimental context (which variables you get values for is determined by your interaction Hamiltonian; changing your detector's settings changes its interaction Hamiltonian with the system of interest). The common way of thinking about Bell's theorem misunderstands what realism means for a quantum system. Ordinary realism holds that the quantum state (the density matrix) is physically real and that, together with microscopic degrees of freedom in the measurement apparatus, is fully consistent with the experimental facts of quantum mechanics. Bell-realism holds that the unknown hypothetical outcomes of experiments not performed are real which is both not consistent with experiment and not a useful assumption to guide your quantum mechanical thinking.

In the corrected interpretation of Bell's theorem in which you appropriately account for contextuality, the random variable a_0 only exists when your experiment is set to measure the property associated to $\hat{A}_0$, and similarly so for the other properties. In each of the four possible experimental settings, one can then fully define a probability distribution using the Born rule appropriate for the two variables which are defined in that context and then one sees by a brief calculation that indeed:

$$\mathbb{E}_{00}(a_0 b_0) + \mathbb{E}_{01}(a_0 b_1) + \mathbb{E}_{10}(a_1 b_0) - \mathbb{E}_{11}(a_1 b_1) = 2\sqrt{2} \quad (9.4.23)$$

exactly as is required for consistency. In the above the subscripts on the expectation indicate which experimental context is used (and thus the appropriate Born rule distribution). There is no joint distribution for all four variables because there is no experimental context in which all four variables exist. It is amazing just how wrong the common discussion around Bell's theorem is. Please again refer to [79] for more analysis and references to other works that hath understanding.

Exercises

Problem 9.7: ★ The most important homework question.

- Go take a talk through nature with someone you like, even if that someone is just yourself.
- Go pet a cat, if you can.

9.5 The Path Integral

9.5.1 The Path Integral for Time Evolution

Feynman developed a convenient formula, known as the path integral, for computing the time evolution operator $\hat{U}(t, t_0)$. For ordinary quantum mechanics his formula is actually obnoxiously inconvenient. But, while ordinary operator methods are generally much more painful for calculations in quantum field theory compared to single particle quantum mechanics, the path integral isn't really any worse when we make the leap to field theory. So, it becomes convenient by comparison. Strictly speaking, every calculation in quantum mechanics (including in quantum field theory) can be done without ever using the path integral. However, it is often the most convenient route to take for very complicated calculations. Recall that the unitary time evolution operator $\hat{U}(t, t_0)$ defined by:

$$i\hbar \frac{d\hat{U}(t, t_0)}{dt} = \hat{H}(t)\hat{U}(t, t_0), \quad \hat{U}(t, t) = \mathbb{1}, \quad (9.5.1)$$

can be formally expressed in terms of the Hamiltonian operator using the time ordering transformation as:

$$\hat{U}(t, t_0) = \mathcal{T} : e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt'} \quad (9.5.2)$$

and satisfies the composition property:

$$\hat{U}(t, t_0) = \hat{U}(t, t_1)\hat{U}(t_1, t_0). \quad (9.5.3)$$

The path integral is used to explicitly compute the configuration space propagator $\hat{U}(t, Q, t_0, Q_0)$, which is the matrix element function of $\hat{U}$ in coordinate space:

$$U(t, Q, t_0, Q_0) = \langle Q | \hat{U}(t, t_0) | Q_0 \rangle \quad (9.5.4)$$

Consider a list of $N+1$ times $t_0, t_1, \dots, t_{N-1}, t_N = t$ that divide up the time interval $[t_0, t]$ with $t_n < t_{n+1}$. We will eventually seek to take N large so that we can also take the duration between adjacent times to become arbitrarily small. Using the composition property, we have immediately:

$$\hat{U}(t, t_0) = \hat{U}(t, t_{N-1})\hat{U}(t_{N-1}, t_{N-2})\dots\hat{U}(t_2, t_1)\hat{U}(t_1, t_0) = \mathcal{T} : \prod_{n=0}^{N-1} \hat{U}(t_{n+1}, t_n). \quad (9.5.5)$$

To compute $U(t, Q, t_0, Q_0)$, we insert a complete set of $|Q\rangle$ states between each factor in this product (we use the labels $Q_0, Q_1, \dots, Q_{N-1}, Q_N = Q$):

$$U(t, Q, t_0, Q_0) = \int \langle Q | \hat{U}(t, t_{N-1}) | Q_{N-1} \rangle \langle Q_{N-1} | \hat{U}(t_{N-1}, t_{N-2}) | Q_{N-2} \rangle \dots \cdot \langle Q_2 | \hat{U}(t_2, t_1) | Q_1 \rangle \langle Q_1 | \hat{U}(t_1, t_0) | Q_0 \rangle d^d Q_1 \dots d^d Q_{N-1} \quad (9.5.6)$$

$$= \int U(t, Q, t_{N-1}, Q_{N-1}) U(t_{N-1}, Q_{N-1}, t_{N-2}, Q_{N-2}) \dots \cdot U(t_2, Q_2, t_1, Q_1) U(t_1, Q_1, t_0, Q_0) d^d Q_1 \dots d^d Q_{N-1} \quad (9.5.7)$$

$$= \int \left(\prod_{n=0}^{N-1} U(t_{n+1}, Q_{n+1}, t_n, Q_n) \right) d^d Q_1 \dots d^d Q_{N-1}. \quad (9.5.8)$$

This is true for each N , and so in the $N \rightarrow \infty$ limit:

$$U(t, Q, t_0, Q_0) = \lim_{N \rightarrow \infty} \int \left(\prod_{n=0}^{N-1} U(t_{n+1}, Q_{n+1}, t_n, Q_n) \right) d^d Q_1 \dots d^d Q_{N-1}. \quad (9.5.9)$$

We will now compute each of these factors which in the large N limit causes the time interval $t_{n+1} - t_n$ to become short. Note that because each Q_n is integrated over its all range, the displacement $Q_{n+1} - Q_n$ does not become small.

Consider $U(t + \delta t, Q + \delta Q, t, Q)$ for δt small but δQ arbitrary. Using (9.5.2):

$$U(t + \delta t, Q + \delta Q, t, Q) = \langle Q + \delta Q | \hat{U}(t + \delta t, t) | Q \rangle = \langle Q + \delta Q | \mathcal{T} : e^{-\frac{i}{\hbar} \int_t^{t+\delta t} \hat{H}(t') dt'} | Q \rangle \quad (9.5.10)$$

$$= \langle Q + \delta Q | \left(\mathbb{1} - \frac{i}{\hbar} \int_t^{t+\delta t} \hat{H}(t') dt' + \mathcal{O}(\delta t^2) \right) | Q \rangle \quad (9.5.11)$$

$$= \langle Q + \delta Q | \left(\mathbb{1} - \frac{i}{\hbar} \hat{H}(t) \delta t + \mathcal{O}(\delta t^2) \right) | Q \rangle \quad (9.5.12)$$

$$= \langle Q + \delta Q | Q \rangle - \frac{i}{\hbar} \delta t \langle Q + \delta Q | \hat{H}(t) | Q \rangle + \mathcal{O}(\delta t^2). \quad (9.5.13)$$

Now use (9.2.21) with $H(t, Q, P)$ the Wigner function associated to $\hat{H}$:

$$U(t + \delta t, Q + \delta Q, t, Q) = \delta(\delta Q) - \frac{i}{\hbar} \delta t \int e^{\frac{i}{\hbar} P_a \delta Q^a} H\left(t, Q + \frac{\delta Q}{2}, P\right) \frac{d^d P}{(2\pi\hbar)^d} + \mathcal{O}(\delta t^2) \quad (9.5.14)$$

$$= \int \frac{e^{\frac{i}{\hbar} P_a \delta Q^a}}{(2\pi\hbar)^d} d^d P - \frac{i}{\hbar} \delta t \int e^{\frac{i}{\hbar} P_a \delta Q^a} H\left(t, Q + \frac{\delta Q}{2}, P\right) \frac{d^d P}{(2\pi\hbar)^d} + \mathcal{O}(\delta t^2) \quad (9.5.15)$$

$$= \int e^{\frac{i}{\hbar} P_a \delta Q^a} \left(1 - \frac{i}{\hbar} \delta t H\left(t, Q + \frac{\delta Q}{2}, P\right) + \mathcal{O}(\delta t^2) \right) \frac{d^d P}{(2\pi\hbar)^d} \quad (9.5.16)$$

$$= \int e^{\frac{i}{\hbar} (P_a \delta Q^a - H(t, Q + \delta Q/2, P) \delta t + \mathcal{O}(\delta t^2))} \frac{d^d P}{(2\pi\hbar)^d}. \quad (9.5.17)$$

Define the phase-action change δS by:

$$\delta S = P_a \delta Q^a - H(t, Q + \delta Q/2, P) \delta t \quad (9.5.18)$$

$$\Rightarrow U(t + \delta t, Q + \delta Q, t, Q) = \int e^{\frac{i}{\hbar} \delta S + \mathcal{O}(\delta t^2)} \frac{d^d P}{(2\pi\hbar)^d}. \quad (9.5.19)$$

Returning this to (9.5.9) and noting that if we divide up $[t_0, t_f]$ evenly, $t_{n+1} - t_n = \frac{t_f - t_0}{N}$:

$$U(t_f, Q_f, t_0, Q_0) = \lim_{N \rightarrow \infty} \int \left(\prod_{n=0}^{N-1} \int e^{\frac{i}{\hbar} \delta S_n + \mathcal{O}(1/N^2)} \frac{d^d P_n}{(2\pi\hbar)^d} \right) d^d Q_1 \dots d^d Q_{N-1} \quad (9.5.20)$$

$$= \lim_{N \rightarrow \infty} \int e^{\frac{i}{\hbar} \sum_{n=0}^{N-1} \delta S_n + \mathcal{O}(1/N)} \frac{d^d P_0}{(2\pi\hbar)^d} \frac{d^d Q_1 d^d P_1}{(2\pi\hbar)^d} \dots \frac{d^d Q_{N-1} d^d P_{N-1}}{(2\pi\hbar)^d}. \quad (9.5.21)$$

Here we used that the correction terms $\mathcal{O}(\delta t^2)$ are $\mathcal{O}(1/N^2)$ when written in terms of N and that a sum of N terms which are $\mathcal{O}(1/N^2)$ is $\mathcal{O}(1/N)$. If we now assume that it is safe to “complete” this limit, then in the $N \rightarrow \infty$ limit these $1/N$ terms vanish:

$$U(t_f, Q_f, t_0, Q_0) = \lim_{N \rightarrow \infty} \int e^{\frac{i}{\hbar} \sum_{n=0}^{N-1} \delta S_n} \frac{d^d P_0}{(2\pi\hbar)^d} \frac{d^d Q_1 d^d P_1}{(2\pi\hbar)^d} \dots \frac{d^d Q_{N-1} d^d P_{N-1}}{(2\pi\hbar)^d} \quad (9.5.22)$$

where each δS_n is given by:

$$\delta S_n = P_{na}(Q_{n+1}^a - Q_n^a) - H\left(t_n, \frac{Q_n + Q_{n+1}}{2}, P_n\right) \frac{t_f - t_0}{N} \quad (9.5.23)$$

and $Q_N = Q_f$.

Equation (9.5.22) is the relatively safe formula to use for the path integral, but it is almost never what you will see written. It is called the path integral because we could view $Q_0, Q_1, \dots, Q_{N-1}, Q_f$ and $P_0, \dots, P_{N-1}$ as forming a path through classical phase space associated with the times $t_0, t_1, \dots, t_{N-1}, t_f$ beginning at Q_0 at time t_0 and ending at Q_f at time t_f . We integrate over all the intermediate points. In the $N \rightarrow \infty$ limit, this becomes (at least formally) “an integration over all paths” in phase space connecting (t_0, Q_0) to (t_f, Q_f) . This is somewhat like the classical variational problem which considers variations of all such paths to find the distinguished classical path (by the one that makes the action stationary). Now we are integrating over all such paths. The integral measure over all such paths is quite a mess to write out, and you will note that we perform one more P integration than Q integration. Call the path that we are integrating over $(Q(t), P(t))$. This path then has boundary conditions $Q(t_0) = Q_0$ and $Q(t_f) = Q_f$. For compactness of notation, it is common to make the replacement:

$$\frac{d^d P_0}{(2\pi\hbar)^d} \frac{d^d Q_1 d^d P_1}{(2\pi\hbar)^d} \dots \frac{d^d Q_{N-1} d^d P_{N-1}}{(2\pi\hbar)^d} \rightarrow \mathcal{D}Q \mathcal{D}P = \mathcal{D}\mathbb{P}. \quad (9.5.24)$$

This replacement is just lazy notation and the expression on the far left side should be used when being

careful. The expression in the exponent in the $N \rightarrow \infty$ limit actually goes to the form of a Riemann sum:

$$\lim_{N \rightarrow \infty} \sum_{n=0}^{N-1} \delta S_n = \lim_{N \rightarrow \infty} \sum_{n=0}^{N-1} \left(P_{na} \frac{Q_{n+1}^a - Q_n^a}{t_{n+1} - t_n} - H \left(t_n, \frac{Q_n + Q_{n+1}}{2}, P_n \right) \right) (t_{n+1} - t_n) \quad (9.5.25)$$

$$= \int_{t_0}^{t_f} \left(P_a(t) \dot{Q}^a(t) - H(t, Q(t), P(t)) \right) dt \quad (9.5.26)$$

This integral is precisely the action integral one would get for the path (Q, P) using the Wigner function $H(t, Q, P)$ associated to the Hamiltonian operator $\hat{H}$ as if it were the Hamiltonian for the quantities (Q, P) . Thus, define the Wigner action functional:

$$S[Q, P] = \int_{t_0}^{t_f} \left(P_a \dot{Q}^a - H(t, Q, P) \right) dt. \quad (9.5.27)$$

In terms of this functional, the condensed expression for the path integral becomes:

$$U(t_f, Q_f, t, Q) = \int_{Q(t_0)=Q_0}^{Q(t_f)=Q_f} e^{\frac{i}{\hbar} S[Q, P]} \mathcal{D}Q \mathcal{D}P. \quad (9.5.28)$$

Equation (9.5.28) has a very nice interpretation and that interpretation significantly predates Feynman – it was identified by Huygens nearly 300 years prior – the path integral gives the propagation amplitude for an initial wave disturbance (localized at Q_0 at time t_0) to a final wave disturbance (localized at Q_f at time t_f) by summing (integrating) over all paths that connect the initial and final points (paths taken in phase space) and weighted by the phase accumulated along that particularly trajectory. Feynman’s identification was to appreciate that the phase is itself given by (up to a multiplier) a functional of a very similar form to the classical action.

9.5.2 Important Subtleties

There are a few common errors made in the use of the path integral. These errors are common because they are safe for some common special cases but they fail in general. You should view them as useful shortcuts that are valid under appropriate circumstances, and you should remember to actually check the circumstances before you use them. First, the $H(t, Q, P)$ function in the path integral is the Wigner function associated to the Hamiltonian operator $\hat{H}$, it is **NOT** the Hamiltonian function of the classical system gotten by taking the classical limit of the quantum theory. It is a common error to think of the path integral as a “quantization scheme” (which you know by now doesn’t exist) where you take the Hamiltonian function of a classical system and put it into (9.5.27). This is **WRONG**. Because generators in classical mechanics transform quantities by the Poisson bracket while functions on phase space in quantum mechanics transform according to the Moyal bracket, if you perform “path integral quantization” in one coordinate system and your friend performs the same process on the same classical system expressed in different coordinates, the resulting quantum theories will not generally be equivalent. You used the wrong transformation properties! In one perspective, $\mathcal{H}$ (the classical Hamiltonian) is the $\hbar \rightarrow 0^+$ limit of H and $\hbar$ corrections are mixed around by quantum coordinate transformations. Throwing them away in one coordinate system (unphysically) designates a preferred coordinate system. This distinction is very important for symmetry considerations. In order for the quantum system to have a desired symmetry, the Wigner function H must have appropriate symmetry under the Moyal bracket with the generator of that symmetry. If you look solely for a function symmetric under the Poisson bracket with the generator, your theory will not in general actually have the right symmetry (people may call this an anomaly, but it isn’t very anomalous to get the wrong answer by doing wrong math). The reason this error is sometimes safe is that sometimes all of our symmetry transformations of interest act linearly on our coordinates and momenta. If Q and P transform linearly then the generator of that transformation is necessarily a quadratic polynomial in Q and P and as we showed when proving Groenewold’s theorem, there is a unique faithful quantization scheme of polynomials of quadratic degree or less and it is equivalent to identifying Wigner functions with classical generators. In essence, if at least one of the two functions in a bracket is a quadratic polynomial in Q and P , then the Moyal and Poisson brackets of those functions agree. So, if *all* of our symmetry generators of interest other than the Hamiltonian are classically (at most) quadratic polynomials of Q and P and we develop a classical Hamiltonian with all of those symmetries, then using that Hamiltonian as the Wigner H of a quantum theory will give a quantum theory with the correct symmetries.

Those who commit the second error have almost always committed the first. So, suppose for now you have already mistakenly replaced H with the classical Hamiltonian $\mathcal{H}$. In that case, the functional S in (9.5.27) becomes the classical Hamiltonian action. The second oft repeated error with the path integral is to claim that the momentum integrals can generally be completed so that afterward the integrand of the Q integrals is of the form $e^{\frac{i}{\hbar} S_{\mathcal{L}}}$ where $S_{\mathcal{L}}$ is now the Lagrangian action of the classical theory. Let me explain where this incorrect claim comes from. Suppose that H happens to depend on P only as a quadratic polynomial and that the coefficients of the term quadratic in P do not depend on Q . Such a simple H takes the form:

$$H(t, Q, P) = \frac{1}{2} W^{ab}(t) P_a P_b + \Gamma^a(t, Q) P_a + V(t, Q) \quad (9.5.29)$$

for some functions W^{ab} , Γ^a , V . For shorthand, define:

$$\bar{Q}_n = \frac{Q_n + Q_{n+1}}{2}, \quad \dot{Q}_n = \frac{Q_{n+1} - Q_n}{t_{n+1} - t_n}, \quad \delta t_n = t_{n+1} - t_n. \quad (9.5.30)$$

Now using our simple form of H and returning to (9.5.22), we can explicitly complete the P integrals using the results of the multivariable Gaussian integral. In particular, if $\vec{x}$ is a vector in $\mathbb{R}^n$ and $A_{ab} = A_{ba}$, B_a , and C are some real coefficients independent of x and the matrix A_{ab} is positive definite, then:

$$\int_{\mathbb{R}^n} e^{-\frac{i}{2} A_{ab} x^a x^b + i B_a x^a + i C} d^n \vec{x} = \frac{(2\pi)^{\frac{n}{2}}}{i^{\frac{n}{2}} \sqrt{\det A}} e^{\frac{i}{2} A^{-ab} B_a B_b + i C} \quad (9.5.31)$$

where A^{-ab} is the inverse matrix of A_{ab} (this result is proven in the homework). With these, in this special case we can simplify (9.5.22) to:

$$U(t_f, Q_f, t_0, Q_0) = \lim_{N \rightarrow \infty} \int e^{\frac{i}{\hbar} \sum_{n=0}^{N-1} \delta S_{\mathcal{L}_n}} \prod_{n=0}^{N-1} \left(\frac{1}{(2\pi i \hbar \delta t_n)^{\frac{d}{2}} \sqrt{\det W(t_n)}} \right) d^d Q_1 \dots d^d Q_{N-1} \quad (9.5.32)$$

where we have defined:

$$\delta S_{\mathcal{L}_n} = \frac{1}{2} W_{ab}^{-1}(t_n) (\dot{Q}_n^a - \Gamma_n^a(t_n, \bar{Q}_n)) (\dot{Q}_n^b - \Gamma_n^b(t_n, \bar{Q}_n)) \delta t_n - V(t_n, \bar{Q}_n) \delta t_n. \quad (9.5.33)$$

Notice that if H happens to be the classical Hamiltonian $\mathcal{H}$ and it takes the form (9.5.29) then by the Legendre transformation, the classical Lagrangian is:

$$\mathcal{L} = \frac{1}{2} W_{ab}^{-1} (\dot{Q}^a - \Gamma^a) (\dot{Q}^b - \Gamma^b) - V \quad (9.5.34)$$

and so in this very special case:

$$\lim_{N \rightarrow \infty} \sum_{n=0}^{N-1} \delta S_{\mathcal{L}_n} = S_{\mathcal{L}} \quad (9.5.35)$$

where $S_{\mathcal{L}}$ is the classical Lagrangian action. As well, factors in the extra product appearing in (9.5.32) are all independent of Q . Because of this, in our super special case we can rewrite $U(t_f, Q_f, t_0, Q_0)$ as:

$$U(t_f, Q_f, t_0, Q_0) = \mathcal{N}(t_f, f_0) \int_{Q(t_0)=Q_0}^{Q(t_f)=Q_f} e^{\frac{i}{\hbar} S_{\mathcal{L}}} \mathcal{D}Q \quad (9.5.36)$$

where $\mathcal{N}$ is some complex function independent of Q and we have made the replacement:

$$d^d Q_1 \dots d^d Q_{N-1} \rightarrow \mathcal{D}Q. \quad (9.5.37)$$

Because of the unitarity of $\hat{U}$ and the fact that $\mathcal{N}$ does not depend on Q , it is possible to cancel $\mathcal{N}$ from any computations of operator summaries:

$$\langle \hat{G} \rangle(t) = \text{Tr}(\hat{\rho}(t) \hat{G}) = \frac{\text{Tr}(\hat{U}(t, 0) \hat{\rho}_0 \hat{U}^\dagger(t, 0) \hat{G})}{\text{Tr}(\hat{U}(t, 0) \hat{\rho}_0 \hat{U}^\dagger(t, 0))} \quad (9.5.38)$$

$$= \frac{\int \langle Q_0 | \hat{\rho}_0 | Q'_0 \rangle \langle Q'_0 | \hat{U}^\dagger | Q'_f \rangle \langle Q'_f | \hat{G} | Q_f \rangle \langle Q_f | \hat{U} | Q_0 \rangle d^d Q_0 d^d Q'_0 d^d Q_f d^d Q'_f}{\int \langle Q_0 | \hat{\rho}_0 | Q'_0 \rangle \langle Q'_0 | \hat{U}^\dagger | Q'_f \rangle \langle Q_f | \hat{U} | Q_0 \rangle d^d Q_0 d^d Q'_0 d^d Q_f} \quad (9.5.39)$$

$$= \frac{\int \langle Q_0 | \hat{\rho}_0 | Q'_0 \rangle \int_{Q(0)=Q'_0}^{Q(t)=Q'_f} e^{-\frac{i}{\hbar} S_{\mathcal{L}}} \mathcal{D}Q \langle Q'_f | \hat{G} | Q_f \rangle \int_{Q(0)=Q_0}^{Q(t)=Q_f} e^{\frac{i}{\hbar} S_{\mathcal{L}}} \mathcal{D}Q d^d Q_0 d^d Q'_0 d^d Q_f d^d Q'_f}{\int \langle Q_0 | \hat{\rho}_0 | Q'_0 \rangle \int_{Q(0)=Q'_0}^{Q(t)=Q_f} e^{-\frac{i}{\hbar} S_{\mathcal{L}}} \mathcal{D}Q \int_{Q(0)=Q_0}^{Q(t)=Q_f} e^{\frac{i}{\hbar} S_{\mathcal{L}}} \mathcal{D}Q d^d Q_0 d^d Q'_0 d^d Q_f} \quad (9.5.40)$$

Equation (9.5.36) is a very useful special case of the path integral, because half of the integrals have

already been performed, but very importantly if H is not of the form of (9.5.29) then it is just a wrong formula. Regardless of the form taken by H , one can in principle complete the P integrals in (9.5.22) and leave behind something that now is purely a function of all of the time steps and Q_n . In the $N \rightarrow \infty$ limit this leaves a function of t_0, t_f, Q_0, Q_f and a functional of the path connecting Q_0 and Q_f . Thus, formally for some such functional S' and some arbitrary function $\mathcal{N}'(t_f, t_0)$:

$$\mathcal{N}'(t_f, t_0) e^{\frac{i}{\hbar} S'[Q]} = \lim_{N \rightarrow \infty} \int e^{\frac{i}{\hbar} \sum_{n=0}^{N-1} \delta S_n} \frac{d^d P_0}{(2\pi\hbar)^d} \frac{d^d P_1}{(2\pi\hbar)^d} \cdots \frac{d^d P_{N-1}}{(2\pi\hbar)^d}. \quad (9.5.41)$$

From this it automatically follows that:

$$U(t_f, Q_f, t_0, Q_0) = \mathcal{N}'(t_f, t_0) \int_{Q(t_0)=Q_0}^{Q(t_f)=Q_f} e^{\frac{i}{\hbar} S'[Q]} \mathcal{D}Q. \quad (9.5.42)$$

This of course bears a striking resemblance to (9.5.36). However, there is absolutely no reason to believe that $S'[Q]$ has any relationship whatsoever to the classical Lagrangian action in general. In fact, in general you cannot even guarantee that it is possible to select $\mathcal{N}'$ so that the functional $S'[Q]$ is real-valued (which of course $S_{\mathcal{L}}[Q]$ always is) nor do you have any reasonable expectation of $S'[Q]$ generically manifesting the symmetries of your theory in an obvious way.

9.5.3 The Path Integral for Vacuum Expectation Values

The path integral is especially useful for computing so-called “vacuum expectation values” or vevs for short. Many quantities of interest in quantum mechanics, in particular scattering amplitudes, can be computed from vevs. We will see precisely how over the coming chapters. A vev specifically is an operator summary, typically of operators in the active picture, taken in the ground state (lowest energy state) of the quantum system. Let us now establish how vevs are related to the path integral. Let $\hat{Q}_A^a(t)$ represent our coordinate operators in the active picture. As always, the $\hat{Q}_A^a(t)$ are related to our usual coordinate operators by:

$$\hat{Q}_A^a(t) = \hat{U}^\dagger(t, t_0) \hat{Q}^a \hat{U}(t, t_0) \quad (9.5.43)$$

where t_0 is the time at which we choose to define the passive picture coordinate operators $\hat{Q}^a$. At each t , we can define normalized eigenstates $|Q(t)\rangle$ of the $\hat{Q}_A^a(t)$ operators:

$$\hat{Q}_A^a(t) |Q(t)\rangle = Q^a |Q(t)\rangle \quad (9.5.44)$$

$$\implies \hat{Q}^a (\hat{U}(t, t_0) |Q(t)\rangle) = Q^a (\hat{U}(t, t_0) |Q(t)\rangle) \quad (9.5.45)$$

$$\implies |Q(t_0)\rangle = \hat{U}(t, t_0) |Q(t)\rangle. \quad (9.5.46)$$

Immediately it follows that:

$$\langle Q(t) | Q_0(t_0) \rangle = U(t, Q, t_0, Q_0) \quad (9.5.47)$$

and so these time-dependent eigenstates are closely related to the path integral.

Now suppose we have some list of operators in the active picture $\hat{O}_n(t_n), \dots, \hat{O}_1(t_1)$ where $t_n > t_{n-1} > \dots > t_2 > t_1$. We can use the path integral to compute the matrix elements of the time ordered product of these operators. Let $T > t_n$ and $T_0 = t_0 < t_1$. Then:

$$\begin{aligned} \langle Q(T) | \hat{O}_n(t_n) \dots \hat{O}_1(t_1) | Q_0(T_0) \rangle \\ = \langle Q(t_0) | \hat{U}(T, t_0) \hat{U}^\dagger(t_n, t_0) \hat{O}_n(t_n) \hat{U}(t_n, t_0) \dots \hat{U}^\dagger(t_1, t_0) \hat{O}_1(t_1) \hat{U}(t_1, t_0) \hat{U}^\dagger(T_0, t_0) | Q_0(t_0) \rangle \end{aligned} \quad (9.5.48)$$

$$= \langle Q | \hat{U}(T, t_n) \hat{O}_n \hat{U}(t_n, t_{n-1}) \dots \hat{O}_2 \hat{U}(t_2, t_1) \hat{O}_1 \hat{U}(t_1, t_0) | Q_0 \rangle \quad (9.5.49)$$

where in the last line we stop writing that the operators or eigenstates are evaluated at t_0 because we can simply view them as in the passive picture at that time. We can now insert the Wigner representation of each operator in this product to achieve:

$$\begin{aligned} \langle Q_f(T) | \hat{O}_n(t_n) \dots \hat{O}_1(t_1) | Q_0(T_0) \rangle \\ = \int U(T, Q_f, t_n, Q'_n) \prod_{k=1}^n \left(e^{\frac{i}{\hbar} P_{ka} (Q_k'^a - Q_k^a)} \mathcal{O}_k \left(\frac{Q_k + Q_k'}{2}, P_k \right) U(t_k, Q_k, t_{k-1}, Q_{k-1}) \right) \end{aligned}$$

$$\cdot d^d Q'_1 \frac{d^d Q_1 d^d P_1}{(2\pi\hbar)^d} \dots d^d Q'_n \frac{d^d Q_n d^d P_n}{(2\pi\hbar)^d}. \quad (9.5.50)$$

Each factor of U in this expression will give a path integral between the different times of operator evaluation. We then see that between these path integrals the operator's Wigner function is evaluated at the averaged coordinate and that the momentum and coordinate different are integrated over. Therefore, we see that ultimately this is also of the form of an integration over all paths between Q_0 at T_0 and Q_f at T in which the operators to be evaluated are inserted as Wigner functions at the correct time step. The exponential factor with the momentum is simply the correct contribution to the Wigner action functional appropriate for change between Q_k and Q'_k without a change in time. Thus, this formula when fully expressed in terms of the path integral simply becomes:

$$\langle Q_f(T) | \mathcal{T} : \hat{O}_n(t_n) \dots \hat{O}_1(t_1) | Q_0(T_0) \rangle = \int_{Q(T_0)=Q_0}^{Q(T)=Q_f} e^{\frac{i}{\hbar} S[Q,P]} \mathcal{O}_n(Q(t_n), P(t_n)) \dots \mathcal{O}_1(Q(t_1), P(t_1)) \mathcal{D}Q \mathcal{D}P \quad (9.5.51)$$

where we have manually written in the time ordering for clarity of when this formula is valid.

Equation (9.5.51) is not obviously a vev, but we will now see that it is very closely related to one. Suppose we have a quantum system with a time independent Hamiltonian operator $\hat{H}$ and let $|n\rangle$ be an orthonormal basis of eigenstates of $\hat{H}$ and $\psi_n(Q) = \langle Q | n \rangle$ be the corresponding eigenstate wavefunctions. Let $|\Omega\rangle$ be used to denote the ground state (lowest energy state) among these and let its energy eigenvalue be E_Ω . Assume our system is such that this ground state is unique. Let $\hat{O} = \hat{O}_n(t_n) \dots \hat{O}_1(t_1)$ be a shorthand for our operator from before. Let T, t, T_0, t_0 be times such that $T > t > t_n, t_1 > t_0 > T_0$. Then, time evolution from T_0 to T can be broken into three sections. In the first, from T_0 to t_0 , we simply exponentiate the Hamiltonian operator. In particular, we have:

$$\langle Q(T) | Q'(t) \rangle = \langle Q(t_0) | \hat{U}(T, t_0) \hat{U}^\dagger(t, t_0) | Q'(t_0) \rangle = \langle Q(t_0) | e^{-\frac{i}{\hbar} \hat{H}(T-t)} | Q'(t_0) \rangle = \sum_n e^{-\frac{i}{\hbar} E_n(T-t)} \psi_n(Q) \psi_n^*(Q'). \quad (9.5.52)$$

In the second, from t_0 to t , we will not explicitly evaluate the time evolution. Finally, from t to T we again exponentiate. Thus:

$$\begin{aligned} \langle Q(T) | \hat{O} | Q_0(T_0) \rangle &= \int \langle Q(T) | Q'(t) \rangle \langle Q'(t) | \hat{O} | Q'_0(t_0) \rangle \langle Q'_0(t_0) | Q_0(T_0) \rangle d^d Q'_0 d^d Q' \\ &= \int \sum_{nn'} e^{-\frac{i}{\hbar} E_n(T-t) - \frac{i}{\hbar} E_{n'}(t_0-T_0)} \psi_n(Q) \psi_n^*(Q') \psi_{n'}(Q'_0) \psi_{n'}^*(Q_0) \langle Q'(t) | \hat{O} | Q'_0(t_0) \rangle d^d Q'_0 d^d Q'. \end{aligned} \quad (9.5.53)$$

We are now going to do a subtle trick which is possible specifically because the Hamiltonian is bounded below (so that it is capable of thermodynamic equilibrium, which is required by the experimental success of thermodynamics). This trick is called a **Wick rotation**. The Schrödinger equation, or equivalently the von Neumann equation, gives time evolution in a way which formally depends analytically on time, even if the time parameter is viewed as a complex number. So, for times between t and T and between t_0 and T_0 we can "tilt the time axis" in the complex plane so that our ultimate initial time is $T_0 e^{-i\delta}$ and our final time is $T e^{-i\delta}$ with δ a small positive real number. By *can* do this, I mean that the path integral formula (9.5.51) will still hold with these replacements because the realness of t was never used in the calculation. That is, we have:

$$\langle Q_f(T e^{-i\delta}) | \mathcal{T} : \hat{O}_n(t_n) \dots \hat{O}_1(t_1) | Q_0(T_0 e^{-i\delta}) \rangle = \int_{Q(T_0 e^{-i\delta})=Q_0}^{Q(T e^{-i\delta})=Q_f} e^{\frac{i}{\hbar} S[Q,P]} \mathcal{O}_n \dots \mathcal{O}_1 \mathcal{D}Q \mathcal{D}P. \quad (9.5.55)$$

Applying this principle to (9.5.54) we have:

$$\begin{aligned} &\frac{\langle Q(T e^{-i\delta}) | \hat{O} | Q_0(T_0 e^{-i\delta}) \rangle}{\langle Q(T e^{-i\delta}) | Q_0(T_0 e^{-i\delta}) \rangle} \\ &= \frac{\int \sum_{nn'} e^{-\frac{i}{\hbar} E_n(T e^{-i\delta}-t) - \frac{i}{\hbar} E_{n'}(t_0-T_0 e^{-i\delta})} \psi_n(Q) \psi_n^*(Q') \psi_{n'}(Q'_0) \psi_{n'}^*(Q_0) \langle Q'(t) | \hat{O} | Q'_0(t_0) \rangle d^d Q'_0 d^d Q'}{\sum_n e^{-\frac{i}{\hbar} E_n(T-T_0) e^{-i\delta}} \psi_n(Q) \psi_n^*(Q_0)}. \end{aligned} \quad (9.5.56)$$

From here we can take the limits $T \rightarrow \infty$ and $T_0 \rightarrow -\infty$ and because of δ , all but the ground state terms in our sum will exponentially decay. (The ground state terms also decay, but the decay rate cancels between

then numerator and denominator while all higher energy terms decay more quickly). Thus, taking the limit:

$$\lim_{\substack{T \rightarrow \infty \\ T_0 \rightarrow -\infty}} \frac{\langle Q(Te^{-i\delta}) | \hat{O} | Q_0(T_0e^{-i\delta}) \rangle}{\langle Q(Te^{-i\delta}) | Q_0(T_0e^{-i\delta}) \rangle} = \int e^{\frac{i}{\hbar} E_{\Omega}(t-t_0)} \psi_{\Omega}^*(Q') \psi_{\Omega}(Q'_0) \langle Q'(t) | \hat{O} | Q'_0(t_0) \rangle d^d Q'_0 d^d Q' \quad (9.5.57)$$

$$= \int e^{\frac{i}{\hbar} E_{\Omega}(t-t_0)} \langle \Omega | Q' \rangle \langle Q' | \hat{U}(t, t_0) \hat{O} | Q'_0 \rangle \langle Q'_0 | \Omega \rangle d^d Q'_0 d^d Q' \quad (9.5.58)$$

$$= \langle \Omega | \hat{O} | \Omega \rangle \quad (9.5.59)$$

which is precisely a vev. Because vevs will be common, we introduce the shorthand for the time ordered vacuum expectation value:

$$\text{Vev}(\hat{O}_n(t_n) \dots \hat{O}_1(t_1)) = \langle \Omega | \mathcal{T} : \hat{O}_n(t_n) \dots \hat{O}_1(t_1) | \Omega \rangle. \quad (9.5.60)$$

Because of the time ordering used in the definition of the **Vev**, the operators within it commute if evaluated at different times.

By combining (9.5.55) and (9.5.59) we have:

$$\text{Vev}(\hat{O}_n(t_n) \dots \hat{O}_1(t_1)) = \lim_{\delta \rightarrow 0^+} \lim_{\substack{T \rightarrow \infty \\ T_0 \rightarrow -\infty}} \frac{\int_{Q(T_0e^{-i\delta})=Q_0}^{Q(Te^{-i\delta})=Q_f} e^{\frac{i}{\hbar} S[Q,P]} \mathcal{O}_n \dots \mathcal{O}_1 \mathcal{D}Q \mathcal{D}P}{\int_{Q(T_0e^{-i\delta})=Q_0}^{Q(Te^{-i\delta})=Q_f} e^{\frac{i}{\hbar} S[Q,P]} \mathcal{D}Q \mathcal{D}P} \quad (9.5.61)$$

This equation is very interesting because the left hand side does not depend on Q_f or Q_0 while the right hand side does. Thus, the boundary conditions Q_f and Q_0 are arbitrary, provided they are consistent between the numerator and denominator. Almost all practical calculations involving the path integral are done as perturbations around a quantum harmonic oscillator, and the standard boundary conditions to take in such a case are to set the initial and final coordinates to the equilibrium position of the oscillator. Just as with the Fourier transform, the δ damping is typically not written explicitly unless it is of specific computational importance for a particular equation. That said, you should not forget that it is there when it is time to be careful. In fact, the δ damping can be interpreted directly in terms of the Fourier transform. Consider the use of a new time coordinate t' for times outside of the interval (t, t_0) which is related to our previous time coordinate by $t' = e^{i\delta}t$. Now the initial and final values of t' are T_0 and T respectively, which are purely real. A function of frequency ω when written in terms of t , meaning containing a component $e^{-i\omega t}$, then becomes a function of frequency $\omega' = e^{-i\delta}\omega$ so that $e^{-i\omega t} = e^{-i\omega' t'}$. Thus the Wick rotation can also be viewed as adding a small negative imaginary component to the frequency, precisely how the usual Fourier damping works. Understanding these finer points of the meaning of equation (9.5.61), we write more easily and less clearly:

$$\text{Vev}(\hat{O}_n(t_n) \dots \hat{O}_1(t_1)) = \frac{\int e^{\frac{i}{\hbar} S[Q,P]} \mathcal{O}_n(Q(t_n), P(t_n)) \dots \mathcal{O}_1(Q(t_1), P(t_1)) \mathcal{D}Q \mathcal{D}P}{\int e^{\frac{i}{\hbar} S[Q,P]} \mathcal{D}Q \mathcal{D}P}. \quad (9.5.62)$$

Because the path integral integrates over the entire path through phase space, we can nicely reexpress this result in terms of our usual $\Phi(t) = (Q(t), P(t))$ condensed phase space coordinates as:

$$\text{Vev}(\hat{O}_n(t_n) \dots \hat{O}_1(t_1)) = \frac{\int e^{\frac{i}{\hbar} S[\Phi]} \mathcal{O}_n(\Phi(t_n)) \dots \mathcal{O}_1(\Phi(t_1)) \mathcal{D}\mathbb{P}}{\int e^{\frac{i}{\hbar} S[\Phi]} \mathcal{D}\mathbb{P}}. \quad (9.5.63)$$

As usual, generators of interest are typically analytic functions of our phase space variables. If all of the $\hat{O}_k$ above are such, we can replace them by their series representations in terms of the Φ^a and thus develop a series representation of the above vev in terms of vevs of products of the Φ^a evaluated at various times. Such vevs are called the **Green's functions** of the quantum theory. So, the typical vevs of most interest are:

$$G_n^{a_1 \dots a_n}(t_1, \dots, t_n) = \text{Vev}(\hat{\Phi}^{a_1}(t_1) \dots \hat{\Phi}^{a_n}(t_n)). \quad (9.5.64)$$

(The Green's function with n copies of $\Phi^a(t)$ is typically called the n -point Green's function or n -point correlator.) All of these Green's functions can be recovered from a single functional which is called the generating functional of the quantum theory. Let $J_a(t)$ be a smooth function of compact support which transforms inversely to the $\Phi^a(t)$ under a canonical transformation. Then, define the functional:

$$\mathcal{Z}[J] = \langle \Omega | \mathcal{T} : e^{\frac{i}{\hbar} \int_{-\infty}^{\infty} J_a(t) \hat{\Phi}^a(t) dt} | \Omega \rangle. \quad (9.5.65)$$

Series expanding in powers of $J_a(t)$, we find:

$$\mathcal{Z}[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar} \right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} J_{a_1}(t_1) \dots J_{a_n}(t_n) \langle \Omega | \mathcal{T} : \hat{\Phi}^{a_1}(t_1) \dots \hat{\Phi}^{a_n}(t_n) | \Omega \rangle dt_1 \dots dt_n. \quad (9.5.66)$$

Thus:

$$G_n^{a_1 \dots a_n}(t_1, \dots, t_n) = \left(\frac{\hbar}{i} \right)^n \frac{\delta^n \mathcal{Z}[J]}{\delta J_{a_1}(t_1) \dots \delta J_{a_n}(t_n)} \Big|_{J=0}. \quad (9.5.67)$$

As well, by using (9.5.63) in the definition of $\mathcal{Z}[J]$, we have:

$$\mathcal{Z}[J] = \frac{\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\hbar} \right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} J_{a_1}(t_1) \dots J_{a_n}(t_n) \int e^{\frac{i}{\hbar} S[\Phi]} \Phi^{a_1}(t_1) \dots \Phi^{a_n}(t_n) \mathcal{D}\mathbb{P} dt_1 \dots dt_n}{\int e^{\frac{i}{\hbar} S[\Phi]} \mathcal{D}\mathbb{P}} \quad (9.5.68)$$

$$\Rightarrow \mathcal{Z}[J] = \frac{\int e^{\frac{i}{\hbar} (S[\Phi] + \int_{-\infty}^{\infty} J_a(t) \Phi^a(t) dt)} \mathcal{D}\mathbb{P}}{\int e^{\frac{i}{\hbar} S[\Phi]} \mathcal{D}\mathbb{P}}. \quad (9.5.69)$$

The denominator is simply the numerator evaluated at $J_a(t) = 0$. Thus, by completing the single path integral for general $J_a(t)$ in the numerator we can determine $\mathcal{Z}[J]$. From $\mathcal{Z}[J]$ we can determine all of the Green's functions of the theory by using (9.5.67). From those Green's functions we can calculate (9.5.63) for any $\hat{\mathcal{O}}_k$ which have Wigner functions that are analytic in the coordinates and momenta. The vevs in (9.5.63) can be used to determine almost all quantities of interest in many quantum mechanical models. Thus, the ultimate utility of the path integral is in setting up $\mathcal{Z}[J]$ as the central quantity of interest for further calculation.

The quantum generating functional isn't really computed by literally evaluating the path integral. Instead, in practical terms it is computed by perturbing a few known path integral results (Gaussian – the quantum harmonic oscillator and other very simple systems) systematically. Suppose that the Wigner action functional can be split into a solvable part S_0 and a perturbation S_1 which may reasonably be considered small (solvable here means that if that were the only contribution to the Wigner action functional then the resulting path integral would be doable explicitly):

$$S[\Phi] = S_0[\Phi] + S_1[\Phi]. \quad (9.5.70)$$

Let $\mathcal{Z}_0[J]$ be the generating functional computed when using $S_0[\Phi]$. Then, recklessly commuting limits:

$$\int e^{\frac{i}{\hbar} (S[\Phi] + \int_{-\infty}^{\infty} J_a(t) \Phi^a(t) dt)} \mathcal{D}\mathbb{P} = \int e^{\frac{i}{\hbar} S_1[\frac{\hbar}{i} \frac{\delta}{\delta J}]} e^{\frac{i}{\hbar} (S_0[\Phi] + \int_{-\infty}^{\infty} J_a(t) \Phi^a(t) dt)} \mathcal{D}\mathbb{P} \quad (9.5.71)$$

$$\Rightarrow \mathcal{Z}[J] = \mathcal{N} e^{\frac{i}{\hbar} S_1[\frac{\hbar}{i} \frac{\delta}{\delta J}]} \mathcal{Z}_0[J] \quad (9.5.72)$$

where by evaluating the functional S_1 at $\frac{\hbar}{i} \frac{\delta}{\delta J}$ we mean that we express S_1 formally as a series and replace its argument with this functional derivative at each order and $\mathcal{N}$ is a normalization factor necessary because by definition $\mathcal{Z}[0] = 1$. Many limits were commuted in this calculation and the effect of this is that (9.5.72) is not typically exactly true. Instead, the right hand side of (9.5.72) can be expanded in powers of S_1 to give a reasonable perturbation series and that will be the correct perturbative expansion of the left hand side. The issue is that it is unlikely that the full series converges to the true exact $\mathcal{Z}[J]$, that is, there is no reason to believe $\mathcal{Z}[J]$ depends analytically on whatever series expansion parameter is used when considering S_1 as small. Perturbation theory is almost always this way and the resulting series are called **asymptotic series**. Asymptotic series are extremely useful for getting excellent approximations to true answers, even if the series does not converge to the true answer (and possibly doesn't converge at all) because in any practical calculation we will only compute to finite order of perturbation theory (and typically only a very low order).

The generating functional satisfies a sort of “equation of motion” called the **Schwinger-Dyson equation**. Consider:

$$\int e^{\frac{i}{\hbar} (S[\Phi] + \int_{-\infty}^{\infty} J_b \Phi^b dt')} \frac{\delta S}{\delta \Phi^a(t)} [\Phi] \mathcal{D}\mathbb{P} = \frac{\hbar}{i} \int e^{\frac{i}{\hbar} \int_{-\infty}^{\infty} J_b \Phi^b dt'} \frac{\delta}{\delta \Phi^a(t)} e^{\frac{i}{\hbar} S[\Phi]} \mathcal{D}\mathbb{P}. \quad (9.5.73)$$

We now perform functional integration by parts. The boundary terms of the integration are necessarily negligible for the path integral to converge. This situation is helped by the δ damping from before. For large Φ , S is typically also large. Then, because t has been slightly rotated it develops a small imaginary part so that the argument of the exponential develops a negative real part and so decays for large Φ . Thus we have:

$$\int e^{\frac{i}{\hbar} (S[\Phi] + \int_{-\infty}^{\infty} J_b \Phi^b dt')} \frac{\delta S}{\delta \Phi^a(t)} [\Phi] \mathcal{D}\mathbb{P} = -\frac{\hbar}{i} \int e^{\frac{i}{\hbar} S[\Phi]} \frac{\delta}{\delta \Phi^a(t)} e^{\frac{i}{\hbar} \int_{-\infty}^{\infty} J_b \Phi^b dt'} \mathcal{D}\mathbb{P} \quad (9.5.74)$$

$$= -J_a(t) \int e^{\frac{i}{\hbar}(S[\Phi] + \int_{-\infty}^{\infty} J_b \Phi^b dt')} \mathcal{D}\mathbb{P}. \quad (9.5.75)$$

Alternatively:

$$\frac{\delta S}{\delta \Phi^a} \left[\frac{\hbar}{i} \frac{\delta}{\delta J} \right] \int e^{\frac{i}{\hbar}(S[\Phi] + \int_{-\infty}^{\infty} J_b \Phi^b dt')} \mathcal{D}\mathbb{P} = \int e^{\frac{i}{\hbar}(S[\Phi] + \int_{-\infty}^{\infty} J_b \Phi^b dt')} \frac{\delta S}{\delta \Phi^a(t)} [\Phi] \mathcal{D}\mathbb{P}. \quad (9.5.76)$$

With these together then, we have the Schwinger-Dyson equation:

$$\boxed{\frac{\delta S}{\delta \Phi^a(t)} \left[\frac{\hbar}{i} \frac{\delta}{\delta J} \right] \mathcal{Z}[J] = -J_a \mathcal{Z}[J].} \quad (9.5.77)$$

This functional differential equation can be solved order by order in J_a and order by order in perturbation theory to determine the quantum generating functional. Doing so explicitly we will save for later chapters.

9.5.4 The Path Integral for the Quantum Harmonic Oscillator

One of the only path integrals that can be computed exactly is the quantum harmonic oscillator. Consequently, perturbation theory for the path integral is essentially only useful when perturbing near the qho limit. Suppose we have a system of interacting quantum harmonic oscillators. The resulting Wigner Hamiltonian function is then a quadratic polynomial in the coordinates and momenta. The Wigner action functional then is automatically a quadratic functional of the coordinates and momenta (as the only additional contribution beyond the integral of the Wigner Hamiltonian is the integral of $P_a \dot{Q}^a$ which is also quadratic). By a quadratic functional, I mean that the third functional derivative vanishes everywhere:

$$\frac{\delta^3 S}{\delta \Phi^a(t) \delta \Phi^b(t') \delta \Phi^c(t'')} = 0. \quad (9.5.78)$$

We will see that the entire path integral for the qho is determined by its 2-point Green's function, which is given a special name as the **Feynman propagator** and written as $D^{ab}(t, t')$:

$$\boxed{D^{ab}(t, t') = G_2^{ab}(t, t') = \langle \Omega | \mathcal{T} : \hat{\Phi}^a(t) \hat{\Phi}^b(t') | \Omega \rangle.} \quad (9.5.79)$$

The reason for designating the Feynman propagator with a special symbol is that when doing perturbative calculations the Feynman propagator of the unperturbed theory will appear all over the place.

Define $S_J[\Phi]$ as the functional:

$$S_J[\Phi] = S[\Phi] + \int_{-\infty}^{\infty} J_a(t) \Phi^a(t) dt. \quad (9.5.80)$$

Automatically it follows that: S_J is also a quadratic functional:

$$\frac{\delta^3 S_J}{\delta \Phi^a(t) \delta \Phi^b(t') \delta \Phi^c(t'')} = 0. \quad (9.5.81)$$

When S_J is viewed as an action, there will be some classical solution $\phi_J(t)$ achieved by taking the stationary variation of S_J with initial and final conditions $\phi_J = 0$ at the times T_0 and T (which we eventually will take to $-\infty, +\infty$) and solving the Euler-Lagrange equations of motion:

$$\frac{\delta S_J}{\delta \Phi^a}[\phi_J] = 0. \quad (9.5.82)$$

We can write any trajectory $\Phi^a(t)$ as a deviation from that solution as:

$$\Phi^a(t) = \phi_J^a(t) + \delta \Phi^a(t). \quad (9.5.83)$$

Decomposed this way, we view $\phi_J^a(t)$ as a shift of our integration variables and $\delta \Phi^a(t)$ as our new integration variables. Because $S_J[\Phi]$ is a quadratic functional, its functional Taylor series terminates after only 3 terms:

$$S_J[\Phi] = S_J[\phi_J + \delta \Phi] = S_J[\phi_J] + \int_{-\infty}^{\infty} \delta \Phi^a(t) \frac{\delta S_J}{\delta \Phi^a(t)}[\phi_J] dt + \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta \Phi^a(t) \delta \Phi^b(t') \frac{\delta^2 S_J}{\delta \Phi^a(t) \delta \Phi^b(t')}[\phi_J] dt' dt. \quad (9.5.84)$$

The second term on the right hand side vanishes identically by (9.5.82). As well, the second functional derivative in the third term is automatically independent of both J . This is because it is independent of being evaluated at ϕ_J as by taking another functional derivative we achieve 0 by (9.5.81) and the only other J dependent piece in S_J is linear in Φ (as introduced in (9.5.80)) which doesn't contribute to the second

functional derivative. Therefore, for some $M_{ab}(t, t')$:

$$M_{ab}(t, t') = \frac{\delta^2 S_J}{\delta \Phi^a(t) \delta \Phi^b(t')} [\phi_J] = \frac{\delta^2 S}{\delta \Phi^a(t) \delta \Phi^b(t')} [\Phi]. \quad (9.5.85)$$

With these simplifications we have:

$$S_J[\Phi] = S_J[\phi_J] + \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta \Phi^a \delta \Phi^b M_{ab}(t, t') dt' dt. \quad (9.5.86)$$

With this, we can now evaluate the path integral very simply, letting ϕ_0 mean ϕ_J with $J = 0$:

$$\mathcal{Z}[J] = \frac{\int e^{\frac{i}{\hbar} S_J[\Phi]} \mathcal{D}\Phi}{\int e^{\frac{i}{\hbar} S[\Phi]} \mathcal{D}\Phi} = \frac{e^{\frac{i}{\hbar} S_J[\phi_J]} \int e^{\frac{i}{2\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta \Phi^a \delta \Phi^b M_{ab}(t, t') dt' dt} \mathcal{D}\delta\Phi}{e^{\frac{i}{\hbar} S[\phi_0]} \int e^{\frac{i}{2\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta \Phi^a \delta \Phi^b M_{ab}(t, t') dt' dt} \mathcal{D}\delta\Phi} = e^{\frac{i}{\hbar} (S_J[\phi_J] - S[\phi_0])}. \quad (9.5.87)$$

The actual integrations completely cancel!

In order to fully simplify $\mathcal{Z}[J]$, we need to evaluate $S_J[\phi_J]$. Let us assume we have defined our harmonic oscillator variables so that the minimum of the Wigner Hamiltonian is at the origin of phase space and let us set its minimum value to 0. Then, automatically the linear in Φ pieces of $S[\Phi]$ are 0. From (9.5.85) then we have:

$$S[\Phi] = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} M_{ab}(t, t') \Phi^a(t) \Phi^b(t') dt dt'. \quad (9.5.88)$$

From this it follows that (9.5.82) becomes:

$$\int_{-\infty}^{\infty} M_{ab}(t, t') \phi_J^b(t') dt' = -J_a(t). \quad (9.5.89)$$

This is a linear equation, which in actual practice becomes a linear differential equation ($M_{ab}(t, t')$ will be a sum of Dirac deltas and derivatives of deltas of $t - t'$). The initial and final condition on ϕ_J are arbitrary (as long as they are the same for ϕ_0) and we take $\phi_J(T_0) = \phi_J(T) = 0$ for convenience. This differential equation with those boundary conditions will have some solution and due to linearity, it will be linear in $J_a(t)$. Therefore, for some function $\mathcal{G}^{ab}(t, t')$:

$$\phi_J^a(t) = \int_{-\infty}^{\infty} \mathcal{G}^{ab}(t, t') J_b(t') dt'. \quad (9.5.90)$$

We can view $M_{ab}(t, t')$ and $\mathcal{G}^{ab}(t, t')$ as operators on functions (which act by multiplication followed by integration over t') and in this view $\mathcal{G}^{ab}(t, t')$ is the operator inverse (up to a minus sign) of $M_{ab}(t, t')$ on the space of functions with the specified boundary conditions. Plainly, $\mathcal{G}^{ab}$ is the Green's function of the differential equation. Define the functional $W[J]$ by:

$$\mathcal{Z}[J] = e^{\frac{i}{\hbar} W[J]}. \quad (9.5.91)$$

For our qho it automatically follows that:

$$W[J] = S_J[\phi_J] - S[\phi_0] = S[\phi_J] - S[\phi_0] + \int_{-\infty}^{\infty} J_a(t) \phi_J^a(t) dt. \quad (9.5.92)$$

Because ϕ_J is linear in $J_a(t)$ and $S[\Phi]$ is quadratic in Φ , we immediately have that $W[J]$ is quadratic in $J_a(t)$. Therefore, its functional Taylor series truncates after only three terms:

$$W[J] = W[0] + \int_{-\infty}^{\infty} \frac{\delta W}{\delta J_a(t)} [0] J_a(t) dt + \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\delta^2 W}{\delta J_a(t) \delta J_b(t')} [0] J_a(t) J_b(t') dt dt'. \quad (9.5.93)$$

From the definition of $W[J]$ it is immediate that $W[0] = 0$. Differentiating the definition of $W[J]$ gives:

$$\frac{\delta W}{\delta J_a(t)} [J] = \phi_J^a(t) + \int_{-\infty}^{\infty} \frac{\delta \phi_J^b(t')}{\delta J_a(t)} \left(\frac{\delta S}{\delta \Phi^b(t')} [\phi_J] + J_b(t') \right) dt' = \phi_J^a(t) = \int_{-\infty}^{\infty} \mathcal{G}^{ab}(t, t') J_b(t') dt' \quad (9.5.94)$$

after using (9.5.82) and (9.5.90). Thus:

$$\frac{\delta W}{\delta J_a(t)} [0] = 0, \quad \frac{\delta^2 W}{\delta J_a(t) \delta J_b(t')} = \mathcal{G}^{ab}(t, t'). \quad (9.5.95)$$

Returning to (9.5.93) we have:

$$W[J] = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{G}^{ab}(t, t') J_a(t) J_b(t') dt dt'. \quad (9.5.96)$$

Using (9.5.67), (9.5.79), and (9.5.91) we see:

$$D^{ab}(t, t') = -i\hbar \mathcal{G}^{ab}(t, t'). \quad (9.5.97)$$

Therefore, for a system of interacting quantum harmonic oscillators, the entire path integral is given by:

$$\mathcal{Z}[J] = e^{-\frac{1}{2\hbar^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} D^{ab}(t, t') J_a(t) J_b(t') dt' dt} \quad (9.5.98)$$

where $D^{ab}(t, t')$ is just the Feynman propagator of the oscillators.

We will now explicitly compute the Feynman propagator for a system of harmonic oscillators. The general Wigner Hamiltonian function for a system of quantum harmonic oscillators takes the form of (1.15.7) without the need for higher order terms (and using that we have set the origin of the phase space as the minimum of the Wigner Hamiltonian). By the theorem of normal modes (Theorem 1.14) there exists a constant symplectic matrix $\hat{\Lambda}$ which relate our coordinates and momenta (Q, P) to new coordinates and momenta (q, p) by:

$$\Phi = \begin{pmatrix} Q \\ P \end{pmatrix} = \hat{\Lambda} \begin{pmatrix} q \\ p \end{pmatrix} = \hat{\Lambda} \phi \quad (9.5.99)$$

so that the Wigner Hamiltonian expressed in terms of these new coordinates takes the form:

$$H = \sum_n \frac{p_n^2 + \omega_n^2 q_n^2}{2}. \quad (9.5.100)$$

Let $d^{ab}(t, t')$ be the Feynman propagator for the normal mode coordinates (q, p) :

$$d^{ab}(t, t') = \langle \Omega | \mathcal{T} : \hat{\phi}^a(t) \hat{\phi}^b(t') | \Omega \rangle. \quad (9.5.101)$$

Immediately then:

$$D^{ab}(t, t') = \Lambda^a{}_c \Lambda^b{}_d d^{cd}(t, t'). \quad (9.5.102)$$

Because each of the oscillators (q, p) are decoupled, $d^{ab}(t, t')$ simply decomposes into a list of Feynman propagators each for an individual oscillator. So, all we need to do is compute the Feynman propagator for a single oscillator.

For an individual oscillator of angular frequency ϖ the Feynman propagator can be computed easily using standard quantum mechanical techniques. The Hamiltonian operator is:

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{1}{2} \varpi^2 \hat{q}^2 = \hbar \varpi \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \mathbb{1} \right) \quad (9.5.103)$$

where we as always define the lowering operator as:

$$\hat{a} = \sqrt{\frac{\varpi}{2\hbar}} \hat{q} + \frac{i}{\sqrt{2\varpi\hbar}} \hat{p}. \quad (9.5.104)$$

Using the Schrödinger equation it quickly follows that the active picture lowering operator $\hat{a}(t)$ satisfies:

$$i\hbar \frac{d\hat{a}(t)}{dt} = [\hat{a}(t), \hat{H}] = \hbar \varpi \hat{a}(t) \implies \hat{a}(t) = e^{-i\varpi t} \hat{a}_0. \quad (9.5.105)$$

The coordinate and momenta operators become simply:

$$\hat{q}(t) = \sqrt{\frac{\hbar}{2\varpi}} (\hat{a}(t) + \hat{a}^\dagger(t)), \quad \hat{p}(t) = \frac{d\hat{q}(t)}{dt}. \quad (9.5.106)$$

The 2-point vevs of $\hat{a}(t)$ and $\hat{a}^\dagger(t)$ are:

$$\text{Vev}(\hat{a}(t)\hat{a}(t')) = \vartheta(t-t') e^{-i\varpi(t+t')} \langle 0 | \hat{a}_0^2 | 0 \rangle + \vartheta(t'-t) e^{-i\varpi(t+t')} \langle 0 | \hat{a}_0^2 | 0 \rangle = 0 \quad (9.5.107)$$

$$\text{Vev}(\hat{a}(t)\hat{a}^\dagger(t')) = \vartheta(t-t') e^{-i\varpi(t-t')} \langle 0 | \hat{a}_0 \hat{a}_0^\dagger | 0 \rangle + \vartheta(t'-t) e^{-i\varpi(t-t')} \langle 0 | \hat{a}_0^\dagger \hat{a}_0 | 0 \rangle = e^{-i\varpi(t-t')} \vartheta(t-t') \quad (9.5.108)$$

$$\text{Vev}(\hat{a}^\dagger(t)\hat{a}^\dagger(t')) = \vartheta(t-t') e^{i\varpi(t+t')} \langle 0 | \left(\hat{a}_0^\dagger \right)^2 | 0 \rangle + \vartheta(t'-t) e^{i\varpi(t+t')} \langle 0 | \left(\hat{a}_0^\dagger \right)^2 | 0 \rangle = 0. \quad (9.5.109)$$

Only the mixed $\hat{a}, \hat{a}^\dagger$ vev is nonzero. Due to time translational symmetry, it is only a function of $t - t'$ and so we can define the function $f(t)$:

$$f(t) = e^{-i\varpi t} \vartheta(t), \quad \text{Vev}(\hat{a}(t)\hat{a}^\dagger(t')) = f(t-t'). \quad (9.5.110)$$

When doing real calculations, the Fourier transform of $f(t)$ tends to be more useful. Remember the ε damping

always used in the definition of the Fourier transform as it is important here:

$$\int_{-\infty}^{\infty} e^{i\omega t} f(t) dt = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} e^{-\varepsilon|t| - i\omega t} \vartheta(t) dt = \lim_{\varepsilon \rightarrow 0^+} \frac{i}{\omega - \varpi + i\varepsilon} \quad (9.5.111)$$

$$\implies f(t) = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{i}{\omega - \varpi + i\varepsilon} e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (9.5.112)$$

We now compute the vevs of our coordinates and momenta in terms of this representation of $f(t)$:

$$\text{Vev}(\hat{q}(t)\hat{q}(t')) = \frac{\hbar}{2\varpi} \text{Vev}(\hat{a}(t)\hat{a}(t') + \hat{a}^\dagger(t)\hat{a}(t') + \hat{a}(t)\hat{a}^\dagger(t') + \hat{a}^\dagger(t)\hat{a}^\dagger(t')) \quad (9.5.113)$$

$$= \frac{\hbar}{2\varpi} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \left(\frac{i}{-\omega - \varpi + i\varepsilon} + \frac{i}{\omega - \varpi + i\varepsilon} \right) e^{-i\omega(t-t')} \frac{d\omega}{2\pi} \quad (9.5.114)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{i\hbar(1 - i\frac{\varepsilon}{\varpi})}{\omega^2 - \varpi^2 + 2i\varpi\varepsilon + \varepsilon^2} e^{-i\omega(t-t')} \frac{d\omega}{2\pi}. \quad (9.5.115)$$

The ε piece in the numerator makes a vanishing contribution to the integral in the $\varepsilon \rightarrow 0^+$ limit, as does the ε^2 piece in the denominator. The only ε dependent piece that makes a nonzero contribution to the result is the $+2i\varpi\varepsilon$ and so it is the only one necessary to keep (this can be checked by simply carrying out the integration). As well, because we only require $\varepsilon \rightarrow 0^+$ we can rescale the definition of ε to absorb the factor of 2ϖ . So:

$$\boxed{\text{Vev}(\hat{q}(t)\hat{q}(t')) = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{i\hbar}{\omega^2 - \varpi^2 + i\varepsilon} e^{-i\omega(t-t')} \frac{d\omega}{2\pi}.} \quad (9.5.116)$$

The appearance of $+i\varepsilon$ in the denominator here is often called the Feynman $i\varepsilon$ or Feynman prescription. The vevs of other combinations of momenta and coordinates are simply:

$$\text{Vev}(\hat{q}(t)\hat{p}(t')) = \frac{\partial}{\partial t'} \text{Vev}(\hat{q}(t)\hat{q}(t')), \quad \text{Vev}(\hat{p}(t)\hat{p}(t')) = \frac{\partial^2}{\partial t \partial t'} \text{Vev}(\hat{q}(t)\hat{q}(t')). \quad (9.5.117)$$

Now let k and l be indices which run over 1, 2 with 1 indicating a coordinate q and 2 indicating a momentum p and let n run over the different pairs of normal modes. So, we write $\Lambda^a_{n,k}$ to mean that a is a component of our original Q, P coordinates and n, k specifies a particular coordinate or momentum of our normal mode coordinates. With this notation, we have finally that the Feynman propagator of a general system of interacting quantum harmonic oscillators is given by (with implicit summation over k, l and explicit summation over n):

$$\boxed{D^{ab}(t, t') = \sum_n \Lambda^a_{n,k} \Lambda^b_{n,l} \left(\frac{1}{\partial} \quad \frac{\partial}{\partial t \partial t'} \right)^{kl} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{i\hbar}{\omega^2 - \omega_n^2 + i\varepsilon} e^{-i\omega(t-t')} \frac{d\omega}{2\pi}.} \quad (9.5.118)$$

In the path integral perspective, the $+i\varepsilon$ in the denominator appears the way it does because of the boundary conditions on the path integral (fixing the initial and final coordinates and applying the time Wick rotation). If you use different boundary conditions for computing which $\mathcal{G}^{ab}$ satisfies (9.5.90), you will find different appearances of $i\varepsilon$. The most common useful alternative boundary conditions in some calculations are delayed boundary conditions (also called causal boundary conditions) in which the initial coordinates and initial momenta are specified. These boundary conditions lead to the familiar causal Green's function for the harmonic oscillator. Importantly, the use of the path integral (and equivalently the fact that vevs are time ordered) imposes the Feynman $+i\varepsilon$ upon us; it is not a choice. Other boundary conditions are only ever useful when computing something other than a time ordered vev.

Exercises

Problem 9.8: Multivariate Gaussian Integrals. Recall the result of the single variable Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-\frac{a}{2}x^2 + bx + c} dx = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a} + c}$$

valid for $a > 0$ and b, c arbitrary complex numbers that we have shown previously.

- (a) Let $F(a, b, c)$ be given by the integral above, now considering a, b, c to be generic complex numbers. Decompose a into its real and imaginary parts and show that for $\text{Re}(a) > 0$ $F(a, b, c)$ is analytic in both the real and imaginary parts of a . Thus, conclude that in fact the integral given above is valid for all complex a with $a > 0$.

- (b) Consider b to be purely imaginary. Show that even for $\text{Re}(a) = 0$ the quoted integral remains analytic in the imaginary part of a in a neighborhood away from the point $a = 0$ and use this to show that in fact the quoted integral is valid for $\text{Re}(a) \geq 0$ if $\text{Re}(b) = 0$.
- (c) Consider now the integral:

$$G(A, B, C) = \int_{\mathbb{R}^n} e^{-\frac{i}{2} A_{ab} x^a x^b + i B_a x^a + i C} d^n \vec{x}$$

for a real symmetric positive definite matrix A_{ab} , a real vector B_a , and real number C . Show that by diagonalizing A_{ab} and changing coordinates in the integral, the result becomes a product of n independent integrals of the type of $F(a, b, c)$ with $\text{Re}(a) = \text{Re}(b) = 0$. Then, use the results of the previous parts to evaluate $G(A, B, C)$ and confirm that it agrees with (9.5.31).

Problem 9.9: Be careful, even with quadratic path integrals. The ability to put $U(t_f, Q_f, t_0, Q_0)$ into the form of (9.5.36) depends fully on the special form of the Hamiltonian Wigner function (9.5.29). It has often been tempting to others to attempt to use (9.5.36) even when W^{ab} in (9.5.29) is Q dependent. Here we will see how this goes wrong.

- (a) Show that if $W^{ab} = W^{ab}(t, Q)$ then by following the steps leading to (9.5.32) we have:

$$U(t_f, Q_f, t_0, Q_0) = \lim_{N \rightarrow \infty} \int e^{\frac{i}{\hbar} \sum_{n=0}^{N-1} \delta S_{\mathcal{L}}} \prod_{n=0}^{N-1} \left(\frac{1}{(2\pi i \hbar \delta t_n)^{\frac{d}{2}} \sqrt{\det W(t_n, Q_n)}} \right) d^d Q_1 \dots d^d Q_{N-1}.$$

From this show that the $\sqrt{\det W}$ factors now no longer cancel in calculations of operator summaries such as in (9.5.40); they matter!

- (b) Show formally (because the notation is plainly only schematic) that the above $U(t_f, Q_f, t_0, Q_0)$ can be put into the form:

$$U(t_f, Q_f, t_0, Q_0) = \mathcal{N}(t_f, t_0) \int e^{\frac{i}{\hbar} (S_{\mathcal{L}} + \frac{i\hbar}{2} \int_{t_0}^{t_f} \delta(0) \ln \det W(t, Q) dt)} \mathcal{D}Q$$

for some function $\mathcal{N}(t_f, t_0)$ and where $\delta(0)$ is understood as the $N \rightarrow \infty$ limit of $\frac{1}{\delta t_n}$. Thus the effective action functional S' receives a correction which is neither real nor finite. Again, the details of (9.5.29) matter for justifying (9.5.36).

Problem 9.10: Time Domain Representation of the Feynman Propagator. Complete the Fourier transform on the right hand side of (9.5.116) to show explicitly that:

$$\text{Vev}(\hat{q}(t)\hat{q}(t')) = \frac{\hbar}{2\varpi} e^{-i\varpi|t-t'|}.$$

You may be initially surprised that this vev is not real valued, given that $\hat{q}(t)$ is self-adjoint at each t . However, because $\hat{q}(t)$ and $\hat{q}(t')$ do not commute for $t \neq t'$, the product $\hat{q}(t)\hat{q}(t')$ is not self-adjoint and so the vev is fully allowed to be complex valued.

9.6 Quantum Statistical Mechanics

Fundamentally, we got started in the business of quantum mechanics because of statistical mechanics. In the case of particles, the macroscopic properties of matter are inconsistent with the existence of point particles. We have since replaced point particles with Schrödinger wave packets, which are able to explain the macroscopic properties of matter. As well, the inability for classical field theories to reach thermodynamic equilibrium (illustrated by the ultraviolet catastrophe in black body radiation) has shown us that we need to alter classical field theory as well. Its replacement is quantum field theory, which we will delve fully into next chapter. However, the very little bit of quantum field theory we developed in section 8.10 will be enough for us to finally solve the ultraviolet catastrophe, thus showing the power of quantum mechanics to solve a fundamental problem of classical mechanics. It is time to learn quantum statistical mechanics.

In quantum statistical mechanics we are interested in the statistical expected values of the physical properties of interest of an ensemble of “equivalent” systems, just as in classical statistical mechanics. We again can have this ensemble originating from many trials of an experiment where we only have imperfect control over the initial conditions (and thus use a distribution to model our ignorance of them) or from us uncontrolledly selecting a subsystem from a single system comprised of many mechanically identical subsystems (one particle in a box of gas). As we have established in quantum mechanics, all symmetry generators from Noether’s theorem are extensive and take the form of the operator summary of a self-adjoint operator. Further, we have already shown that the statistical expectation of an operator summary is still of the form of an operator summary but now with that summary taken by using the statistical expectation of the system’s density matrix. Thus, in quantum statistical mechanics all of the physical properties of interest are characterized by the statistical expectation of the system’s density matrix, which we will just call $\hat{\rho}$ as it acts as the effective density matrix of the full ensemble. Of course, the full density matrix of our system satisfies the von Neumann equation (9.1.80).

9.6.1 The First Law of Thermodynamics

The fundamental results of thermodynamics carry over to quantum mechanics with hardly any change. Let us begin with the first law of thermodynamics. Consider our system in the active picture so that now the density matrix is constant $\hat{\rho}_0$ and the coordinate and momentum operators evolve with time. Suppose our system has free Hamiltonian operator $\hat{H}$ and is subject to some external forces which cause modification to the evolution of the momentum operators as usual:

$$\frac{d\hat{Q}^a}{dt} = \frac{1}{i\hbar}[\hat{Q}^a, \hat{H}], \quad \frac{d\hat{P}_a}{dt} = \frac{1}{i\hbar}[\hat{P}_a, \hat{H}] + \hat{F}_a^{\text{ext}}. \quad (9.6.1)$$

We now want to compute the time evolution of the expected energy of the system. We write our Hamiltonian operator in the form of (9.2.45):

$$\hat{H} = \sum_{m=0}^{\infty, \infty} \sum_{n=0}^{\infty, \infty} H^{(m,n)}_{a_1 \dots a_m b_1 \dots b_n} \text{Sym}(\hat{Q}^{a_1}, \dots, \hat{Q}^{a_m}, \hat{P}_{b_1}, \dots, \hat{P}_{b_n}) \quad (9.6.2)$$

where we have taken the point $(q, p) = (0, 0)$ and given an abbreviated name to the coefficients of the expansion. Those coefficients are constant because the underlying system has time translational symmetry. Now we can directly compute:

$$\frac{d\hat{H}}{dt} = \sum_{m=0}^{\infty, \infty} \sum_{n=0}^{\infty, \infty} H^{(m,n)}_{a_1 \dots a_m b_1 \dots b_n} \left(m \text{Sym} \left(\frac{d\hat{Q}^{a_1}}{dt}, \dots, \hat{Q}^{a_m}, \hat{P}_{b_1}, \dots, \hat{P}_{b_n} \right) + n \text{Sym} \left(\hat{Q}^{a_1}, \dots, \hat{Q}^{a_m}, \frac{d\hat{P}_{b_1}}{dt}, \dots, \hat{P}_{b_n} \right) \right) \quad (9.6.3)$$

$$= \frac{1}{i\hbar} [\hat{H}, \hat{H}] + \sum_{m=0}^{\infty, \infty} \sum_{n=0}^{\infty, \infty} H^{(m,n)}_{a_1 \dots a_m b_1 \dots b_n} n \text{Sym} \left(\hat{Q}^{a_1}, \dots, \hat{Q}^{a_m}, \hat{F}_{b_1}^{\text{ext}}, \dots, \hat{P}_{b_n} \right). \quad (9.6.4)$$

This last series can be understood as effectively differentiating $\hat{H}$ as a function with respect to $\hat{P}_a$ and inserting $\hat{F}_a^{\text{ext}}$ at each place $\hat{P}_a$ was removed. Therefore, we define as a piece of notation:

$$\left(\hat{F}_a^{\text{ext}} \frac{\partial}{\partial \hat{P}_a} \right) \hat{H} = \sum_{m=0}^{\infty, \infty} \sum_{n=0}^{\infty, \infty} H^{(m,n)}_{a_1 \dots a_m b_1 \dots b_n} n \text{Sym} \left(\hat{Q}^{a_1}, \dots, \hat{Q}^{a_m}, \hat{F}_{b_1}^{\text{ext}}, \dots, \hat{P}_{b_n} \right) \quad (9.6.5)$$

$$\Rightarrow \frac{d\hat{H}}{dt} = \left(\hat{F}_a^{\text{ext}} \frac{\partial}{\partial \hat{P}_a} \right) \hat{H}. \quad (9.6.6)$$

Immediately then, because $E = \langle \hat{H} \rangle$:

$$\frac{dE}{dt} = \left\langle \left(\hat{F}_a^{\text{ext}} \frac{\partial}{\partial \hat{P}_a} \right) \hat{H} \right\rangle. \quad (9.6.7)$$

If we now divide our variables as usual in statistical mechanics into microscopic m and macroscopic M degrees of freedom we have (simply by expanding the sum):

$$\frac{dE}{dt} = \left\langle \left(\hat{F}_{ma}^{\text{ext}} \frac{\partial}{\partial \hat{P}_{ma}} \right) \hat{H} \right\rangle + \left\langle \left(\hat{F}_{Ma}^{\text{ext}} \frac{\partial}{\partial \hat{P}_{Ma}} \right) \hat{H} \right\rangle. \quad (9.6.8)$$

So, just as in classical mechanics the contributions to the change in energy decompose nicely into effects due to macroscopic external forces and effects due to microscopic external forces. Just as in classical mechanics then, these contributions provide the fundamental definitions of work and heat:

$$\frac{dW}{dt} = \left\langle \left(\hat{F}_{Ma}^{\text{ext}} \frac{\partial}{\partial \hat{P}_{Ma}} \right) \hat{H} \right\rangle, \quad \frac{dQ}{dt} = \left\langle \left(\hat{F}_{ma}^{\text{ext}} \frac{\partial}{\partial \hat{P}_{ma}} \right) \hat{H} \right\rangle \quad (9.6.9)$$

and the first law of thermodynamics is entirely unchanged:

$$\frac{dE}{dt} = \frac{dW}{dt} + \frac{dQ}{dt}. \quad (9.6.10)$$

9.6.2 Thermodynamic Equilibrium

The notion of thermodynamic equilibrium and the generalized Boltzmann distribution also carry over very nicely into quantum mechanics. Let us return to the passive picture and consider the evolution of the density matrix under the von Neumann equation. Let $\hat{\rho}$ indicate the time-averaged density matrix:

$$\hat{\rho} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \hat{\rho}(t) dt. \quad (9.6.11)$$

So, $\hat{\rho}$ captures the long term behavior of our system. Using the von Neumann equation, we have that:

$$[\hat{\rho}, \hat{H}] = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau i\hbar \frac{d\hat{\rho}(t)}{dt} dt = i\hbar \lim_{\tau \rightarrow \infty} \frac{\hat{\rho}(\tau) - \hat{\rho}(0)}{\tau}. \quad (9.6.12)$$

The numerator will always remain a bounded operator while the denominator goes to 0 and so in fact:

$$[\hat{\rho}, \hat{H}] = 0. \quad (9.6.13)$$

The steady state density matrix must commute with the Hamiltonian operator.

Suppose our system has K independent extensive conserved quantities $G_1, \dots, G_K$. In quantum mechanics, these can be written as the operator summaries of K self-adjoint operators $\hat{G}_1, \dots, \hat{G}_K$ and each of these operators must commute with the Hamiltonian operator in order to have the conservation law:

$$[\hat{G}_k, \hat{H}] = 0. \quad (9.6.14)$$

By independent we require that these quantities cannot be written in terms of each other and that their operators commute:

$$[\hat{G}_k, \hat{G}_l] = 0. \quad (9.6.15)$$

Because we assume these are a complete list of our system's conserved quantities, in order for $\hat{\rho}$ to commute with $\hat{H}$ it must be a function of the operators $\hat{G}_1, \dots, \hat{G}_K$. That is, for some functional form F :

$$\hat{\rho} = F(\hat{G}_1, \dots, \hat{G}_K). \quad (9.6.16)$$

The particulars of this functional form are fixed by the initial conditions of the system. However, if our experimental design is unbiased in certain ways we can determine a specific function F just like in classical statistical mechanics. For example, if we always prepare our system to identically have energy E and to be totally unbiased otherwise on average, then necessarily the only one of the $\hat{G}_k$ that F depends on is $\hat{H}$ itself and $\hat{\rho}$ will take the form:

$$\hat{\rho} = N\delta(\hat{H} - E) \quad (9.6.17)$$

where N is a normalization factor. Because $\hat{\rho}$ must have trace 1 we can determine this normalization factor

in terms of the density of states $g(E)$:

$$g(E) = \text{Tr}(\delta(\hat{H} - E)) \quad (9.6.18)$$

and in doing so we achieve the quantum microcanonical ensemble:

$$\hat{\rho}_{\text{micro}} = \frac{1}{g(E)} \delta(\hat{H} - E). \quad (9.6.19)$$

Alternatively, we can say that if we bring together two subsystems which are noninteracting but under the same thermodynamic conditions then they should be statistically independent of each other and their extensive conserved quantities should add. Independence requires that their density matrices multiply by (9.1.128):

$$\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2. \quad (9.6.20)$$

The additivity of extensive conserved quantities then means:

$$F(\vec{\hat{G}}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \vec{\hat{G}}_2) = F(\vec{\hat{G}}_1) \otimes F(\vec{\hat{G}}_2) \quad (9.6.21)$$

where we have formed a vector $\vec{\hat{G}} = (\hat{G}_1, \dots, \hat{G}_K)$. By the identical calculation leading to (5.5.49), we have that for some real numbers β_a and Z :

$$F(\vec{\hat{G}}) = \frac{e^{-\beta_a \hat{G}^a}}{Z}. \quad (9.6.22)$$

Thus we recover the generalized Boltzmann distribution as the generalized canonical ensemble in quantum mechanics. The most common special case of course is when all of our conserved quantities other than the energy are 0 on average and so happen to have vanishing multipliers β_a , leaving us with the usual canonical ensemble:

$$\hat{\rho}_{\text{canon}} = \frac{e^{-\beta \hat{H}}}{Z}. \quad (9.6.23)$$

The temperature is (in direct analog of classical statistical mechanics) defined as the reciprocal of the β factor corresponding to the energy:

$$T = \frac{1}{\beta} \quad (9.6.24)$$

and the partition function Z is fixed as always by requiring appropriate normalization of the distribution:

$$\text{Tr}(\hat{\rho}_{\text{canon}}) \stackrel{!}{=} 1 \implies Z = \text{Tr}(e^{-\beta \hat{H}}). \quad (9.6.25)$$

It is clear how (9.6.18) and (9.6.25) reduce in the classical limit to the classical definitions of the density of states and the partition function by using (9.2.153) and that in the classical limit the Wigner function associated to H will become the classical Hamiltonian $\mathcal{H}$. This also explains the inclusion of factors $2\pi\hbar$ all the way back in the phase space measure in (5.2.4); those factors were put there to make this classical limit as simple as possible due to the factors of $2\pi\hbar$ which appear automatically in the Weyl transform.

The familiar formula (5.5.23) for the expected energy in the canonical ensemble even holds in quantum mechanics! By an essentially identical calculation:

$$\frac{\partial Z}{\partial \beta} = \frac{\partial}{\partial \beta} \text{Tr}(e^{-\beta \hat{H}}) = -\text{Tr}(\hat{H} e^{-\beta \hat{H}}) = -Z \text{Tr}(\hat{H} \hat{\rho}) = -EZ \implies E = -\frac{\partial}{\partial \beta} \ln Z. \quad (9.6.26)$$

Unsurprisingly given how much of the rest of thermodynamic structure is shared between classical and quantum mechanics, the free energy is defined in exactly the same way between them:

$$\mathcal{F} = -T \ln Z. \quad (9.6.27)$$

The T derivative of $\mathcal{F}$ immediately then gives (using (9.6.24) and (9.6.26)):

$$E = \mathcal{F} - T \frac{\partial \mathcal{F}}{\partial T}. \quad (9.6.28)$$

9.6.3 Von Neumann Entropy

The classical formula for the entropy of a phase space density (5.6.77) can't directly apply to the density matrix because the density matrix is not a function on the phase space. An obvious suggestion would be to take (5.6.77) and replace the phase space density by the Wigner function associated to the density matrix, however this is not a valid definition of entropy because the Wigner function associated to the density matrix can be negative, rendering the logarithm meaningless (on real numbers). Because the density matrix is a nonnegative self-adjoint operator of unit trace, we can diagonalize it into the form:

$$\hat{\rho} = \sum_n p_n \hat{\pi}_n \quad (9.6.29)$$

where the $\hat{\pi}_n$ are projectors and satisfy:

$$\pi_n \pi_k = \delta_{nk} \pi_n, \quad \sum_n \hat{\pi}_n = \mathbb{1} \quad (9.6.30)$$

and the eigenvalues p_n of $\hat{\rho}$ satisfy:

$$p_n \geq 0, \quad \sum_n p_n = 1. \quad (9.6.31)$$

By (9.1.97), the density matrix (9.6.29) behaves identically to randomly sampling from the $\hat{\pi}_n$ as a list of density matrices with associated probability p_n for the purposes of computing expectations. So, a possible natural definition of the entropy of the density matrix is then:

$$S = - \sum_n p_n \ln p_n \quad (9.6.32)$$

as this is the information entropy you would get by using that probability distribution. This entropy is known as the von Neumann entropy and we will now show that it does in fact have the desired properties we would like the entropy to have. Recall that a function of a diagonalizable operator is defined to act with that function on the operators eigenvalues in the diagonal basis. With this in mind, we can immediately rewrite the von Neumann entropy as:

$$S = -\text{Tr}(\hat{\rho} \ln \hat{\rho}). \quad (9.6.33)$$

Because the von Neumann entropy is an information entropy of a probability distribution, it is automatically nonnegative:

$$S \geq 0. \quad (9.6.34)$$

This is superior to the situation in classical mechanics where the entropy can become arbitrarily negative (because differential entropy is cursed). The explanation for how the possible negativity arises in classical mechanics is in how the classical phase space density is generally not the Wigner function associated to a valid density matrix. Throwing away the $\hbar$ and higher order corrections changes the value of the entropy in a way that does not disappear in the classical limit (and may not even be finite).

In classical statistical mechanics, the various ensembles of interest have the maximum possible entropy consistent with their relevant constraints. The very same is true in quantum mechanics. Let us show this for the canonical ensemble, as for the other ensembles the calculations follow essentially the same steps. We wish to maximize the von Neumann entropy for a $\hat{\rho}$ with a given expected energy E and so consider the variations of:

$$S(\hat{\rho}) = -\text{Tr}(\hat{\rho} \ln \hat{\rho}) + \alpha(1 - \text{Tr}(\hat{\rho})) + \beta(E - \text{Tr}(\hat{H}\hat{\rho})) \quad (9.6.35)$$

with the Lagrange multipliers α and β . Varying with respect to $\hat{\rho}$ yields:

$$\frac{\partial S}{\partial \hat{\rho}} = -\ln \hat{\rho} - \mathbb{1} - \alpha \mathbb{1} - \beta \hat{H} \stackrel{!}{=} 0 \quad (9.6.36)$$

The derivative of a scalar function with respect to an operator is really defined in an arbitrary orthonormal basis as:

$$\frac{\partial S}{\partial \hat{\rho}} = \sum_{mn} \frac{\partial S}{\partial \rho_{nm}} |m\rangle \langle n| \quad (9.6.37)$$

where the components ρ_{nm} are defined as usual by:

$$\rho_{nm} = \langle n | \hat{\rho} | m \rangle. \quad (9.6.38)$$

Continuing from (9.6.36) we have:

$$\hat{\rho} = e^{-\alpha} e^{-\beta \hat{H}} \quad (9.6.39)$$

which upon normalization just recovers the canonical ensemble. The second derivative of the entropy again reveals that this is the maximum value attained.

Another foundational argument in favor of the suitability of von Neumann's definition of the entropy of a density matrix is that it precisely recovers the usual relationship between the entropy and the free energy. In particular, for the canonical ensemble:

$$S = -\text{Tr}(\hat{\rho} \ln \hat{\rho}) = -\text{Tr}(\hat{\rho}(-\beta \hat{H} - \mathbb{1} \ln Z)) = \beta E + \ln Z = \frac{E - \mathcal{F}}{T} = -\frac{\partial \mathcal{F}}{\partial T} \quad (9.6.40)$$

totally identically to classical statistical mechanics. The von Neumann entropy is extensive. If two systems are independent so that their combined density matrix factorizes as $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$ then:

$$\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2 \implies \ln \hat{\rho} = \ln \hat{\rho}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \ln \hat{\rho}_2 \implies S(\hat{\rho}) = S(\hat{\rho}_1) + S(\hat{\rho}_2). \quad (9.6.41)$$

Von Neumann's entropy is also subadditive, just like classical information entropy. Unfortunately, the proof is a bit more complicated. First we need a few smaller results. Let $\hat{A}$ and $\hat{B}$ be self-adjoint operators and let $f(x)$ be a differentiable real valued function of a real variable. Define the operator:

$$\hat{C}(t) = (1-t)\hat{A} + t\hat{B} \implies \hat{C}(0) = \hat{A}, \quad \hat{C}(1) = \hat{B}. \quad (9.6.42)$$

Let $|n(t)\rangle$ be a set of orthonormal eigenvectors of $\hat{C}(t)$ with eigenvalues $\lambda_n(t)$. Then, by perturbation theory around t (from t to $t + \delta t$, say) it follows that:

$$\lambda'_n(t) = \langle n(t) | (\hat{B} - \hat{A}) | n(t) \rangle \quad (9.6.43)$$

where the prime indicates the derivative with respect to t . So:

$$\text{Tr}(f(\hat{C}(t + \delta t))) = \sum_n f(\lambda_n(t + \delta t)) = \sum_n f(\lambda_n(t)) + \delta t \sum_n \lambda'_n(t) f'(\lambda_n(t)) + \mathcal{O}(\delta t^2) \quad (9.6.44)$$

$$= \sum_n \langle n(t) | f(\hat{C}(t)) | n(t) \rangle + \delta t \sum_n \langle n(t) | (\hat{B} - \hat{A}) f'(\hat{C}(t)) | n(t) \rangle + \mathcal{O}(\delta t^2) \quad (9.6.45)$$

$$\implies \frac{d}{dt} \text{Tr}(f((1-t)\hat{A} + t\hat{B})) = \text{Tr}((\hat{B} - \hat{A}) f'((1-t)\hat{A} + t\hat{B})). \quad (9.6.46)$$

Now consider $f(x)$ to be a concave up function. A concave up function is a function for which for $x \neq y$ and $t \in (0, 1)$:

$$f((1-t)x + ty) < (1-t)f(x) + tf(y). \quad (9.6.47)$$

Let $|m'\rangle$ denote any orthonormal basis of our Hilbert space which is not an eigenbasis of $\hat{A}$. Using the concave up-ness of $f(x)$ and the diagonal representation of $\hat{A}$:

$$\text{Tr}(f(\hat{A})) = \sum_m \langle m' | f(\hat{A}) | m' \rangle = \sum_{mn} f(\lambda_n(0)) \langle m' | n(0) \rangle \langle n(0) | m' \rangle \quad (9.6.48)$$

$$> \sum_m f \left(\sum_n a_n |\langle m' | n(0) \rangle|^2 \right) = \sum_m f(\langle m' | \hat{A} | m' \rangle). \quad (9.6.49)$$

If we instead have $|m'\rangle = |n_A\rangle$ we get exact equality immediately and so in general:

$$\text{Tr}(f(\hat{A})) \geq \sum_m f(\langle m' | \hat{A} | m' \rangle) \quad (9.6.50)$$

for any concave up $f(x)$, self-adjoint $\hat{A}$, and generic orthonormal basis $|m'\rangle$ with equality holding if and only if $|m'\rangle$ is an eigenbasis of $\hat{A}$. Let us now apply this result with $\hat{A}$ replaced by $\hat{C}(t)$. Let us first assume $\hat{A}$ and $\hat{B}$ commute but $\hat{A} \neq \hat{B}$. Then, we can select $|n(t)\rangle$ to be a simultaneous eigenbasis of them and because $\hat{A} \neq \hat{B}$ there is at least one n so that $\langle n(t) | \hat{A} | n(t) \rangle \neq \langle n(t) | \hat{B} | n(t) \rangle$. With this, (9.6.47), (9.6.50) we have:

$$\text{Tr}(f((1-t)\hat{A} + t\hat{B})) = \sum_n f((1-t)\langle n(t) | \hat{A} | n(t) \rangle + t\langle n(t) | \hat{B} | n(t) \rangle) \quad (9.6.51)$$

$$< \sum_n \left((1-t)f(\langle n(t) | \hat{A} | n(t) \rangle) + tf(\langle n(t) | \hat{B} | n(t) \rangle) \right) = (1-t)\text{Tr}(f(\hat{A})) + t\text{Tr}(f(\hat{B})). \quad (9.6.52)$$

Now let us assume $\hat{A}$ and $\hat{B}$ do not commute. Then, the eigenbasis $|n(t)\rangle$ will be an eigenbasis of neither $\hat{A}$ nor $\hat{B}$ and so again using (9.6.47) and (9.6.50):

$$\text{Tr}(f((1-t)\hat{A} + t\hat{B})) = \sum_n f((1-t)\langle n(t)|\hat{A}|n(t)\rangle + t\langle n(t)|\hat{B}|n(t)\rangle) \quad (9.6.53)$$

$$\leq \sum_n \left((1-t)f(\langle n(t)|\hat{A}|n(t)\rangle) + tf(\langle n(t)|\hat{B}|n(t)\rangle) \right) < (1-t)\text{Tr}(f(\hat{A})) + t\text{Tr}(f(\hat{B})). \quad (9.6.54)$$

If we had instead chosen $\hat{B} = \hat{A}$ then plainly $\text{Tr}(f((1-t)\hat{A} + t\hat{B})) = (1-t)\text{Tr}(f(\hat{A})) + t\text{Tr}(f(\hat{B}))$. So, we have that for a concave up function $f(x)$, arbitrary self-adjoint $\hat{A}$ and $\hat{B}$, and $t \in (0, 1)$:

$$\text{Tr}(f((1-t)\hat{A} + t\hat{B})) \leq (1-t)\text{Tr}(f(\hat{A})) + t\text{Tr}(f(\hat{B})) \quad (9.6.55)$$

with equality holding if and only if $\hat{A} = \hat{B}$. This is known as the convexity of the trace.

Consider $\hat{B} \neq \hat{A}$ and from our function $f(x)$ define the function $F(t)$:

$$F(t) = \text{Tr}(f((1-t)\hat{A} + t\hat{B})). \quad (9.6.56)$$

It immediately follows for $t \in (0, 1)$ and $x, y \in [0, 1]$ with $y \neq x$ from the convexity of the trace that $F(t)$ is also concave up:

$$(1-t)F(x) + tF(y) = (1-t)\text{Tr}(f((1-x)\hat{A} + x\hat{B})) + t\text{Tr}(f((1-y)\hat{A} + y\hat{B})) \quad (9.6.57)$$

$$> \text{Tr}(f((1-t)(1-x)\hat{A} + (1-t)x\hat{B} + t(1-y)\hat{A} + ty\hat{B})) = F((1-t)x + ty). \quad (9.6.58)$$

As well, define the function $g(t)$:

$$g(t) = \frac{F(t) - F(0)}{t}. \quad (9.6.59)$$

Because $F(t)$ is concave up, it follows that $g(t)$ is increasing. We can see this by evaluating the concave up condition on $F(t)$ in terms of $x = 0$, $y = b$, $t = \frac{a}{b}$ (note $a < b$ because $t < 1$):

$$b > a \implies \frac{F(b) - F(0)}{b} > \frac{F(a) - F(0)}{a} \implies g(b) > g(a). \quad (9.6.60)$$

By applying the concave up condition at $x = 0$, $y = 1$:

$$F(1) - F(0) > g(t). \quad (9.6.61)$$

Because $g(t)$ is an increasing function of t and using its explicit definition, we also have:

$$F(1) - F(0) > g(t) > \lim_{t \rightarrow 0^+} g(t) = F'(0). \quad (9.6.62)$$

Let us now apply (9.6.46) to simplify this inequality into:

$$\text{Tr}(f(\hat{B})) - \text{Tr}(f(\hat{A})) > \text{Tr}((\hat{B} - \hat{A})f'(\hat{A})). \quad (9.6.63)$$

Plainly, if we had used $\hat{B} = \hat{A}$ then both sides of (9.6.63) become 0 and we get equality. Thus we have:

$$\text{Tr}(f(\hat{B})) - \text{Tr}(f(\hat{A})) \geq \text{Tr}((\hat{B} - \hat{A})f'(\hat{A})) \quad (9.6.64)$$

for any differentiable concave up function $f(x)$ and self-adjoint operators $\hat{A}$ and $\hat{B}$ with equality if and only if $\hat{A} = \hat{B}$. This result is known as Klein's inequality.

Using Klein's inequality we can prove the subadditivity of the von Neumann entropy. Consider the function:

$$f(x) = x \ln x. \quad (9.6.65)$$

Plainly for $x > 0$ $f(x)$ is differentiable. As well, its second derivative is positive (simply $1/x$), which we can then integrate from a to $b > a$ to show that $f'(x)$ is an increasing function:

$$f''(x) = \frac{1}{x} > 0 \implies f'(b) - f'(a) > 0. \quad (9.6.66)$$

We can now take this condition and replace b by x and then integrate from a to b or replace a by x and then integrate from a to b . Doing each of these and combining the results gives:

$$f'(a) < \frac{f(b) - f(a)}{b - a} < f'(b). \quad (9.6.67)$$

If we now consider $c > b$, we have:

$$\frac{f(c) - f(a)}{c - a} = \frac{\frac{f(c)-f(b)}{c-b}(c-b) + \frac{f(b)-f(a)}{b-a}(b-a)}{c-a} > \frac{f'(b)(c-b) + \frac{f(b)-f(a)}{b-a}(b-a)}{c-a} \quad (9.6.68)$$

$$> \frac{\frac{f(b)-f(a)}{b-a}(c-b) + \frac{f(b)-f(a)}{b-a}(b-a)}{c-a} = \frac{f(b) - f(a)}{b-a}. \quad (9.6.69)$$

Taking $a = x$, $b = (1-t)x + ty$, and $c = y$ with $y > x$ and $t \in (0, 1)$ we find with a small amount of algebra that indeed $f(x)$ is concave up:

$$f((1-t)x + ty) < (1-t)f(x) + tf(y). \quad (9.6.70)$$

result known as Klein's inequality. Let $f(x)$ be a real valued function of a real variable which is concave up. Now consider two different valid density matrices $\hat{q}$ and $\hat{p}$. Because $f(x)$ is concave up, we can apply Klein's inequality to find:

$$\text{Tr}(\hat{p} \ln \hat{p}) - \text{Tr}(\hat{q} \ln \hat{q}) \geq \text{Tr}((\hat{p} - \hat{q})(\ln \hat{q} + \mathbb{1})) \quad (9.6.71)$$

$$\implies \text{Tr}(\hat{p} \ln \hat{p}) - \text{Tr}(\hat{p} \ln \hat{q}) \geq 0 \quad (9.6.72)$$

with equality holding if and only if $\hat{q} = \hat{p}$. This quantity for two density matrices defines the quantum relative information $\mathcal{I}(\hat{p}|\hat{q})$:

$$\mathcal{I}(\hat{p}|\hat{q}) = \text{Tr}(\hat{p} \ln \hat{p}) - \text{Tr}(\hat{p} \ln \hat{q}). \quad (9.6.73)$$

This is the natural operator generalization of our formula for the relative information between two probability distributions. Due to Klein's inequality, we see that $\mathcal{I}(\hat{p}|\hat{q})$ is nonnegative and it is 0 if and only if $\hat{p} = \hat{q}$:

$$\mathcal{I}(\hat{p}|\hat{q}) \geq 0. \quad (9.6.74)$$

Finally, we can prove the subadditivity of the entropy. Consider a quantum system which decomposes into two subsystems. Let $\hat{\rho}$ be the density matrix of the full system and let $\hat{\rho}_1$ and $\hat{\rho}_2$ be the marginal density matrices of the two subsystems. As well, let $\hat{\rho}_{\text{indep}}$ be the tensor product of $\hat{\rho}_1$ and $\hat{\rho}_2$:

$$\hat{\rho}_1 = \text{Tr}_2(\hat{\rho}), \quad \hat{\rho}_2 = \text{Tr}_1(\hat{\rho}), \quad \hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2. \quad (9.6.75)$$

Of course, $\hat{\rho}_{\text{indep}}$ is the density matrix the system would have if the two subsystems were completely independent and noninteracting. Then:

$$S(\hat{\rho}_1) + S(\hat{\rho}_2) - S(\hat{\rho}) = -\text{Tr}_1(\hat{\rho}_1 \ln \hat{\rho}_1) - \text{Tr}_2(\hat{\rho}_2 \ln \hat{\rho}_2) + \text{Tr}(\hat{\rho} \ln \hat{\rho}) \quad (9.6.76)$$

$$= -\text{Tr}(\hat{\rho} \ln(\hat{\rho}_1 \otimes \mathbb{1})) - \text{Tr}(\hat{\rho} \ln(\mathbb{1} \otimes \hat{\rho}_2)) + \text{Tr}(\hat{\rho} \ln \hat{\rho}) \quad (9.6.77)$$

$$= \text{Tr}(\hat{\rho} \ln \hat{\rho}) - \text{Tr}(\hat{\rho} \ln \hat{\rho}_{\text{indep}}) \quad (9.6.78)$$

$$= \mathcal{I}(\hat{\rho}|\hat{\rho}_{\text{indep}}) \geq 0 \quad (9.6.79)$$

with equality holding if and only if $\hat{\rho} = \hat{\rho}_{\text{indep}}$. After one final step we have, as promised:

$$\boxed{S(\hat{\rho}) \leq S(\hat{\rho}_1) + S(\hat{\rho}_2)} \quad (9.6.80)$$

with equality if and only if $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$.

Just like in classical statistical mechanics, the entropy is conserved by Hamiltonian time evolution. Under Hamiltonian time evolution, the density matrix has the simple time dependence:

$$\hat{\rho}(t) = \hat{U}(t, t_0) \hat{\rho}(t_0) \hat{U}^\dagger(t, t_0). \quad (9.6.81)$$

Any continuous function of $\hat{\rho}(t)$ then satisfies:

$$f(\hat{\rho}(t)) = \hat{U}(t, t_0) f(\hat{\rho}(t_0)) \hat{U}^\dagger(t, t_0) \quad (9.6.82)$$

(to see this, first use that any continuous function can be arbitrarily well approximated by an analytic function and that for an analytic function this follows automatically by using its power series expression). So, the entropy is constant by the cyclicity of the trace:

$$S(t) = -\text{Tr}(\hat{\rho}(t) \ln \hat{\rho}(t)) = -\text{Tr}(\hat{U}(t, t_0) \hat{\rho}(t_0) \ln \hat{\rho}(t_0) \hat{U}^\dagger(t, t_0)) = -\text{Tr}(\hat{\rho}(t_0) \ln \hat{\rho}(t_0)) = S(t_0). \quad (9.6.83)$$

Exactly as in classical mechanics, the entropy of an isolated system only changes due to unaccounted for forces (which we could add by time evolving using (9.6.1)). The combination of the subadditivity of entropy together with its conservation under Hamiltonian time evolution give that the proof of the second law of thermodynamics established in (5.7.29) is completely unchanged in quantum mechanics. The second law of thermodynamics carries over exactly.

9.6.4 Planck's Law

Now that we have shown how thermodynamics plays nicely with quantum mechanics, let us show how quantum field theory explains Planck's law. Because the electromagnetic Hamiltonian in (4.6.29) depends only quadratically on the fields and because all of the symmetries of electromagnetism act linearly on the potentials, we know that we can write down a Hamiltonian operator for quantum electromagnetism with all of the correct symmetries by taking that classical Hamiltonian as the Wigner function of the theory. Because of this, all of the coordinate transformations leading to (5.12.86) remain appropriate in quantum mechanics, with that $\mathcal{H}$ now interpreted as the Wigner function for $\hat{H}$. So, the Hamiltonian operator for quantum mechanical electromagnetic waves in a conducting box of volume side length ℓ is then:

$$\begin{aligned} \hat{H} = & \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{\hat{P}_{\vec{n}-1}^2}{2} + \frac{\hat{P}_{\vec{n}+1}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} (\hat{A}_{\vec{n}-1}^2 + \hat{A}_{\vec{n}+1}^2) \right) + \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{\hat{P}_{x0n_y n_z}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} \hat{A}_{x0n_y n_z}^2 \right) \\ & + \sum_{n_x=1}^{\infty} \sum_{n_z=1}^{\infty} \left(\frac{\hat{P}_{yn_x 0n_z}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} \hat{A}_{yn_x 0n_z}^2 \right) + \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \left(\frac{\hat{P}_{zn_x n_y 0}^2}{2} + \frac{\pi^2 |\vec{n}|^2}{2\ell^2} \hat{A}_{zn_x n_y 0}^2 \right). \end{aligned} \quad (9.6.84)$$

This is now the form of an infinite number of quantum harmonic oscillators! Because the structure of thermodynamics is totally unchanged by quantum mechanics, the Helmholtz free energy remains extensive and so all of the arguments leading to (5.12.98) are unchanged. Therefore, we still have the the free energy of quantum electromagnetism is given by:

$$\mathcal{F} = \frac{\mathbb{V}}{\pi^2} \int_0^{\infty} \mathcal{F}_1(T, \omega) \omega^2 d\omega \quad (9.6.85)$$

where $\mathcal{F}_1(T, \omega)$ is the free energy of a single harmonic oscillator at temperature T of angular frequency ω . However, now it is the free energy of a quantum harmonic oscillator because each mode within (9.6.84) is a qho. The ground state energy of any system is entirely arbitrary and unphysical as we can shift the energy by an overall constant. By convention, we typically set the ground state energy of a quantum field theory to be 0 by definition. Doing so, we have that for a single quantum harmonic oscillator we take the Hamiltonian operator:

$$\hat{H} = \hbar\omega \hat{a}^\dagger \hat{a} \quad (9.6.86)$$

in terms of the creation and annihilation operators of the oscillator. Now using (9.6.25) we have:

$$Z_1 = \text{Tr}(e^{-\beta \hat{H}}) = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-n\beta \hbar\omega} = \frac{1}{1 - e^{-\beta \hbar\omega}} \quad (9.6.87)$$

$$\implies \mathcal{F}_1 = -T \ln Z_1 = T \ln \left(1 - e^{-\frac{\hbar\omega}{T}} \right). \quad (9.6.88)$$

This is *exactly* the same free energy that we guessed in (5.12.126). Therefore, quantum mechanics genuinely explains that formula. From this free energy, we can legitimately follow the rest of the steps of section 5.12 to derive Planck's law and the Stefan-Boltzmann law. We can also explain (5.12.141). Using the density of states definition in (9.6.18):

$$g(E) = \text{Tr}(\delta(\hat{H} - E)) = \sum_n \delta(E_n - E) = \sum_n (E - n\hbar\omega) \quad (9.6.89)$$

exactly as desired. Amazingly, quantum mechanics fully resolves the tension between classical field theory and thermodynamics.

9.6.5 Bose-Einstein and Fermi-Dirac Statistics

In the next chapter we will learn that a quadratic quantum field theory for a field of integer spin has creation and annihilation operators that satisfy the usual commutation relations but for a quadratic quantum field theory for a field of half-integer spin the creation and annihilation operators satisfy a slightly unusual commutation relation. In particular, if $\hat{a}$, $\hat{a}'$ are the annihilation operators for two different modes of angular frequency ω, ω' for an integer spin field, we will find:

$$[\hat{a}, \hat{a}'] = 0, \quad [\hat{a}, \hat{a}'^\dagger] = 0, \quad [\hat{a}, \hat{a}^\dagger] = [\hat{a}', \hat{a}'^\dagger] = 1. \quad (9.6.90)$$

However, if $\hat{a}$ and $\hat{a}'$ the similarly so but for a half-integer spin field, we will find:

$$[\hat{a}, \hat{a}']_+ = 0, \quad [\hat{a}, \hat{a}'^\dagger]_+ = 0, \quad [\hat{a}, \hat{a}^\dagger]_+ = [\hat{a}', \hat{a}'^\dagger]_+ = 1 \quad (9.6.91)$$

where we have defined the anticommutator of two operators:

$$[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}. \quad (9.6.92)$$

Plainly, the anticommutator is simply the symmetrized product of two operators, but for our thinking it will tend to be nicer to represent it in this $[\cdot, \cdot]_+$ notation so that it appears more similar to the usual commutator. This connection between the type of commutator used and the spin of the field is called the **spin-statistics theorem**. While we will have to wait until next chapter to justify it, it has important implications for quantum statistical mechanics, and so we will study some of those consequences here. Fields which have creation and annihilation operators satisfying the usual commutation relations (9.6.90) are called bosons and fields which have creation and annihilation operators satisfying the anticommutation relations (9.6.91) are called fermions. The existence of fermions surprises sane people at first, but you will learn that they make perfectly good sense.

As we have seen, the electromagnetic field is bosonic. Let us see the basics of the statistical mechanics of bosonic fields in general. Suppose we have a quadratic field theory which we have transformed into creation and annihilation operators $\hat{a}_k, \hat{a}_k^\dagger$ where k here is a label identifying which field mode is under consideration (we will not ever intend implicit summation over k). Let E_k be the energy of a single particle state corresponding to mode k . Then, the Hamiltonian operator for the theory is simply:

$$\hat{H} = \sum_k E_k \hat{a}_k^\dagger \hat{a}_k. \quad (9.6.93)$$

From here we can easily compute the partition function of the theory because the modes for different k commute with each other. Define the number operator $\hat{N}$ which counts the total number of particles:

$$\hat{N} = \sum_k \hat{a}_k^\dagger \hat{a}_k. \quad (9.6.94)$$

Then, in exact analogy of (5.10.124), the grand canonical ensemble density matrix is given by:

$$\hat{\rho} = \frac{e^{-\beta(\hat{H} - \mu\hat{N})}}{\mathcal{Z}} \quad (9.6.95)$$

where the grand partition function is determined by the normalization of the density matrix:

$$\text{Tr}(\hat{\rho}) = 1 \implies \mathcal{Z} = \text{Tr}(e^{-\beta(\hat{H} - \mu\hat{N})}). \quad (9.6.96)$$

In the classical statistical mechanics of identical particles we found that the occupation number density was very useful. We can define an exactly analogous and equally useful quantity in the quantum statistical mechanics of identical particles. Define the occupation number n_k of mode k as the expected number of particles in mode k :

$$n_k = \mathbb{E}(\langle \hat{a}_k^\dagger \hat{a}_k \rangle) = \text{Tr}(\hat{a}_k^\dagger \hat{a}_k \hat{\rho}). \quad (9.6.97)$$

Because the Hamiltonian and number operators in the grand canonical ensemble are sums of commuting terms for each different k , we can decompose the density matrix has:

$$\hat{\rho} = \prod_k \left(\frac{e^{-\beta(E_k - \mu)\hat{a}_k^\dagger \hat{a}_k}}{\mathcal{Z}_k} \right) \quad (9.6.98)$$

where each mode's grand partition function is defined by:

$$\mathcal{Z}_k = \text{Tr}_k(e^{-\beta(E_k - \mu)\hat{a}_k^\dagger \hat{a}_k}) \quad (9.6.99)$$

and the trace is only taken over the Hilbert space of mode k . With our decomposition of the density matrix, the computation of n_k becomes quite simple:

$$n_k = \frac{\text{Tr}(\hat{a}_k^\dagger \hat{a}_k e^{-\beta(E_k - \mu)\hat{a}_k^\dagger \hat{a}_k} \prod_{k' \neq k} e^{-\beta(E_{k'} - \mu)\hat{a}_{k'}^\dagger \hat{a}_{k'}})}{\prod_{k'} \mathcal{Z}_{k'}} = \frac{\text{Tr}(\hat{a}_k^\dagger \hat{a}_k e^{-\beta(E_k - \mu)\hat{a}_k^\dagger \hat{a}_k})}{\text{Tr}(e^{-\beta(E_k - \mu)\hat{a}_k^\dagger \hat{a}_k})} = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \mathcal{Z}_k. \quad (9.6.100)$$

We can easily compute $\mathcal{Z}_k$ because we already know the eigenvalues of the (bosonic) quantum harmonic oscillator:

$$\mathcal{Z}_k = \sum_{n=0}^{\infty} e^{-\beta(E_k - \mu)n} = \frac{1}{1 - e^{-\beta(E_k - \mu)}}. \quad (9.6.101)$$

Using this, we immediately have:

$$n_k = \frac{1}{e^{\beta(E_k - \mu)} - 1}. \quad (9.6.102)$$

This is the expected number of particles in mode k at a given temperature and chemical potential. Equation (9.6.102) is called the **Bose-Einstein** occupation formula and the particles of bosonic fields are said to satisfy Bose-Einstein statistics.

It is useful to define the occupation number operator $\hat{n}$ as an operator on the single particle Hilbert space of the field theory by:

$$\hat{n} = \sum_k n_k |k\rangle\langle k| \quad (9.6.103)$$

where $|k\rangle$ indicates a single particle state in mode k . Automatically then, if $\hat{H}_1$ is the effective single particle Hamiltonian operator of the field theory, we have that the total expected number of particles and total expected energy are given by:

$$N = \text{Tr}(\hat{n}), \quad E = \text{Tr}(\hat{H}_1 \hat{n}). \quad (9.6.104)$$

Let $n(Q, P)$ be the Wigner function associated to $\hat{n}$ and Q, P be the phase space coordinates of the phase space of a single particle. Similarly, let H_1 be the Wigner function for $\hat{H}_1$. Then, using (9.2.153) we have:

$$N = \int n(Q, P) d\mathbb{P}_1, \quad E = \int H_1(Q, P) n(Q, P) d\mathbb{P}_1 \quad (9.6.105)$$

in exact analogy with (5.10.141). Very often in applications (but not always), the single particle states can be considered as basically classical because we may have inadequate resolution to notice single particle quantum effects. However, even such a case, quantum mechanics affects the statistics of the many particle system. In this pseudo-classical case, we approximate H_1 simply by the classical Hamiltonian $\mathcal{H}_1$ of a single particle of the field theory in the classical limit. As well, then E_k limits toward being $\mathcal{H}$ evaluated at the relevant point in the single particle phase space. Thus, in this pseudo-classical limit we approximate:

$$\boxed{n_{\text{BE}}(Q, P) \approx \frac{1}{e^{\beta(\mathcal{H}_1 - \mu)} - 1}} \quad (9.6.106)$$

where the subscript BE indicates that this is appropriate for Bose-Einstein particles.

We can perform all of the above analysis for fermionic fields as well, and surprisingly little changes about the calculations. Before we do so, we need to learn some basic facts about how fermions work. For the moment, suppose we have a single fermionic quantum harmonic oscillator. That is, we have an operator $\hat{a}$ that we call an annihilation operator and its adjoint $\hat{a}^\dagger$ which together satisfy:

$$[\hat{a}, \hat{a}]_+ = 0, \quad [\hat{a}, \hat{a}^\dagger]_+ = 1 \quad (9.6.107)$$

and so that the Hamiltonian operator for the system is:

$$\hat{H} = \hbar\omega \hat{a}^\dagger \hat{a}. \quad (9.6.108)$$

We want to now understand the Hilbert space of this system and to find the eigenstates and eigenvalues of $\hat{H}$. Because of the anticommutation relations, we immediately have that $\hat{a}$ and $\hat{a}^\dagger$ as operators square to the zero operator:

$$\hat{a}^2 = (\hat{a}^\dagger)^2 = 0. \quad (9.6.109)$$

Let $|\psi\rangle$ be a normalized eigenstate of $\hat{H}$ of eigenvalue E :

$$\langle\psi|\psi\rangle = 1, \quad \hat{H}|\psi\rangle = E|\psi\rangle. \quad (9.6.110)$$

Now let us act $\hat{a}^\dagger$ on the eigenvalue equation:

$$\hbar\omega \hat{a}^\dagger \hat{a}^\dagger \hat{a} |\psi\rangle = E \hat{a}^\dagger |\psi\rangle. \quad (9.6.111)$$

The left-hand side is automatically zero because $\hat{a}^\dagger \hat{a}^\dagger = 0$. Therefore:

$$\hat{H}|\psi\rangle = E|\psi\rangle \implies E \hat{a}^\dagger |\psi\rangle = 0. \quad (9.6.112)$$

So, each eigenstate of $\hat{H}$ either has eigenvalue 0 or satisfies $\hat{a}^\dagger |\psi\rangle = 0$. Let us first consider an eigenstate of eigenvalue 0 and let us call it $|\psi_0\rangle$. Then, acting $\hat{a}$ on the eigenvalue equation:

$$\hat{H}|\psi_0\rangle = 0 \implies \hat{a} \hat{a}^\dagger \hat{a} |\psi_0\rangle = 0 \quad (9.6.113)$$

$$\implies (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})\hat{a}|\psi_0\rangle - \hat{a}^\dagger\hat{a}\hat{a}|\psi_0\rangle = 0 \quad (9.6.114)$$

$$\implies \hat{a}|\psi_0\rangle = 0. \quad (9.6.115)$$

So, if an eigenstate of $\hat{H}$ has eigenvalue 0 then it is annihilated by the annihilation operator. Now let us see how $|\psi_0\rangle$ is affected by the creation operator. Let $|\psi_1\rangle$ be given by:

$$|\psi_1\rangle = \hat{a}^\dagger|\psi_0\rangle \quad (9.6.116)$$

$$\implies \langle\psi_1|\psi_1\rangle = \langle\psi_0|\hat{a}\hat{a}^\dagger|\psi_0\rangle = \langle\psi_0|(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|\psi_0\rangle - \langle\psi_0|\hat{a}^\dagger\hat{a}|\psi_0\rangle = 1 \quad (9.6.117)$$

and so $|\psi_1\rangle$ is properly normalized. As well:

$$\hat{H}|\psi_1\rangle = \hbar\omega\hat{a}^\dagger\hat{a}\hat{a}^\dagger|\psi_0\rangle = \hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)|\psi_1\rangle - \hbar\omega\hat{a}\hat{a}^\dagger\hat{a}|\psi_0\rangle = \hbar\omega|\psi_1\rangle \quad (9.6.118)$$

and so $|\psi_1\rangle$ is also an eigenstate of $\hat{H}$, but with eigenvalue $\hbar\omega$. Because $\omega \neq 0$ and all of $\hat{H}$'s eigenstates satisfy $E\hat{a}^\dagger|\psi\rangle = 0$, we immediately have that $|\psi_1\rangle$ cannot be raised any further:

$$\hat{a}^\dagger|\psi_1\rangle = 0. \quad (9.6.119)$$

We can also recover $|\psi_0\rangle$ from $|\psi_1\rangle$ by lowering in the usual way:

$$\hat{a}|\psi_1\rangle = \hat{a}\hat{a}^\dagger|\psi_0\rangle = (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|\psi_0\rangle - \hat{a}^\dagger\hat{a}|\psi_0\rangle = |\psi_0\rangle. \quad (9.6.120)$$

So, given an eigenstate of $\hat{H}$ with eigenvalue 0 we can produce a state of eigenvalue $\hbar\omega$ and neither can be raised or lowered to achieve any new independent states beyond these two.

Next let us consider an eigenstate of $\hat{H}$ which does not have eigenvalue 0. Such a state must have $\hat{a}^\dagger|\psi\rangle = 0$. Let us now act $\hat{a}$ on this equation:

$$\hat{a}\hat{a}^\dagger|\psi\rangle = 0 \implies (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|\psi\rangle - \hat{a}^\dagger\hat{a}|\psi\rangle = 0 \quad (9.6.121)$$

$$\implies \hat{H}|\psi\rangle = \hbar\omega|\psi\rangle. \quad (9.6.122)$$

Thus, if an eigenstate of $\hat{H}$ does not have eigenvalue 0 then it must have eigenvalue $\hbar\omega$. By our previous calculation, we know from this state we can produce a state of eigenvalue 0 by simply considering $\hat{a}|\psi\rangle$. Thus, the eigenstate of $\hat{H}$ comes precisely in disjoint pairs with one member of each pair having eigenvalue 0 and the other having eigenvalue $\hbar\omega$ and the two elements of the pair related by raising/lowering. We can refine our definition of $\hat{H}$ slightly to guarantee that it possesses precisely one such pair. If $\hat{H}$ had multiple pairs of eigenvalues, we could define a creation operator for each pair by projecting the full creation operator onto that pair's subspace of the Hilbert space. Then, the full Hamiltonian operator is given by summing over Hamiltonian operators of the sum form but now manifestly with each only having a two dimensional Hilbert space. Therefore, as part of the definition of a fermionic quantum harmonic oscillator we include the condition that its Hilbert space be purely two dimensional. This is a very stark difference to the bosonic oscillator which had an infinite dimensional Hilbert space! We now call the two eigenstates of $\hat{H}$ $|0\rangle$ and $|1\rangle$ and the number simply refers to the mode occupation number, or in other words, the number of particles in this mode. Surprisingly, a fermionic field can never have more than one particle in any specific state. This enormously affects the statistical behavior of fermions. We can summarize our conclusions on fermions by saying that the Hamiltonian is simply diagonalized by states $|0\rangle$ and $|1\rangle$ satisfying:

$$\langle 0|0\rangle = \langle 1|1\rangle = 1, \quad \langle 0|1\rangle = 0, \quad |1\rangle = \hat{a}^\dagger|0\rangle, \quad |0\rangle = \hat{a}|1\rangle, \quad \hat{H}|0\rangle = 0, \quad \hat{H}|1\rangle = \hbar\omega|1\rangle. \quad (9.6.123)$$

Now let us determine the occupation number distribution for fermionic fields. All of the analysis of (9.6.93) through (9.6.100) and (9.6.103) through (9.6.105) is completely unchanged from the bosonic case. The only thing we need to treat differently is the calculation of $\mathcal{Z}_k$ and the resulting expression for n_k . Now the eigenvalues of $\hat{a}_k^\dagger\hat{a}_k$ are simply 0 and 1 and so:

$$\mathcal{Z}_k = \sum_{n=0}^1 e^{-\beta(E_k - \mu)n} = 1 + e^{-\beta(E_k - \mu)} \quad (9.6.124)$$

$$\implies n_k = \frac{1}{e^{\beta(E_k - \mu)} + 1}. \quad (9.6.125)$$

What a small change from the bosonic case! However, that -1 versus $+1$ is qualitatively hugely important. If the exponential is small in the bosonic case, the denominator approaches 0 and the occupation number becomes arbitrarily large. Because n_k is necessarily nonnegative from its definition, $E_k > \mu$ always in the bosonic case. If the exponential is small in the fermionic case, the denominator approaches 1 and the

occupation number never exceeds 1, consistent with what we have just learned about fermions. In the pseudo-classical limit, we naturally have the Fermi-Dirac (FD) occupation number distribution:

$$n_{\text{FD}}(Q, P) \approx \frac{1}{e^{\beta(\mathcal{H}_1 - \mu)} + 1}. \quad (9.6.126)$$

Both the Fermi-Dirac and Bose-Einstein distributions recover the classical Maxwell-Boltzmann distribution in the classical limit. At very low temperatures β is large and so the eigenvalues of the operator $e^{-\beta\hat{H}}$ fall off very quickly. Because of this, the density matrix at low temperatures is very small except near the lowest energy states of the system. In the bosonic case, this causes all of the particles to cram together in the lowest energy states of the system (known as a Bose-Einstein condensate). In the fermionic case, this causes all of the lowest energy states to have essentially filled occupation number 1 and for that to be a cutoff energy (called the Fermi energy) above which the occupation number drops to 0. Thus at very low temperatures the different statistics of the particles matters a lot. Away from the extremely low temperature limit, in regions of the phase space where single particles have high energy compared to the chemical potential then $e^{\beta(\mathcal{H}_1 - \mu)}$ becomes much greater than 1 and the exponential dominates the denominator in the both the Bose-Einstein and Fermi-Dirac cases. The leading order result simply reduces then to the Maxwell-Boltzmann distribution in (5.10.149).

9.6.6 The Lindblad Equation

This subsection will closely follow [67]. In general, the density matrix of a subsystem of a larger quantum system does not satisfy a closed equation of motion in terms of itself. This is completely unsurprising, because the subsystem will generically interact with other degrees of freedom outside of the subsystem. However, just as how in classical mechanics a mass moving on a table (after a little bit of averaging) approximately satisfies a closed equation of motion with dissipation from friction, it is often possible to approximately describe the statistically averaged (also often with some short-time averaging) dynamics of a subsystem density matrix with a closed equation of motion. What form can such an equation of motion take? That is, we are looking for the most general possible closed equation of motion for a statistically averaged open quantum system. It will not simply be the von Neumann equation, as that would represent a subsystem without dissipation.

Without statistical averaging or when the subsystem is strongly coupled to the rest of the quantum system, the effective dynamics of the subsystem density matrix are generally not even linear (see for example [9]). We will assume (for now) that after statistical averaging and for the subsystem interactions we are interested in it is still possible to find an effective linear equation of motion for the subsystem density matrix. Later, we will justify this assumption by a more direct derivation where these conditions directly enter. For now we will only be concerned with our subsystem and so we will think about it more as an open system with density matrix $\hat{\rho}(t)$. Because we assume there is a linear effective equation of motion for this density matrix, we equivalently assume that there will be some linear map $\mathcal{V}$ that relates the density matrix at time t to the density matrix at time 0:

$$\hat{\rho}(t) = \mathcal{V}(\hat{\rho}(0)). \quad (9.6.127)$$

This must be a map from the space of valid density matrices into itself which acts linearly on density matrices:

$$\mathcal{V}(a\hat{\rho}_1 + b\hat{\rho}_2) = a\mathcal{V}(\hat{\rho}_1) + b\mathcal{V}(\hat{\rho}_2). \quad (9.6.128)$$

A valid density matrix necessarily is self-adjoint and nonnegative and has trace 1. So, we need the outputs of $\mathcal{V}$ to also satisfy these. Because of this, $\mathcal{V}$ must be a so-called Completely Positive Trace Preserving Map (CPTP map). A map is called trace preserving if for any operator $\hat{A}$ on which it is defined it satisfies:

$$\text{Tr}(\mathcal{V}(\hat{A})) = \text{Tr}(\hat{A}). \quad (9.6.129)$$

This will protect the trace of our density matrix. Complete positivity is a bit more complicated. A linear map on operators is called positive if, for any nonnegative operator $\hat{A}$ on which it is defined, the operator $\mathcal{V}(\hat{A})$ is also nonnegative. A linear map $\mathcal{V}$ is called completely positive if the linear map $\mathcal{V} \otimes \mathbb{1}$ is positive for any size of identity matrix $\mathbb{1}$. It is plain that we need $\mathcal{V}$ to be positive so that the density matrix remains positive under time evolution. We additionally need complete positivity because if our open system is embedded in a system with some other degrees of freedom that it do not evolve, the combined system density matrix must also be a valid density matrix. Such a system would evolve by the map $\mathcal{V} \otimes \mathbb{1}$, and thus this map must also be positive. It is surprising at first that complete positivity and positivity are distinct, but there are actually pretty simple examples to see how this happens. Let us consider the standard example. Consider a system of

two spin-1/2 particles and the wavefunction:

$$|\psi\rangle = \frac{|+-\rangle + |-+\rangle}{\sqrt{2}}. \quad (9.6.130)$$

We will represent wavefunctions and operators as explicit vectors as:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |++\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |+-\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |-+\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad |--\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (9.6.131)$$

The resulting density matrix for this system is:

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2} \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right) \quad (9.6.132)$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (9.6.133)$$

Now consider the transpose only of the first particle. Suppose $\hat{A}$ is nonnegative. For any $|\phi\rangle$:

$$0 \leq \langle\phi|\hat{A}|\phi\rangle = \langle\phi^*|\hat{A}^T|\phi^*\rangle. \quad (9.6.134)$$

Because this is true for any $|\phi\rangle$ and the complex conjugate is invertible (by just conjugating again), we have equivalently that for all $|\phi\rangle$:

$$\langle\phi|\hat{A}^T|\phi\rangle \geq 0. \quad (9.6.135)$$

Therefore the transpose is a positive map. We will now see that it is not completely positive because $T \otimes \mathbb{1}$ is not positive. Acting $T \otimes \mathbb{1}$ on $\hat{\rho}$ we have:

$$(T \otimes \mathbb{1})\hat{\rho} = \frac{1}{2} \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right) \quad (9.6.136)$$

$$= \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (9.6.137)$$

This operator has $-\frac{1}{2}$ as an eigenvalue (under the eigenvector $\frac{|++\rangle - |--\rangle}{\sqrt{2}}$) and so it isn't positive. Because of these, the transpose is not completely positive. This establishes clearly why we need to assume the map $\mathcal{V}$ be a proper CPTP map.

Okay, so $\mathcal{V}$ must be a linear CPTP map. We will now find the general form of such a map. Consider an operator $\hat{V}$. Plainly, the map $\mathcal{V}(\hat{\rho}) = \hat{V}\hat{\rho}\hat{V}^\dagger$ is positive. We can see this because for any $|\psi\rangle$ we can define the vector $|\phi\rangle = \hat{V}^\dagger|\psi\rangle$ and thus have that for all $|\psi\rangle$:

$$\langle\psi|\mathcal{V}(\hat{\rho})|\psi\rangle = \langle\psi|\hat{V}\hat{\rho}\hat{V}^\dagger|\psi\rangle = \langle\phi|\hat{\rho}|\phi\rangle \geq 0 \quad (9.6.138)$$

by the nonnegativity of the density matrix. It is also true that an $\mathcal{V}$ of this form is completely positive. We can see this as the map $\mathcal{V} \otimes \mathbb{1}$ can be written on a tensor product space simply as:

$$(\mathcal{V} \otimes \mathbb{1})\hat{\rho} = (\hat{V} \otimes \mathbb{1})\hat{\rho}(\hat{V}^\dagger \otimes \mathbb{1}) \quad (9.6.139)$$

which is also of the same form as $\mathcal{V}$ with $\hat{V}$ replaced by $\hat{V} \otimes \mathbb{1}$. While every map of this form is completely positive, not every completely positive map takes this form.

Suppose the Hilbert space $\mathbb{H}$ for our system has dimension d and let $|n\rangle$ be an arbitrary orthonormal basis of $\mathbb{H}$. For helping with calculation, we introduce a second ancillary Hilbert space $\mathbb{H}_A$ of the same dimension with arbitrary orthonormal basis $|n_A\rangle$. Now define the vector $|\psi\rangle$:

$$|\psi\rangle = \sum_n |n\rangle \otimes |n_A\rangle. \quad (9.6.140)$$

Of course, $|\psi\rangle\langle\psi|$ is a positive operator, because that form is positive for any nonzero vector. If $\mathcal{V}$ is a completely positive map acting on our system, then it must be a positive map acting on the combined system plus ancillary system when we lift it to act on the combined system as:

$$\mathcal{V}' = \mathcal{V} \otimes \mathbb{1}_A. \quad (9.6.141)$$

We can immediately compute:

$$\mathcal{V}'(|\psi\rangle\langle\psi|) = \sum_{mn} \mathcal{V}(|m\rangle\langle n|) \otimes |m_A\rangle\langle n_A| \quad (9.6.142)$$

$$\implies \mathcal{V}(|m\rangle\langle n|) = \langle m_A | \mathcal{V}'(|\psi\rangle\langle\psi|) | n_A \rangle. \quad (9.6.143)$$

Therefore, we can recover how $\mathcal{V}$ acts on our original system solely from the matrix elements of how $\mathcal{V}'$ acts on $|\psi\rangle$. Because $\mathcal{V}'$ is positive, the operator $\mathcal{V}'(|\psi\rangle\langle\psi|)$ is nonnegative and thus can be diagonalized with an orthonormal basis of eigenvectors and nonnegative eigenvalues. That is, there exists an orthonormal basis $|\ell_V\rangle$ so that for some nonnegative coefficients a_ℓ :

$$\mathcal{V}'(|\psi\rangle\langle\psi|) = \sum_{\ell} a_{\ell} |\ell_V\rangle\langle\ell_V|. \quad (9.6.144)$$

If for a given ℓ the coefficient a_{ℓ} is nonzero, define the (unnormalized) vector:

$$|v_{\ell}\rangle = \sqrt{a_{\ell}} |\ell_V\rangle. \quad (9.6.145)$$

Then, we have that there exist vectors $|v_{\ell}\rangle$ so that $\mathcal{V}'(|\psi\rangle\langle\psi|)$ can be written as:

$$\mathcal{V}'(|\psi\rangle\langle\psi|) = \sum_{\ell} |v_{\ell}\rangle\langle v_{\ell}|. \quad (9.6.146)$$

Each vector $|v_{\ell}\rangle$ can be decomposed into the basis $|m\rangle \otimes |n_A\rangle$ with some coefficients:

$$|v_{\ell}\rangle = \sum_{mn} V_{\ell mn} |m\rangle \otimes |n_A\rangle. \quad (9.6.147)$$

From these coefficients we define the operators $\hat{V}_{\ell}$:

$$\hat{V}_{\ell} = \sum_{mn} V_{\ell mn} |m\rangle\langle n|. \quad (9.6.148)$$

From this definition, it immediately follows that:

$$(\hat{V}_{\ell} \otimes \mathbb{1}_A) |\psi\rangle = |v_{\ell}\rangle. \quad (9.6.149)$$

And from this we have:

$$\langle n_A | v_{\ell} \rangle = \hat{V}_{\ell} |n\rangle. \quad (9.6.150)$$

Now by combining (9.6.143), (9.6.146), and (9.6.150):

$$\mathcal{V}(|m\rangle\langle n|) = \sum_{\ell} \langle m_A | v_{\ell} \rangle \langle v_{\ell} | n_A \rangle = \sum_{\ell} \hat{V}_{\ell} |m\rangle\langle n| \hat{V}_{\ell}^{\dagger}. \quad (9.6.151)$$

Any operator $\hat{A}$ on our open system can be decomposed into components A_{mn} as:

$$A_{mn} = \langle m | \hat{A} | n \rangle \quad (9.6.152)$$

$$\implies \hat{A} = \sum_{mn} A_{mn} |m\rangle\langle n|. \quad (9.6.153)$$

Then, using the linearity of $\mathcal{V}$:

$$\mathcal{V}(\hat{A}) = \sum_{\ell} \hat{V}_{\ell} \hat{A} \hat{V}_{\ell}^{\dagger}. \quad (9.6.154)$$

So, any completely positive linear map can be written in this form. Similarly, anything of this form is plainly completely positive because each term in the sum is. Thus, we have Choi's theorem: a linear map is completely positive if and only if it takes the form of (9.6.154) for some operators $\hat{V}_{\ell}$.

Now that we understand completely positive maps, let us see how to enforce trace preservation upon them. Suppose $\mathcal{V}$ is a completely positive map and we have expressed it in the form of (9.6.154). In order for it to be trace preserving, we require that for any $\hat{A}$:

$$\text{Tr}(\mathcal{V}(\hat{A})) = \text{Tr}(\hat{A}). \quad (9.6.155)$$

Consider $\hat{A} = |m\rangle\langle n|$. Then, simplifying both sides while using (9.6.154) yields:

$$\langle n | \sum_{\ell} \hat{V}_{\ell}^{\dagger} \hat{V}_{\ell} | m \rangle = \delta_{mn}. \quad (9.6.156)$$

If we now multiply $|n\rangle\langle m|$ onto both sides and sum over m and n we find:

$$\sum_{\ell} \hat{V}_{\ell}^{\dagger} \hat{V}_{\ell} = \mathbb{1}. \quad (9.6.157)$$

Thus the $\hat{V}_{\ell}$ operators must satisfy this in order for the map to be trace preserving. Further, if they do satisfy this the trace is in fact preserved by using the cyclicity of the trace:

$$\text{Tr}(\mathcal{V}(\hat{A})) = \sum_{\ell} \text{Tr}(\hat{V}_{\ell}^{\dagger} \hat{V}_{\ell} \hat{A}) = \text{Tr}(\hat{A}). \quad (9.6.158)$$

So, we have the Choi-Krauss theorem: a map $\mathcal{V}$ is linear completely positive trace preserving if and only if it can be put into the form:

$$\mathcal{V}(\hat{A}) = \sum_{\ell} \hat{V}_{\ell} \hat{A} \hat{V}_{\ell}^{\dagger} \quad (9.6.159)$$

for some operators $\hat{V}_{\ell}$, called the Krauss operators of the map, which satisfy:

$$\sum_{\ell} \hat{V}_{\ell}^{\dagger} \hat{V}_{\ell} = \mathbb{1}. \quad (9.6.160)$$

Returning to (9.6.127), by assuming our open quantum system has a closed linear equation of motion, it must be the case that for some operators $\hat{V}_{\ell}(t, t_0)$:

$$\hat{\rho}(t) = \sum_{\ell} \hat{V}_{\ell}(t, t_0) \hat{\rho}(t_0) \hat{V}_{\ell}^{\dagger}(t, t_0) \quad (9.6.161)$$

where the $\hat{V}_{\ell}(t, t_0)$ operators satisfy:

$$\sum_{\ell} \hat{V}_{\ell}^{\dagger}(t, t_0) \hat{V}_{\ell}(t, t_0) = \mathbb{1}. \quad (9.6.162)$$

To proceed, we first introduce a useful basis of operators. On a d dimensional Hilbert space, a generic operator has d^2 independent matrix elements and the set of such operators forms a vector space (of dimension d^2). We introduce the inner product on operators $\hat{A}, \hat{B}$ by:

$$(\hat{A}, \hat{B}) = \text{Tr}(\hat{A}^{\dagger} \hat{B}). \quad (9.6.163)$$

This inner product satisfies all of the usual conditions on the definition of an inner product. Let $\hat{f}_{\ell}$ be a list of d^2 operators which are orthonormal under this inner product:

$$\text{Tr}(\hat{f}_k^{\dagger} \hat{f}_{\ell}) = \delta_{k\ell}. \quad (9.6.164)$$

Thus, this set of d^2 operators form an orthonormal basis of the vector space of operators on our Hilbert space. So, there must exist coefficients $\alpha_{\ell k}(t, t_0)$ so that:

$$\hat{V}_{\ell}(t, t_0) = \sum_k \alpha_{\ell k}(t, t_0) \hat{f}_k. \quad (9.6.165)$$

Returning this form to (9.6.161), we have that:

$$\hat{\rho}(t) = \sum_{kk'} \left(\sum_{\ell} \alpha_{\ell k}(t, t_0) \alpha_{\ell k'}^*(t, t_0) \right) \hat{f}_k \hat{\rho}(t_0) \hat{f}_{k'}^{\dagger} = \sum_{k\ell} \beta_{k\ell}(t, t_0) \hat{f}_k \hat{\rho}(t_0) \hat{f}_{\ell}^{\dagger} \quad (9.6.166)$$

where we have introduced the coefficients:

$$\beta_{kk'}(t, t_0) = \sum_{\ell} \alpha_{\ell k}(t, t_0) \alpha_{\ell k'}^*(t, t_0). \quad (9.6.167)$$

Immediately, these coefficients satisfy:

$$\beta_{kk'}^*(t, t_0) = \beta_{k'k}(t, t_0). \quad (9.6.168)$$

We can simplify further by choosing the $\hat{f}_k$ intelligently. We can take by definition one of the $\hat{f}_k$ to be proportional to the identity operator (call it $\hat{f}_0 = \frac{1}{\sqrt{d}} \mathbb{1}$). Then, orthonormality requires all of the other $\hat{f}_k$ to be traceless. So, now write $\hat{F}_k$ for the traceless $\hat{F}_k$ and when the index of $\hat{F}_k$ is summed over understood

that it is covering all of the $\hat{f}_k$ except the term proportional to the identity operator. Expanding in this way, (9.6.166) becomes:

$$\hat{\rho}(t) = \sum_{k\ell} \beta_{k\ell}(t, t_0) \hat{F}_k \hat{\rho}(t_0) \hat{F}_\ell^\dagger + \frac{1}{\sqrt{d}} \sum_k \beta_{k0}(t, t_0) \hat{F}_k \hat{\rho}(t_0) + \frac{1}{\sqrt{d}} \sum_k \beta_{0k}(t, t_0) \hat{\rho}(t_0) \hat{F}_k^\dagger + \frac{1}{d} \beta_{00}(t, t_0) \hat{\rho}(t_0). \quad (9.6.169)$$

The limit $t_0 \rightarrow t$ gives that necessarily:

$$\beta_{k\ell}(t, t) = 0 \quad (k \text{ or } \ell \text{ nonzero}), \quad \beta_{00}(t, t) = d. \quad (9.6.170)$$

Now differentiate both sides of (9.6.169) with respect to t , multiply by $i\hbar$, and evaluate in the limit $t_0 \rightarrow t$. After doing so:

$$i\hbar \dot{\hat{\rho}}(t) = \sum_{k\ell} ig_{k\ell}(t) \hat{F}_k \hat{\rho}(t) \hat{F}_\ell^\dagger + \frac{1}{\sqrt{d}} \sum_k i_k(t) \hat{F}_k \hat{\rho}(t) - \frac{1}{\sqrt{d}} \sum_k i_k^*(t) \hat{\rho}(t) \hat{F}_k^\dagger + \frac{i}{d} h(t) \hat{\rho}(t) \quad (9.6.171)$$

where we have introduced the coefficients:

$$g_{k\ell}(t) = \hbar \left. \frac{\partial \beta_{k\ell}(t', t)}{\partial t'} \right|_{t'=t}, \quad i_k(t) = i\hbar \left. \frac{\partial \beta_{k0}(t', t)}{\partial t'} \right|_{t'=t}, \quad h(t) = \hbar \left. \frac{\partial \beta_{00}(t', t)}{\partial t'} \right|_{t'=t} \quad (9.6.172)$$

and in the definition of $g_{k\ell}$ both k and ℓ are nonzero. Yes, we intentionally only included the i in the definition of $i_k(t)$. Let $\hat{F}(t)$ be defined by:

$$\hat{F}(t) = \frac{1}{\sqrt{d}} \sum_k i_k(t) \hat{F}_k. \quad (9.6.173)$$

Then:

$$i\hbar \dot{\hat{\rho}}(t) = \sum_{k\ell} ig_{k\ell}(t) \hat{F}_k \hat{\rho}(t) \hat{F}_\ell^\dagger + \hat{F}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{F}^\dagger(t) + \frac{i}{d} h(t) \hat{\rho}(t) \quad (9.6.174)$$

Decompose $\hat{F}(t)$ into its self-adjoint and anti-self-adjoint parts:

$$\hat{H}(t) = \frac{\hat{F}(t) + \hat{F}^\dagger(t)}{2}, \quad \hat{G}(t) = \frac{\hat{F}(t) - \hat{F}^\dagger(t)}{2i} \implies \hat{F}(t) = \hat{H}(t) + i\hat{G}(t) \quad (9.6.175)$$

where $\hat{G}(t)$ and $\hat{H}(t)$ are now automatically self-adjoint. From these, we can put (9.6.174) into the form:

$$i\hbar \dot{\hat{\rho}}(t) = [\hat{H}(t), \hat{\rho}(t)] + \sum_{k\ell} ig_{k\ell}(t) \hat{F}_k \hat{\rho}(t) \hat{F}_\ell^\dagger + i\hat{G}(t) \hat{\rho}(t) + i\hat{\rho}(t) \hat{G}(t) + \frac{i}{d} h(t) \hat{\rho}(t). \quad (9.6.176)$$

We haven't yet imposed that our time evolution should be trace preserving. Doing so requires here that the trace of both sides is 0, so that $\hat{\rho}(t)$ maintains a constant trace of 1. Taking the trace and simplifying gives:

$$\text{Tr} \left(\hat{\rho} \left(2\hat{G} + \frac{h}{d} \mathbb{1} + \sum_{k\ell} g_{k\ell} \hat{F}_\ell^\dagger \hat{F}_k \right) \right) \stackrel{!}{=} 0 \quad (9.6.177)$$

As this must hold for any density matrix, we must have:

$$\hat{G}(t) = -\frac{h(t)}{2d} \mathbb{1} - \frac{1}{2} \sum_{k\ell} g_{k\ell}(t) \hat{F}_\ell^\dagger \hat{F}_k. \quad (9.6.178)$$

Using this to simplify (9.6.176), we have:

$$i\hbar \frac{d\hat{\rho}(t)}{dt} = [\hat{H}(t), \hat{\rho}(t)] + i \sum_{k\ell} g_{k\ell}(t) (\hat{F}_k \hat{\rho}(t) \hat{F}_\ell^\dagger - \text{Sym}(\hat{F}_\ell^\dagger \hat{F}_k, \hat{\rho}(t))). \quad (9.6.179)$$

By using the definition of $g_{k\ell}(t)$, we can continue to simplify. Because of (9.6.168), it follows from the definition of $g_{k\ell}(t)$ that:

$$g_{\ell k}^*(t) = g_{k\ell}(t). \quad (9.6.180)$$

Therefore, if the $g_{k\ell}(t)$ coefficients are viewed as the entries of a matrix then that matrix is self-adjoint. Consequently, at each t it can be diagonalized by an orthonormal basis of eigenvectors $\iota_b(t)$ (with b labeling which eigenvector is considered) and it has real eigenvalues $\lambda_b(t)$. We refer to the components of the eigenvector ι_b by $(\iota_b)_k$. So, $g_{k\ell}(t)$ can in fact be written in the form:

$$g_{k\ell}(t) = \sum_b \lambda_b(t) (\iota_b(t))_k (\iota_b(t))_\ell^*. \quad (9.6.181)$$

We can go even further using the properties of $\beta_{k\ell}(t, t_0)$. Consider a list of complex coefficients ϕ_k with k taking the same index range as the indices of $\beta_{k\ell}$ (except for the value 0). Then, by (9.6.167):

$$\sum_{kk'} \beta_{kk'}(t, t_0) \phi_k^* \phi_{k'} = \sum_{\ell} \left| \sum_k \alpha_{\ell k}(t, t_0) \phi_k \right|^2 \geq 0. \quad (9.6.182)$$

So, viewed as the entries of a matrix, the $\beta_{kk'}(t, t_0)$ form a nonnegative matrix. By (9.6.170) at $t_0 = t$ we have $\beta_{kk'} = 0$ and so by the definition of $g_{k\ell}$:

$$g_{k\ell}(t) = \lim_{\varepsilon \rightarrow 0} \frac{\beta_{k\ell}(t + \varepsilon, t)}{\varepsilon}. \quad (9.6.183)$$

The right hand side forms the entries of a nonnegative matrix for all ε and therefore the $g_{k\ell}(t)$ form the entries of a nonnegative matrix. Because of this, the eigenvalues $\lambda_b(t)$ are nonnegative allowing us to unambiguously take their square root along its principle branch. Now define the “Jump Operators” $\hat{L}_k(t)$ by:

$$\hat{L}_k(t) = \sum_{\ell} \sqrt{\lambda_k(t)} (\iota_k(t))_{\ell} \hat{F}_{\ell}. \quad (9.6.184)$$

The jump operators are automatically orthogonal to each other under the operator inner product by using the orthonormality of the $\hat{F}_k$ and the ι_b :

$$\text{Tr}(\hat{L}_{\ell}^{\dagger}(t) \hat{L}_k(t)) = 0 \quad (k \neq \ell). \quad (9.6.185)$$

With these, we can now reexpress (9.6.179) as:

$$i\hbar \frac{d\hat{\rho}(t)}{dt} = [\hat{H}(t), \hat{\rho}(t)] + i \sum_k (\hat{L}_k(t) \hat{\rho}(t) \hat{L}_k^{\dagger}(t) - \text{Sym}(\hat{L}_k^{\dagger}(t) \hat{L}_k(t), \hat{\rho}(t))). \quad (9.6.186)$$

This result is known as the **Lindblad Equation**. Therefore, we see that the most general possible linear closed equation of motion for an open quantum system is given by (9.6.186) with $\hat{H}(t)$ some self-adjoint operator (which we call as always the Hamiltonian operator of the system) and some orthogonal set of traceless operators $\hat{L}_k(t)$ known as the jump operators of the system. All dissipative effects of an open quantum system that can be expressed in a closed equation of motion for the subsystem are determined by whatever the jump operators of the system are.

While the Lindblad equation as derived is general and exact (supposing a linear closed equation of motion exists for our open system), it leaves some important questions unanswered. Should the Hamiltonian operator simply be the free Hamiltonian of the subsystem? (No.) How do you determine what the jump operators should be for the system? (It tells you nothing.) We will now perform a less rigorous analysis that will provide some insight on these questions. Consider a total system with total Hamiltonian operator $\hat{H}_T$ which consists of two interacting subsystems, the first being the open system we care about with free Hamiltonian operator $\hat{H}_0$ and the second being a set of environmental degrees of freedom with free Hamiltonian operator $\hat{H}_E$. The two interact with some interaction term $\hat{H}_1$. So, we write the full Hamiltonian operator as:

$$\hat{H}_T = \hat{H}_0 \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_E + \hat{H}_1 \quad (9.6.187)$$

where as usual we will typically be lazy about the distinction between $\hat{H}_0 \otimes \mathbb{1}$ and $\hat{H}_0$ going forward. We will find later that it is convenient to slightly shift some pieces of $\hat{H}_0$ into $\hat{H}_1$ so for now we will actually use:

$$\hat{H}_T = \hat{H}'_0 \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_E + \hat{H}'_1 \quad (9.6.188)$$

where $\hat{H}'_0$ will differ slightly from $\hat{H}_0$ in a way we will make precise very soon and $\hat{H}'_1$ differs from $\hat{H}_1$ precisely to compensate so that $\hat{H}_T$ is unchanged. The full passive picture density matrix $\hat{\rho}_T(t)$ of the total system then evolves according to the von Neumann equation as:

$$i\hbar \frac{d\hat{\rho}_T(t)}{dt} = [\hat{H}_T, \hat{\rho}_T(t)]. \quad (9.6.189)$$

Let $\hat{U}_T(t)$ be the time evolution operator for the total time evolution:

$$\hat{U}_T(t) = e^{-\frac{i}{\hbar} \hat{H}_T t}. \quad (9.6.190)$$

Then as always the total density matrix depends on time as:

$$\hat{\rho}_T(t) = \hat{U}_T(t) \hat{\rho}_T(0) \hat{U}_T^{\dagger}(t). \quad (9.6.191)$$

For actually performing our analysis it is useful to go instead to the interaction picture and so let $\hat{U}_S(t)$

be the time evolution operator for the subsystem if the interaction is neglected and let $\hat{U}_E(t)$ be the time evolution operator for the environment if the interaction is neglected:

$$\hat{U}_S(t) = e^{-\frac{i}{\hbar}\hat{H}_0't}, \quad \hat{U}_E(t) = e^{-\frac{i}{\hbar}\hat{H}_E't}. \quad (9.6.192)$$

Define $\hat{U}_0(t)$ as the combined system's time evolution operator if the interaction is neglected:

$$\hat{U}_0(t) = \hat{U}_S(t) \otimes \hat{U}_E(t). \quad (9.6.193)$$

The interaction picture density matrix $\hat{\rho}_{TI}(t)$ of the total system is then defined by:

$$\hat{\rho}_{TI}(t) = \hat{U}_0^\dagger(t) \hat{\rho}_T(t) \hat{U}_0(t). \quad (9.6.194)$$

Differentiating this definition and using the von Neumann equation yields:

$$i\hbar \frac{d\hat{\rho}_{TI}}{dt} = \hat{U}_0^\dagger [\hat{H}_1', \hat{\rho}_T] \hat{U}_0. \quad (9.6.195)$$

Define then the interaction picture Hamiltonian operator $\hat{H}_I(t)$:

$$\hat{H}_I(t) = \hat{U}_0^\dagger(t) \hat{H}_1'(t) \hat{U}_0(t). \quad (9.6.196)$$

In terms of this operator, we have the interaction picture von Neumann equation:

$$i\hbar \frac{d\hat{\rho}_{TI}}{dt} = [\hat{H}_I, \hat{\rho}_{TI}]. \quad (9.6.197)$$

As usual, the interaction picture is only useful in-so-far as the interaction terms can be treated with perturbation theory. Exactly integrating the interaction picture von Neumann equation from 0 to t gives:

$$\hat{\rho}_{TI}(t) = \hat{\rho}_T(0) - \frac{i}{\hbar} \int_0^t [\hat{H}_I(t'), \hat{\rho}_{TI}(t')] dt'. \quad (9.6.198)$$

Using this back in the von Neumann equation turns it into:

$$i\hbar \frac{d\hat{\rho}_{TI}}{dt} = [\hat{H}_I(t), \hat{\rho}_T(0)] - \frac{i}{\hbar} \int_0^t [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}_{TI}(t')]] dt'. \quad (9.6.199)$$

Because of the von Neumann equation, $\hat{\rho}_{TI}(t)$ and $\hat{\rho}_{TI}(t')$ differ on the order of $\hat{H}_I$ and so if we now approximate the interaction as small we can approximate $\hat{\rho}_{TI}(t')$ appearing in the integral by $\hat{\rho}_T(0)$:

$$i\hbar \frac{d\hat{\rho}_{TI}}{dt} \approx [\hat{H}_I(t), \hat{\rho}_T(0)] - \frac{i}{\hbar} \int_0^t [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}_T(0)]] dt'. \quad (9.6.200)$$

We don't want an equation of motion for $\hat{\rho}_{TI}$, we want one for the subsystem density matrix. As always, we define the subsystem density matrix $\hat{\rho}(t)$ by tracing over the environmental degrees of freedom:

$$\hat{\rho}(t) = \text{Tr}_E(\hat{\rho}_T(t)). \quad (9.6.201)$$

The interaction picture subsystem density matrix is given by again factoring off its free evolution:

$$\hat{\rho}_I(t) = \hat{U}_S^\dagger(t) \hat{\rho}(t) \hat{U}_S(t). \quad (9.6.202)$$

Cyclicity of the partial trace (which is valid for operators acting only on the traced over degrees of freedom) together with the unitarity of $\hat{U}_E(t)$ allow us to express $\hat{\rho}_I(t)$ nicely in terms of $\hat{\rho}_{TI}(t)$:

$$\hat{\rho}_I(t) = \hat{U}_S^\dagger(t) \text{Tr}_E(\hat{U}_E(t) \hat{U}_E^\dagger(t) \hat{\rho}_T(t)) \hat{U}_S(t) = \text{Tr}_E(\hat{U}_0^\dagger(t) \hat{\rho}_T(t) \hat{U}_0(t)) = \text{Tr}_E(\hat{\rho}_{TI}(t)). \quad (9.6.203)$$

Tracing over (9.6.200) then gives:

$$i\hbar \frac{d\hat{\rho}_I(t)}{dt} \approx \text{Tr}_E([\hat{H}_I(t), \hat{\rho}_T(0)]) - \frac{i}{\hbar} \int_0^t \text{Tr}_E([\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}_T(0)]]) dt'. \quad (9.6.204)$$

In order to proceed further we need to make further reasonable assumptions on the relationship between our open subsystem and its environment and to intelligently represent our interaction term. We assume that at time $t = 0$ they are completely independent and so:

$$\hat{\rho}_T(0) = \hat{\rho}(0) \otimes \hat{\rho}_E(0). \quad (9.6.205)$$

We further assume that at $t = 0$ the environment is in equilibrium so that under free time evolution by the environment Hamiltonian operator it remains stationary:

$$[\hat{H}_E, \hat{\rho}_E(0)] = 0. \quad (9.6.206)$$

The space of operators acting on the subsystem's Hilbert space is itself a vector space. Therefore, we can find a basis of operators $\hat{S}_k$ (not necessarily self-adjoint) so that any operator on the subsystem's Hilbert space

can be written as a linear combination of these. Let $|n_E\rangle$ be an orthonormal basis for the environment's Hilbert space. Then, the combination $\langle m_E|\hat{H}_1|n_E\rangle$ is an operator on the subsystem's Hilbert space and thus can be written, for some coefficients h_{kmn} as a linear combination of the $\hat{S}_k$:

$$\langle m_E|\hat{H}_1|n_E\rangle = \sum_k h_{kmn} \hat{S}_k. \quad (9.6.207)$$

By inserting complete sets of states on the environment, this allows us to write the full $\hat{H}_1$ as:

$$\hat{H}_1 = \sum_{kmn} \hat{h}_{kmn} \hat{S}_k \otimes |m_E\rangle\langle n_E|. \quad (9.6.208)$$

So, define the operators $\hat{E}_k$ on the environment's Hilbert space as:

$$\hat{E}_k = \sum_{mn} h_{kmn} |m_E\rangle\langle n_E|. \quad (9.6.209)$$

With these, $\hat{H}_1$ now takes the form:

$$\hat{H}_1 = \sum_k \hat{S}_k \otimes \hat{E}_k. \quad (9.6.210)$$

It is now time to specify how $\hat{H}'_0$ and $\hat{H}_0$ are related (and consequently how $\hat{H}'_1$ and $\hat{H}_1$ are related). $\hat{H}'_0 - \hat{H}_0$ is some operator on the subsystem Hilbert space, and so there exist some constants c_k so that:

$$\hat{H}'_0 = \hat{H}_0 + \sum_k c_k \hat{S}_k. \quad (9.6.211)$$

To compensate the inclusion of this difference, we need:

$$\hat{H}'_1 = \hat{H}_1 - \sum_k c_k \hat{S}_k \quad (9.6.212)$$

so that the total Hamiltonian operator is unchanged. In terms of this decomposition, the first term on the right hand side of (9.6.204) becomes:

$$\text{Tr}_E([\hat{H}_I(t), \hat{\rho}_T(0)]) = \sum_k [\hat{U}_S^\dagger(t) \hat{S}_k \hat{U}_S(t), \hat{\rho}_S(0)] \text{Tr}_E((\hat{E}_k - c_k \mathbb{1}) \hat{U}_E(t) \hat{\rho}_E(0) \hat{U}_E^\dagger(t)) \quad (9.6.213)$$

Because of (9.6.206):

$$\hat{U}_E(t) \hat{\rho}_E(0) \hat{U}_E^\dagger(t) = \hat{\rho}_E(0) \quad (9.6.214)$$

and so:

$$\text{Tr}_E([\hat{H}_I(t), \hat{\rho}_T(0)]) = \sum_k [\hat{U}_S^\dagger(t) \hat{S}_k \hat{U}_S(t), \hat{\rho}_S(0)] (\text{Tr}_E(\hat{E}_k \hat{\rho}_E(0)) - c_k). \quad (9.6.215)$$

We now define $\hat{H}'_0$ by choosing the constants c_k as:

$$c_k = \text{Tr}_E(\hat{E}_k \hat{\rho}_E(0)). \quad (9.6.216)$$

With this separation:

$$\text{Tr}_E([\hat{H}_I(t), \hat{\rho}_T(0)]) = 0. \quad (9.6.217)$$

The reason $\hat{H}'_0$ is useful over $\hat{H}_0$ is that we want to approximate the interaction term $\hat{H}_1$ as having a small effect for perturbation theory; our choice of c_k is precisely such that the expectation value of $\hat{H}_1$ is 0 in the initial state which prevents a constant accumulating drift that would happen if the c_k were not included. It just helps perturbation theory be more accurate. As the subsystem and the environment interact, they will necessarily develop correlations and the total density matrix will no longer cleanly factor into the density matrix of the system and the density matrix of the environment. However, if we assume the environment is macroscopically large compared to the subsystem (containing many degrees of freedom), in statistical mechanical equilibrium, and very difficult to perturb from that equilibrium (due to its macroscopic scale), then we can approximate the total density matrix as factoring:

$$\hat{\rho}_{TI}(t) \approx \hat{\rho}_I(t) \otimes \hat{\rho}_E(0) \quad (9.6.218)$$

where $\hat{\rho}_E$ always remains at its $t = 0$ value because of the equilibrium of the environment. This intentional discarding of correlations is precisely the information loss necessary to explain the change in apparent entropy

during the system's evolution. With these considerations, (9.6.204) now becomes:

$$i\hbar \frac{d\hat{\rho}_I(t)}{dt} \approx -\frac{i}{\hbar} \int_0^t \text{Tr}_E([\hat{H}_I(t), [\hat{H}_I(t-t'), \hat{\rho}_I(t) \otimes \hat{\rho}_E(0)]] dt' \quad (9.6.219)$$

where I have redefined the integration variable from t' to $t-t'$ for later convenience.

So far we have allowed the basis $\hat{S}_k$ of subsystem operators to be generic. It is now time to make an intelligent choice for them. $\hat{H}'_0$ is a self-adjoint operator on the subsystem's Hilbert space. Consider two operators $\hat{A}$ and $\hat{B}$ (not necessarily self-adjoint) on that same Hilbert space. A one line calculation shows:

$$[\hat{H}'_0, \hat{A}]^\dagger = [\hat{A}^\dagger, \hat{H}'_0]. \quad (9.6.220)$$

Immediately then it follows from the cyclicity of the trace that:

$$\text{Tr}(\hat{B}^\dagger [\hat{H}'_0, \hat{A}]) = \text{Tr}([\hat{H}'_0, \hat{B}]^\dagger \hat{A}). \quad (9.6.221)$$

The space of operators on the subsystem's Hilbert space is itself a vector space and itself becomes a Hilbert space when equipped with the inner product defined by (9.6.163). The map $[\hat{H}'_0, \cdot]$ is then a linear operator on that Hilbert space and this calculation shows that it is in fact a self-adjoint operator on that Hilbert space. Therefore, it can be diagonalized by an orthonormal basis of eigenvectors (which are now eigenoperators) with real eigenvalues. That is, there exists a basis $\hat{S}_k$ for the vector space of operators on the subsystem's Hilbert space so that:

$$[\hat{H}'_0, \hat{S}_k] = -\hbar\omega_k \hat{S}_k \quad (9.6.222)$$

with real eigenvalues $-\hbar\omega_k$. Because $\hat{H}'_0$ acts so simply on this basis, we can explicitly compute $\hat{U}_S^\dagger \hat{S}_k \hat{U}_S$ as:

$$\frac{d}{dt}(\hat{U}_S^\dagger \hat{S}_k \hat{U}_S) = \frac{i}{\hbar} \hat{U}_S^\dagger [\hat{H}'_0, \hat{S}_k] \hat{U}_S = -i\omega_k \hat{U}_S^\dagger \hat{S}_k \hat{U}_S \implies \hat{U}_S^\dagger \hat{S}_k \hat{U}_S = e^{-i\omega_k t} \hat{S}_k. \quad (9.6.223)$$

Now the interaction Hamiltonian operator can be computed quite simply as:

$$\hat{H}_I(t) = \sum_k e^{-i\omega_k t} \hat{S}_k \otimes (\hat{U}_E^\dagger \hat{E}_k \hat{U}_E - \text{Tr}(\hat{\rho}_E(0) \hat{E}_k) \mathbb{1}) = \sum_k e^{i\omega_k t} \hat{S}_k^\dagger \otimes (\hat{U}_E^\dagger \hat{E}_k^\dagger \hat{U}_E - \text{Tr}_E(\hat{\rho}_E(0) \hat{E}_k^\dagger) \mathbb{1}) \quad (9.6.224)$$

where the second equation follows because $\hat{H}_I(t)$ is self-adjoint. We now expand out both commutators in (9.6.219) and use the expression for $\hat{H}_I$ in terms of $\hat{S}_k^\dagger$ for terms which (cyclically under the trace) are next to $\hat{\rho}_E(0)$ and the corresponding expression in terms of $\hat{S}_k$ for terms which (cyclically under the trace) are not next to $\hat{\rho}_E(0)$. Doing so yields:

$$\int_0^t \text{Tr}_E([\hat{H}_I(t), [\hat{H}_I(t-t'), \hat{\rho}_I(t) \otimes \hat{\rho}_E(0)]] dt' = \sum_{k\ell} e^{i(\omega_k - \omega_\ell)t} \left(\gamma_{k\ell}(t, \omega_\ell) [\hat{S}_k^\dagger, \hat{S}_\ell \hat{\rho}_I(t)] + \gamma_{\ell k}^*(t, \omega_\ell) [\hat{\rho}_I(t) \hat{S}_k^\dagger, \hat{S}_\ell] \right) \quad (9.6.225)$$

where we have defined the $\gamma_{k\ell}(t, \omega)$ coefficients by:

$$\gamma_{k\ell}(t, \omega) = \int_0^t e^{i\omega t'} \text{Tr}_E \left(\hat{\rho}_E(0) (\hat{U}_E^\dagger(t) \hat{E}_k^\dagger \hat{U}_E(t) - \text{Tr}_E(\hat{\rho}_E(0) \hat{E}_k^\dagger) \mathbb{1}) (\hat{U}_E^\dagger(t-t') \hat{E}_\ell \hat{U}_E(t-t') - \text{Tr}_E(\hat{\rho}_E(0) \hat{E}_\ell) \mathbb{1}) \right) dt'. \quad (9.6.226)$$

We still have more approximations to make. We now approximate that in (9.6.225) for $\omega_k \neq \omega_\ell$ the phase $e^{i(\omega_k - \omega_\ell)t}$ oscillates very rapidly on the time scale we are sensitive to. This is justified by considering that we are looking at the evolution of the interaction picture $\hat{\rho}_I(t)$, which should evolve on the time scale of the interaction, which being with a macroscopic environment we expect to be larger than the intrinsic time scales of the subsystem (which are contained in ω_k, ω_ℓ). If this phase oscillates much more rapidly than anything else in this equation, we can time average it to vanish for $\omega_k \neq \omega_\ell$, giving us:

$$\int_0^t \text{Tr}_E([\hat{H}_I(t), [\hat{H}_I(t-t'), \hat{\rho}_I(t) \otimes \hat{\rho}_E(0)]] dt' \approx \sum_{\substack{k\ell \\ \omega_k = \omega_\ell}} \left(\gamma_{k\ell}(t, \omega_\ell) [\hat{S}_k^\dagger, \hat{S}_\ell \hat{\rho}_I(t)] + \gamma_{\ell k}^*(t, \omega_\ell) [\hat{\rho}_I(t) \hat{S}_k^\dagger, \hat{S}_\ell] \right). \quad (9.6.227)$$

By expanding fully the definition of $\gamma_{k\ell}(t, \omega)$ it becomes:

$$\gamma_{k\ell}(t, \omega) = \int_0^t e^{i\omega t'} \text{Tr}_E(\hat{\rho}_E(0) \hat{U}_E^\dagger(t') (\hat{E}_k^\dagger - c_k^* \mathbb{1}) \hat{U}_E(t') (\hat{E}_\ell - c_\ell \mathbb{1})) dt'. \quad (9.6.228)$$

The integrand here is essentially the operator correlation of $\hat{E}_\ell \mathbb{1}$ at the initial time and $\hat{E}_k^\dagger$ at the time t' (evolved in the active picture). If the environment is very macroscopic, its degrees of freedom will quickly become uncorrelated with each other and so we approximate the above integrand as falling to 0 very quickly for large t' . Because of this, we can effectively extend the upper integration limit to ∞ provided t is not extremely small. That is, we approximate:

$$\gamma_{k\ell}(t, \omega) \approx \lim_{t \rightarrow \infty} \gamma_{k\ell}(t, \omega) = \int_0^\infty e^{i\omega t'} \text{Tr}_E(\hat{\rho}_E(0) \hat{U}_E^\dagger(t') (\hat{E}_k^\dagger - c_k^* \mathbb{1}) \hat{U}_E(t') (\hat{E}_\ell - c_\ell \mathbb{1})) dt'. \quad (9.6.229)$$

We now break these coefficients into self-adjoint and anti-self-adjoint parts (viewed as the components of a matrix) as:

$$\Gamma_{k\ell}(\omega) = \lim_{t \rightarrow \infty} \frac{\gamma_{k\ell}(t, \omega) + \gamma_{\ell k}^*(t, \omega)}{\hbar}, \quad \pi_{k\ell}(\omega) = \lim_{t \rightarrow \infty} \frac{\gamma_{k\ell}(t, \omega) - \gamma_{\ell k}^*(t, \omega)}{2i\hbar}. \quad (9.6.230)$$

In terms of this decomposition, returning everything to (9.6.219) gives:

$$i\hbar \frac{d\hat{\rho}_I(t)}{dt} \approx \sum_{\substack{k\ell \\ \omega_k = \omega_\ell}} \pi_{k\ell}(\omega_k) [\hat{S}_k^\dagger \hat{S}_\ell, \hat{\rho}_I] + i \sum_{\substack{k\ell \\ \omega_k = \omega_\ell}} \Gamma_{k\ell}(\omega_k) (\hat{S}_\ell \hat{\rho}_I \hat{S}_k^\dagger - \text{Sym}(\hat{S}_k^\dagger \hat{S}_\ell, \hat{\rho}_I)). \quad (9.6.231)$$

Now this is looking like the Lindblad equation! Because the matrix formed by the components $\Gamma_{k\ell}$ is self-adjoint, we can diagonalize it by some orthonormal basis of eigenvectors ι_b (with components $(\iota_b)_k$) and eigenvalues λ_b :

$$\Gamma_{k\ell}(\omega) = \sum_b \lambda_b(\omega) (\iota_b(\omega))_k (\iota_b(\omega))_\ell^*. \quad (9.6.232)$$

Using the explicit definition of $\Gamma_{k\ell}(\omega)$ and simplifying gives that it is precisely:

$$\Gamma_{k\ell}(\omega) = \frac{1}{\hbar} \int_{-\infty}^\infty e^{i\omega t} \text{Tr}_E(\hat{\rho}_E(0) \hat{U}_E^\dagger(t) (\hat{E}_k^\dagger - c_k^* \mathbb{1}) \hat{U}_E(t) (\hat{E}_\ell - c_\ell \mathbb{1})) dt. \quad (9.6.233)$$

Let $|n_E\rangle$ be an orthonormal simultaneous eigenbasis of $\hat{H}_E$ and $\hat{\rho}_E(0)$ (which is possible because they commute). In this basis we have;

$$\hat{\rho}_E(0) = \sum_n p_n |n_E\rangle \langle n_E|, \quad \hat{H}_E = \sum_n E_n |n_E\rangle \langle n_E| \quad (9.6.234)$$

where p_n and E_n are real numbers, $p_n \geq 0$, and $\sum_n p_n = 1$. If we now contract this with some components ϕ_k as we would for a matrix summary we find (after inserting complete sets of states):

$$\sum_{k\ell} \Gamma_{k\ell} \phi_k^* \phi_\ell = \sum_{mn} \hbar p_n \int_{-\infty}^\infty e^{i(\omega + \frac{E_n - E_m}{\hbar})t} dt \left| \sum_k \langle m | (\hat{E}_k - c_k \mathbb{1}) | n \rangle \phi^k \right|^2 \quad (9.6.235)$$

$$= \sum_{mn} 2\pi \delta(\hbar\omega + E_n - E_m) \left| \sum_k \langle m | (\hat{E}_k - c_k \mathbb{1}) | n \rangle \phi^k \right|^2 \geq 0. \quad (9.6.236)$$

Thus, $\Gamma_{k\ell}$ forms a nonnegative matrix and its eigenvalues λ_b are consequently nonnegative. Define then the jump operators:

$$\hat{L}_b = \sum_k \sqrt{\lambda_b(\omega_k)} (\iota_b(\omega_k))_k \hat{S}_k. \quad (9.6.237)$$

In terms of these, (9.6.231) becomes:

$$i\hbar \frac{d\hat{\rho}_I(t)}{dt} \approx \sum_{\substack{k\ell \\ \omega_k = \omega_\ell}} \pi_{k\ell}(\omega_k) [\hat{S}_k^\dagger \hat{S}_\ell, \hat{\rho}_I] + i \sum_k (\hat{L}_k \hat{\rho}_I(t) \hat{L}_k^\dagger - \text{Sym}(\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}_I(t))). \quad (9.6.238)$$

Now this is really looking like the Lindblad equation. All we have to do to finish it is return to the passive picture. Doing so simply gives:

$$i\hbar \frac{d\hat{\rho}(t)}{dt} \approx [\hat{H}, \hat{\rho}(t)] + i \sum_k (\hat{L}_k \hat{\rho}(t) \hat{L}_k^\dagger - \text{Sym}(\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}(t))) \quad (9.6.239)$$

where we have defined the effective subsystem Hamiltonian as:

$$\hat{H} = \hat{H}_0 + \sum_k \text{Tr}_E(\hat{E}_k \hat{\rho}_E(0)) \hat{S}_k + \sum_{\substack{k\ell \\ \omega_k = \omega_\ell}} \pi_{k\ell}(\omega_k) [\hat{S}_k^\dagger \hat{S}_\ell, \hat{\rho}_I]. \quad (9.6.240)$$

We have recovered the Lindblad equation through a series of (often reasonable) approximations of a full theory! Because of this, by following the chain of definitions for all the quantities appearing here in the Lindblad equation it is possible to go from a full theory description to this reduced effective description while being able to calculate all of the ingredients of the final equation. This has a significant advantage over just asserting (9.6.186) directly as it gives no assistance in selecting $\hat{H}$ or the jump operators.

9.7 Summary and Additional Reading

Chapter 10

Quantum Field Theory

I insist upon the view that all is waves.
– Erwin Schrödinger [\[104\]](#)

The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.
– Sidney Coleman [\[16\]](#)

10.1 Summary and Additional Reading

Chapter 11

Gauge Theory

The world is a dynamic mess of jiggling things.

– Richard Feynman [27]

From time immemorial, man has desired to comprehend the complexity of nature in terms of as few elementary concepts as possible. Among his quests - in Feynman's words - has been the one for "wheels within wheels" - the task of natural philosophy being to discover the innermost wheels if any such exist. A second quest has concerned itself with the fundamental forces which make the wheels go round and enmesh with one another. The greatness of gauge ideas - of gauge field theories - is that they reduce these two quests to just one; elementary particles (described by relativistic quantum fields) are representations of certain charge operators, corresponding to gravitational mass, spin, flavor, color, electric charge and the like, while the fundamental forces are the forces of attraction or repulsion between these same charges. A third quest seeks for a unification between the charges (and thus of the forces) by searching for a single entity, of which the various charges are components in the sense that they can be transformed one into the other.

– Abdus Salam [100]

Chapter 12

The Standard Model

The creation of Physics is the shared heritage of all mankind. East and West, North and South have equally participated in it.

– Abdus Salam [99]

Why is the muon, some dumb particle, 200 times heavier than the electron? Why is the proton about 2,000 times heavier than the electron? Why is the electric charge of the electron what it is? Why are there six quarks in nature? Why not seven or eleven or five? There are many, many “why” questions. Also a number of “how” questions. What is the mechanism that causes the weak interactions to be weak and the electromagnetic interactions not weak? All kinds of questions remain.

– Sheldon Glashow [36]

The years since the mid-1970s have been the most frustrating in the history of particle physics. We are paying the price of our own success: theory has advanced so far that further progress will require the study of processes at energies far beyond the reach of existing facilities.

– Steven Weinberg [126]

12.1 Summary and Additional Reading

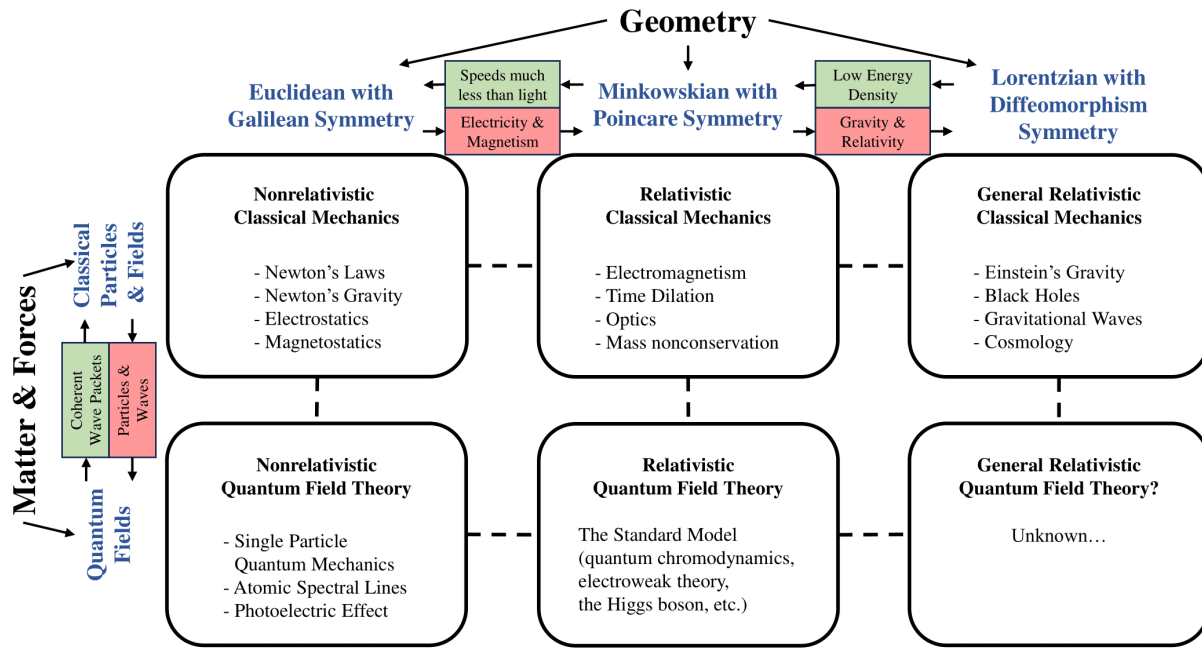


Figure 12.1: ???

Chapter 13

Quantum Gravity

Physics is becoming too difficult for the physicists
– David Hilbert [\[94\]](#)

*In science we must all submit not to what seems to us attractive
from one point of view or another, but to what represents an
agreement between theory and experiment.*
– Dmitri Mendeleev [\[68\]](#)

lol sike.

Appendix A

Mathematical Identities

A.1 Coordinate Systems

We will use R, C, and S as shorthand for Rectangular, Cylindrical, and Spherical coordinates. The atan function is defined by:

$$\text{atan}(y, x) = \begin{cases} \arctan\left(\frac{y}{x}\right), & x > 0 \\ \arctan\left(\frac{y}{x}\right) + \pi, & x < 0 \text{ \& } y \geq 0 \\ \arctan\left(\frac{y}{x}\right) - \pi, & x < 0 \text{ \& } y < 0 \\ \frac{\pi}{2}, & x = 0 \text{ \& } y > 0 \\ -\frac{\pi}{2}, & x = 0 \text{ \& } y < 0 \\ \text{undefined} & x = y = 0. \end{cases}$$

Coordinate Conversions. (φ is defined modulo shifts by 2π .)

System:	R:	C:	S:
Coordinates:	(x, y, z)	(r, φ, z)	(r, θ, φ)
Range:	$x \in \mathbb{R}$ $y \in \mathbb{R}$ $z \in \mathbb{R}$	$r \geq 0$ $0 \leq \varphi < 2\pi$ $z \in \mathbb{R}$	$r \geq 0$ $0 \leq \theta \leq \pi$ $0 \leq \varphi < 2\pi$
to R:	–	$r = \sqrt{x^2 + y^2}$ $\varphi = \text{atan}(y, x)$ $z = z$	$r = \sqrt{x^2 + y^2 + z^2}$ $\theta = \text{atan}(\sqrt{x^2 + y^2}, z)$ $\varphi = \text{atan}(y, x)$
to C:	$x = r \cos \varphi$ $y = r \sin \varphi$ $z = z$	–	$r = \sqrt{r^2 + z^2}$ $\theta = \text{atan}(r, z)$ $\varphi = \varphi$
to S:	$x = r \sin \theta \cos \varphi$ $y = r \sin \theta \sin \varphi$ $z = r \cos \theta$	$r = r \sin \theta$ $\varphi = \varphi$ $z = r \cos \theta$	–

Coordinate Differentials.

	R:	C:	S:
to R:	–	$dr = \frac{xdx+yd y}{\sqrt{x^2+y^2}}$ $d\varphi = \frac{-ydx+xd y}{\sqrt{x^2+y^2}}$ $dz = dz$	$dr = \frac{xdx+ydy+zd z}{\sqrt{x^2+y^2+z^2}}$ $d\theta = \frac{xzdx+yzdy-(x^2+y^2)dz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}}$ $d\varphi = \frac{-ydx+xd y}{\sqrt{x^2+y^2}}$
to C:	$dx = \cos \varphi dr - r \sin \varphi d\varphi$ $dy = \sin \varphi dr + r \cos \varphi d\varphi$ $dz = dz$	–	$dr = \frac{rdr+zd z}{\sqrt{r^2+z^2}}$ $d\theta = \frac{zdr-rdz}{\sqrt{r^2+z^2}}$ $d\varphi = d\varphi$
to S:	$dx = \sin \theta \cos \varphi dr + r \cos \theta \cos \varphi d\theta - r \sin \theta \sin \varphi d\varphi$ $dy = \sin \theta \sin \varphi dr + r \cos \theta \sin \varphi d\theta + r \sin \theta \cos \varphi d\varphi$ $dz = \cos \theta dr - r \sin \theta d\theta$	$dr = \sin \theta dr + r \cos \theta d\theta$ $d\varphi = d\varphi$ $dz = \cos \theta dr - r \sin \theta d\theta$	–

Coordinate Basis Vectors. $\vec{e}_a = \frac{\partial \vec{x}}{\partial x^a}$.

	R:	C:	S:
to R:	–	$\vec{e}_r = \frac{x\vec{e}_x+y\vec{e}_y}{\sqrt{x^2+y^2}}$ $\vec{e}_\varphi = -y\vec{e}_x + x\vec{e}_y$ $\vec{e}_z = \vec{e}_z$	$\vec{e}_r = \frac{x\vec{e}_x+y\vec{e}_y+z\vec{e}_z}{\sqrt{x^2+y^2+z^2}}$ $\vec{e}_\theta = \frac{xz\vec{e}_x+yz\vec{e}_y-(x^2+y^2)\vec{e}_z}{\sqrt{x^2+y^2}}$ $\vec{e}_\varphi = -y\vec{e}_x + x\vec{e}_y$
to C:	$\vec{e}_x = \cos \varphi \vec{e}_r - \frac{\sin \varphi}{r} \vec{e}_\varphi$ $\vec{e}_y = \sin \varphi \vec{e}_r + \frac{\cos \varphi}{r} \vec{e}_\varphi$ $\vec{e}_z = \vec{e}_z$	–	$\vec{e}_r = \frac{r\vec{e}_r+z\vec{e}_z}{\sqrt{r^2+z^2}}$ $\vec{e}_\theta = z\vec{e}_r - r\vec{e}_z$ $\vec{e}_\varphi = \vec{e}_\varphi$
to S:	$\vec{e}_x = \sin \theta \cos \varphi \vec{e}_r + \frac{\cos \theta \cos \varphi}{r} \vec{e}_\theta - \frac{\sin \varphi}{r \sin \theta} \vec{e}_\varphi$ $\vec{e}_y = \sin \theta \sin \varphi \vec{e}_r + \frac{\cos \theta \sin \varphi}{r} \vec{e}_\theta + \frac{\cos \varphi}{r \sin \theta} \vec{e}_\varphi$ $\vec{e}_z = \cos \theta \vec{e}_r - \frac{\sin \theta}{r} \vec{e}_\theta$	$\vec{e}_r = \sin \theta \vec{e}_r + \frac{\cos \theta}{r} \vec{e}_\theta$ $\vec{e}_\varphi = \vec{e}_\varphi$ $\vec{e}_z = \cos \theta \vec{e}_r - \frac{\sin \theta}{r} \vec{e}_\theta$	–

Coordinate Unit Vectors. $\vec{l}_a = \frac{\vec{e}_a}{|\vec{e}_a|}$. Note, all three coordinate systems here are right handed (in the coordinate order given) and orthogonal thus $\vec{l}_a \times \vec{l}_b = \epsilon_{ab}^c \vec{l}_c$ for each of the systems. (In this section ϵ_{abc} always refers to the fully anti-symmetric symbol with $\epsilon_{123} = 1$ and indices of it raised and lowered using the Kronecker delta, not the coordinate metric.)

	R:	C:	S:
to R:	–	$\vec{l}_r = \frac{x\vec{l}_x+y\vec{l}_y}{\sqrt{x^2+y^2}}$ $\vec{l}_\varphi = \frac{-y\vec{l}_x+x\vec{l}_y}{\sqrt{x^2+y^2}}$ $\vec{l}_z = \vec{l}_z$	$\vec{l}_r = \frac{x\vec{l}_x+y\vec{l}_y+z\vec{l}_z}{\sqrt{x^2+y^2+z^2}}$ $\vec{l}_\theta = \frac{xz\vec{l}_x+yz\vec{l}_y-(x^2+y^2)\vec{l}_z}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}}$ $\vec{l}_\varphi = \frac{-y\vec{l}_x+x\vec{l}_y}{\sqrt{x^2+y^2}}$
to C:	$\vec{l}_x = \cos \varphi \vec{l}_r - \sin \varphi \vec{l}_\varphi$ $\vec{l}_y = \sin \varphi \vec{l}_r + \cos \varphi \vec{l}_\varphi$ $\vec{l}_z = \vec{l}_z$	–	$\vec{l}_r = \frac{r\vec{l}_r+z\vec{l}_z}{\sqrt{r^2+z^2}}$ $\vec{l}_\theta = \frac{z\vec{l}_r-r\vec{l}_z}{\sqrt{r^2+z^2}}$ $\vec{l}_\varphi = \vec{l}_\varphi$
to S:	$\vec{l}_x = \sin \theta \cos \varphi \vec{l}_r + \cos \theta \cos \varphi \vec{l}_\theta - \sin \varphi \vec{l}_\varphi$ $\vec{l}_y = \sin \theta \sin \varphi \vec{l}_r + \cos \theta \sin \varphi \vec{l}_\theta + \cos \varphi \vec{l}_\varphi$ $\vec{l}_z = \cos \theta \vec{l}_r - \sin \theta \vec{l}_\theta$	$\vec{l}_r = \sin \theta \vec{l}_r + \cos \theta \vec{l}_\theta$ $\vec{l}_\varphi = \vec{l}_\varphi$ $\vec{l}_z = \cos \theta \vec{l}_r - \sin \theta \vec{l}_\theta$	–

Coordinate Measurements. $g_{ab} = \vec{e}_a \cdot \vec{e}_b$. $ds^2 = g_{ab} dx^a dx^b$. $d\vec{A} = \frac{1}{2} \sqrt{\det g} \epsilon_{abc} g^{ad} \vec{e}_d dx^b \wedge dx^c$. $dS = \sqrt{\det g} dx^1 dx^2 dx^3$.

	R:	C:	S:
Metric:	$g_{ab} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{ab} = \delta_{ab}$	$g_{ab} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}_{ab}$	$g_{ab} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2 \theta \end{pmatrix}_{ab}$
Line Element:	$ds^2 = dx^2 + dy^2 + dz^2$	$ds^2 = dr^2 + r^2 d\varphi^2 + dz^2$	$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\varphi^2$
Area Element:	$d\vec{A} = \vec{e}_x dy dz + \vec{e}_y dz dx + \vec{e}_z dx dy$	$d\vec{A} = \vec{e}_r r d\varphi dz + \vec{e}_\varphi \frac{1}{r} dz dr + \vec{e}_z r dr d\varphi$	$d\vec{A} = \vec{e}_r r^2 \sin \theta d\theta d\varphi + \vec{e}_\theta \sin \theta dr d\varphi + \vec{e}_\varphi \frac{dr d\theta}{\sin \theta}$
Volume Element:	$dS = dx dy dz$	$dS = r dr d\varphi dz$	$dS = r^2 \sin \theta dr d\theta d\varphi$

Basis Vector Derivatives.

R:	C:	S:
$\partial_x \vec{e}_x = 0$	$\partial_r \vec{e}_r = 0$	$\partial_r \vec{e}_r = 0$
$\partial_y \vec{e}_x = 0$	$\partial_\varphi \vec{e}_r = \frac{1}{r} \vec{e}_\varphi$	$\partial_\theta \vec{e}_r = \frac{1}{r} \vec{e}_\theta$
$\partial_z \vec{e}_x = 0$	$\partial_z \vec{e}_r = 0$	$\partial_\varphi \vec{e}_r = \frac{1}{r} \vec{e}_\varphi$
$\partial_x \vec{e}_y = 0$	$\partial_r \vec{e}_\varphi = \frac{1}{r} \vec{e}_\varphi$	$\partial_r \vec{e}_\theta = \frac{1}{r} \vec{e}_\theta$
$\partial_y \vec{e}_y = 0$	$\partial_\varphi \vec{e}_\varphi = -r \vec{e}_r$	$\partial_\theta \vec{e}_\theta = -r \vec{e}_r$
$\partial_z \vec{e}_y = 0$	$\partial_z \vec{e}_\varphi = 0$	$\partial_\varphi \vec{e}_\theta = \frac{\cos \theta}{\sin \theta} \vec{e}_\varphi$
$\partial_x \vec{e}_z = 0$	$\partial_r \vec{e}_z = 0$	$\partial_r \vec{e}_\varphi = \frac{1}{r} \vec{e}_\varphi$
$\partial_y \vec{e}_z = 0$	$\partial_\varphi \vec{e}_z = 0$	$\partial_\theta \vec{e}_\varphi = \frac{\cos \theta}{\sin \theta} \vec{e}_\varphi$
$\partial_z \vec{e}_z = 0$	$\partial_z \vec{e}_z = 0$	$\partial_\varphi \vec{e}_\varphi = -r \sin^2 \theta \vec{e}_r - \sin \theta \cos \theta \vec{e}_\theta$

Derivative Operators. $\vec{v} = v^a \vec{e}_a$. $v_a = g_{ab} v^b$. $\nabla f = \frac{\partial f}{\partial x^a} g^{ab} \vec{e}_b$. $\nabla^2 f = \frac{1}{\sqrt{\det g}} \frac{\partial}{\partial x^a} \left(g^{ab} \frac{\partial f}{\partial x^b} \sqrt{\det g} \right)$.
 $\nabla \cdot \vec{v} = \frac{1}{\sqrt{\det g}} \frac{\partial}{\partial x^a} (v^a \sqrt{\det g})$. $\nabla \times \vec{v} = \frac{1}{\sqrt{\det g}} \epsilon^{abc} \vec{e}_a \frac{\partial v_b}{\partial x^c}$.

R:	C:	S:
$\nabla f = \frac{\partial f}{\partial x} \vec{e}_x + \frac{\partial f}{\partial y} \vec{e}_y + \frac{\partial f}{\partial z} \vec{e}_z$	$= \frac{\partial f}{\partial r} \vec{e}_r + \frac{1}{r^2} \frac{\partial f}{\partial \varphi} \vec{e}_\varphi + \frac{\partial f}{\partial z} \vec{e}_z$	$= \frac{\partial f}{\partial r} \vec{e}_r + \frac{1}{r^2} \frac{\partial f}{\partial \theta} \vec{e}_\theta + \frac{1}{r^2 \sin^2 \theta} \frac{\partial f}{\partial \varphi} \vec{e}_\varphi$
$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$	$= \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \varphi^2} + \frac{\partial^2 f}{\partial z^2}$	$= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \varphi^2}$
$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$	$= \frac{1}{r} \frac{\partial}{\partial r} (r v^r) + \frac{\partial v^\varphi}{\partial \varphi} + \frac{\partial v^z}{\partial z}$	$= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v^r) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (v^\theta \sin \theta) + \frac{\partial v^\varphi}{\partial \varphi}$
$\nabla \times \vec{v} = \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z} \right) \vec{e}_x + \left(\frac{\partial v_x}{\partial z} - \frac{\partial v_z}{\partial x} \right) \vec{e}_y + \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} \right) \vec{e}_z$	$= \frac{1}{r} \left(\frac{\partial v_z}{\partial \varphi} - \frac{\partial v_\varphi}{\partial z} \right) \vec{e}_r + \frac{1}{r} \left(\frac{\partial v_r}{\partial z} - \frac{\partial v_z}{\partial r} \right) \vec{e}_\varphi + \frac{1}{r} \left(\frac{\partial v_\varphi}{\partial r} - \frac{\partial v_r}{\partial \varphi} \right) \vec{e}_z$	$= \frac{1}{r^2 \sin \theta} \left(\frac{\partial v_\varphi}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} \right) \vec{e}_r + \frac{1}{r^2 \sin \theta} \left(\frac{\partial v_r}{\partial \varphi} - \frac{\partial v_\varphi}{\partial r} \right) \vec{e}_\theta + \frac{1}{r^2 \sin \theta} \left(\frac{\partial v_\theta}{\partial r} - \frac{\partial v_r}{\partial \theta} \right) \vec{e}_\varphi$

A.2 Fourier Transform Conventions

The naive definition of the Fourier transformation is that for functions of time:

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\sqrt{2\pi}} f(t) dt \implies f(t) = \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\sqrt{2\pi}} \tilde{f}(\omega) d\omega. \quad (\text{A.2.1})$$

Similarly, for functions of position:

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{e^{-ikx}}{\sqrt{2\pi}} f(x) dx \implies f(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{\sqrt{2\pi}} \tilde{f}(k) dk. \quad (\text{A.2.2})$$

The difference in sign convention chosen for the exponential is standard in physics. It has two particularly nice features. First, for a right moving function: $f(t, x) = g(x - vt)$ for constant $v > 0$, the double (meaning time and space) Fourier transformation of f is proportional to $\delta(\omega - vk)$ and so represents a wave with

dispersion relation $\omega = vk$ with no minus sign. This leads to the definition of the phase velocity as $\frac{\omega}{k}$. If the sign conventions for t and x are defined to be the same then there would be a negative sign in the definition of the phase velocity. The other nice feature is that if one defines the wavenumber 4-vector $k^\mu = (\omega, \vec{k})^\mu$ then the exponent in the spacetime Fourier transform is easily expressed in terms of $k_\mu x^\mu$ and k^μ transforms properly as a 4-vector.

The Fourier transform is based on the fundamental Fourier integral:

$$\int_{-\infty}^{\infty} e^{ikx} dx = 2\pi\delta(k) \quad (\text{A.2.3})$$

which is a shorthand for the more rigorous statement:

$$\lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} e^{ikx - \varepsilon|x|} f(x) dx = 2\pi f(0) \quad (\text{A.2.4})$$

for any integrable function $f(x)$ which is continuous at 0 and decays sufficiently quickly for large x for the integral on the left hand side to converge for all $\varepsilon > 0$. Because of this ε -damping the more careful way to compute the Fourier transform of a function is to include that damping factor in the integral. Whenever a Fourier integral in practice has trouble converging it is likely to be resolved by making this exponential factor explicit.

In literature there exist multiple different conventions on where to put 2π 's in the Fourier transform. Mathematicians tend to use the actual frequency $f = \frac{\omega}{2\pi}$ instead of the angular frequency ω for computing the Fourier transform. Doing so removes 2π 's from the normalization but places them in the exponent. Physicists tend to only use the angular frequency and wavenumber so that no 2π 's appear in the exponent. However, then there are necessary normalization factors of 2π . I use the symmetric convention defined above because it is the choice for which the Fourier transform is unitary:

$$\int_{-\infty}^{\infty} \tilde{f}^*(\omega) \tilde{g}(\omega) d\omega = \int_{-\infty}^{\infty} f^*(t) g(t) dt. \quad (\text{A.2.5})$$

A.3 Asymptotic notation

The Big-O Notation $\mathcal{O}(g(x))$ and little-o Notation $o(g(x))$ are formal ways of characterizing the behavior of a function $f(x)$ near a point x_0 . We write $f(x) = \mathcal{O}(g(x))$ if for all x sufficiently near x_0 , $|f(x)|$ is less than a fixed multiple of $g(x)$. That is, $f(x) = \mathcal{O}(g(x))$ if there exist positive numbers δ, C so that for all x satisfying $0 < |x - x_0| < \delta$:

$$|f(x)| \leq C|g(x)|. \quad (\text{A.3.1})$$

Similarly, we write $f(x) = o(g(x))$ if for every multiplier $C > 0$, $|f(x)| < C|g(x)|$ for all x sufficiently near x_0 . Precisely, $f(x) = o(g(x))$ if for all $C > 0$ there exists a δ so that for all x satisfying $0 < |x - x_0| < \delta$ we have $|f(x)| \leq C|g(x)|$. Notice that the order of conditions between $\mathcal{O}$ and o is different.

Often when using this notation the point of approximation x_0 is not written directly in the equation. This is a common bad habit. When this is done it is absolutely necessary to make sure that x_0 is clear from the text surrounding the equation. While an equals sign is used in the Big-O Notation, one should make sure to not treat the symbol $\mathcal{O}(g(x))$ as if it is a function in itself. Properly, the Big-O Notation defines an equivalence class of functions based on how they behave near a point of interest. For example, one may have two different functions $f_1(x)$ and $f_2(x)$ which both satisfy $f_1(x) = \mathcal{O}(g(x))$ and $f_2(x) = \mathcal{O}(g(x))$. From this one absolutely cannot infer that f_1 and f_2 are equal. There are systematic combination rules for the Big-O Notation though. In particular, we can infer that:

$$f_1(x) = \mathcal{O}(g(x)), \quad f_2(x) = \mathcal{O}(g(x)) \implies af_1(x) + bf_2(x) = \mathcal{O}(g(x)), \quad f_1(x)f_2(x) = \mathcal{O}(g^2(x)) \quad (\text{A.3.2})$$

for all constants a and b . As well, if the asymptotic behavior of $f_1(x)$ and $f_2(x)$ are different near x_0 :

$$\begin{aligned} f_1(x) &= \mathcal{O}(g_1(x)), & f_2(x) &= \mathcal{O}(g_2(x)) \\ \implies af_1(x) + bf_2(x) &= \mathcal{O}(\max(g_1, g_2)), & f_1(x)f_2(x) &= \mathcal{O}(g_1(x)g_2(x)). \end{aligned} \quad (\text{A.3.3})$$

We will often write expressions of the form:

$$f_1(x) = f_2(x) + \mathcal{O}(g(x)) \quad (\text{A.3.4})$$

which is just an alternate notation for the equation:

$$f_1(x) - f_2(x) = \mathcal{O}(g(x)). \quad (\text{A.3.5})$$

Another useful fact is:

$$f_1(x) = f_2(x)\mathcal{O}(g(x)) \implies f_1(x) = \mathcal{O}(f_2(x)g(x)). \quad (\text{A.3.6})$$

The context in which we will most often apply asymptotic notation is to approximations of functions by series. In particular, we use Taylor's theorem: if $f(x)$ is an N times differentiable function at x_0 then there exists a function $h_N(x)$ so that:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \dots + \frac{f^{(N)}(x_0)}{N!}(x - x_0)^N + h_N(x)(x - x_0)^N \quad (\text{A.3.7})$$

and that function $h_N(x)$ satisfies:

$$\lim_{x \rightarrow x_0} h_N(x) = 0. \quad (\text{A.3.8})$$

(Here $f^{(N)}$ indicates N derivatives of f .) This guarantees that for such $f(x)$:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \dots + \frac{f^{(N)}(x_0)}{N!}(x - x_0)^N + o((x - x_0)^N). \quad (\text{A.3.9})$$

If $f(x)$ is $N + 1$ times differentiable then we can make the stronger statement:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \dots + \frac{f^{(N)}(x_0)}{N!}(x - x_0)^N + \mathcal{O}((x - x_0)^{N+1}). \quad (\text{A.3.10})$$

If the quantity $(x - x_0)^{N+1}$ is approximately 0 within our resolution for the values of x which are relevant to us then this allows us to approximate the exact function $f(x)$ by the degree N polynomial on the right hand side for such values of x .

Appendix B

Systems of Units

Depending on the application, different unit systems can be useful. Here we give a brief overview of a few systems and how to convert between them. We will give a brief discussion of different systems and end with a conversion chart between the systems discussed.

B.1 Discussion of Different Systems

SI: Historical and modern.

For historical reasons SI (the international system) is the most popular system of units for most purposes. In SI there are 7 base units, the second s for measuring time, the meter m for measuring distance, the kilogram kg for measuring mass, the ampere A for measuring electric current, the kelvin K for measuring temperature, the mole mol for measuring amounts of a substance, and the candela cd for measuring luminous intensity. Luminous intensity is a measure of brightness of light as perceived by the human eye. We will not have an application for this unit or type of quantity and so we will only discuss the remaining 6 base SI units. Historically, all 6 of the other base units were defined by an arbitrary reference point. That is, historically the meter was defined as the exact length of a particular metal rod kept in France. The second was defined so that there were precisely 86400 seconds per solar day on Earth. The kilogram was defined by the exact mass of a particular metal block. The ampere was defined as the amount of current which when maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed one meter apart in vacuum, produces an the electromagnetic force per unit length between these conductors of $2 \times 10^{-7} \frac{\text{kg}}{\text{s}^2}$. The kelvin was defined so that the temperature difference between the boiling point and freezing point of water both at sea level pressure is 100 K. The mole is defined as an Avogadro's number of things. Avogadro's number was defined as the number of atoms of carbon in 12 grams of the isotope carbon-12. At the time these historical versions of units were defined it was believed that each of these types of measurement (length and time, for example) were completely independent and there was no physically meaningful way to convert between them. In more recent history we have learned this is not true.

In light of physics learned since the original introduction of SI units, each of the base units has been given a more modern definition. These modern definitions are very close to their historical definitions in the numerical values they produce; the difference is negligible for almost all purposes. But, they provide significant conceptual simplification. In modern SI, the second is defined so that the unperturbed ground state hyperfine transition frequency of the cesium-133 atom is $9192631770 \frac{1}{\text{s}}$. This still defines the second in terms of an arbitrary reference value. However, this point of reference can be reproduced exactly anywhere in the universe and measured by atomic physics and so is not reliant on carefully preserving a specific piece of equipment in a vault somewhere on Earth. The meter is defined so that with the given definition of the second the speed of light in a vacuum is by definition $c = 299792458 \frac{\text{m}}{\text{s}}$. The kilogram is defined so that the “unreduced” Planck's constant $2\pi\hbar$ is by exactly $2\pi\hbar = 6.62607015 \times 10^{-34} \frac{\text{kgm}^2}{\text{s}}$. The ampere is defined so that the magnitude of the charge of the electron is $q_e = 1.602176634 \times 10^{-19} \text{As}$. The kelvin is defined so that the Boltzmann factor k_B , defined as the factor which appears in the ideal gas law as $pV = Nk_B T$, exactly takes the value $k_B = 1.380649 \times 10^{-23} \frac{\text{kg m}^2}{\text{s}^2 \text{K}}$. The mole is still defined as an Avogadro's number of things but Avogadro's number is now defined as exactly $6.02214076 \times 10^{23}$. The modern SI system has the advantage that all arbitrary references used (such as to define the unit of time) are universally reproducible rather than

dependent on the preservation of an arbitrary “special” object. The numerical values of the conversion factors used here for modern SI are very complicated but they are chosen so that the modern base units very closely correspond to the historical base units.

The modern definition of SI units holds many advantages over the historical system, both practical in terms of not relying on a special rod or bar, and conceptual. Most salient of the conceptual advantages of modern SI over historical is that in historical SI the values of c , $\hbar$, ϵ_0 , k_B , and N_A (Avogadro’s number) had to be measured in terms of the arbitrarily defined base units. This leads many people learning physics to believe that these quantities are necessarily “fundamental constants” of the universe, meaning parameters which “could have been different” and had to have their values determined by experiment. However, modern SI elucidates that in all five cases this is incorrect. The numerical value of each of these constants is completely determined by redefining an arbitrary reference unit (the units of length, mass, charge, temperature for c , $\hbar$, ϵ_0 , k_B and what amount of substance is assumed for N_A). They exist and have their particular numerical values for purely social and historical reasons. The inconvenience of converting times to lengths by the nasty value of c in SI units is the modern analog of the inconvenience of converting feet to miles by the nasty value of 1 mile = 5280 feet in the American System of units. The ugliness of the numerical values of c , $\hbar$, ϵ_0 , k_B , N_A in SI units and the fact that these symbols continue to clutter the equations in SI units makes it obvious what improved unit system could be defined, one in which these unnecessary constants simply don’t enter into the equations. We will see over the rest of this chapter how to do this losslessly.

There is one specific way in which modern SI is deficient compared to historical SI. Historic SI’s definition of the Ampere implied an exact value for $\mu_{0\text{Hist}} = 4\pi \times 10^{-7} \frac{\text{kg m}}{\text{s}^2 \text{A}^2}$. Consequently, there is an implied value of ϵ_0 using $\epsilon_0 = \frac{1}{\mu_0 c^2}$. Then, the value for the electron charge q_e in Historic SI is a completely measured quantity. This makes physical sense because the electron charge in SI units is given by:

$$q_e = \sqrt{\epsilon_0 \hbar c e} \quad (\text{B.1.1})$$

where e is the electromagnetic coupling constant (the fine structure constant $\alpha = \frac{e^2}{4\pi}$). The electromagnetic coupling constant e is a dimensionless fundamental parameter of the standard model which has to be measured. By defining q_e to take an exact value, there is an induced error bar on the value of ϵ_0 dependent on the precision with which e can be measured. But, ϵ_0 is relevant for macroscopic experiments (and appears even at the level of completely nonrelativistic classical mechanics) so it is somewhat backward to tie its definition in the unit system to precision high energy or atomic physics. Practically this isn’t typically an actual issue due to the fact that the electromagnetic coupling constant is one of the most precisely measured quantities in physics. But, conceptually it would have been better to define the value of ϵ_0 to be exact, or to keep the exact definition of μ_0 from historic SI. Then, the electron charge would (reasonably) have finite precision, determined by the precision with which e can be measured.

GNU (Galilean Natural Units) or Nonrelativistic Natural Units

GNU is an artificial system we used for the completely classical regime where both relativity and quantum mechanics are unknown. Unfortunately, at everyday scales there aren’t any obvious universally reproducible references one can make with nearly the same precision as the SI definition of the second and so an everyday scale unit system such as GNU realistically would have to rely on the old fashioned rod in a vault method for unit definitions or be derived from a more fundamental unit system, such as the high energy unit system we will discuss later. Any actual application of GNU is essentially derived from high energy units, which is the default unit system used in theoretical physics. (Though as we will see high energy units are also a perfectly good system for experiment.)

At everyday scales the units which appear independent are time, length, and mass. Without access to c , units of length and time are independent. Without access to $\hbar$, the unit of mass is independent from length and time. Historically in this regime temperature was also taken to be an independent unit from energy however using Brownian motion and kinetic theory or Johnson noise in a circuit it is possible to measure temperature directly without a need for introducing k_B or N_A . Thus it is not necessary to introduce the kelvin, even when one knows nothing of relativity or quantum mechanics. Historically the electric charge was also taken to be independent through the use of an arbitrary reference charge. But, as discussed in section 3.7 it is not necessary to introduce the Coulomb. Instead, we define the unit of charge so that $\epsilon_0 = 1$. As discussed in section 3.8 doing so while keeping the kilogram, meter, and second sets the units of charge to be $\frac{\sqrt{\text{kg m}^3}}{\text{s}}$.

There is one obvious missed simplification not made in GNU, which is to use the gravitational constant G

to eliminate mass as an independent unit. There is both strong practical and theoretical reason for not doing this. Practically, gravitational mass measurements have always been significantly less precise than inertial mass measurements at everyday scales and so calibrating the unit of mass by setting G to a preselected value would significantly reduce the precision of measurement of everyday masses. The theoretical reason will be explained thoroughly when we discuss Planck units.

LNU (Lorentz Natural Units) or Relativistic Natural Units

LNU is conceptually like GNU except that now knowledge of relativity is assumed so that units of length can be defined by setting $c = 1$. Said another way, the unit of length used in LNU is the lightsecond so that the speed of light is 1 lightsecond per second. Thus, $\epsilon_0 = c = 1$ in LNU; the unit of length induced by this is simply the second and the unit of charge induced by this is $\sqrt{\text{kg s}}$. This system is well suited to describing classical electromagnetism. LNU can be converted down to GNU by using c as a conversion factor to convert units of time to units of length when needed. Ultimately LNU has only mass and time as independent units.

SNU (Schrödinger Natural Units) or Quantum Natural Units

SNU is conceptually like GNU except that now knowledge of quantum mechanics is assumed so that units of mass can be defined by setting $\hbar = 1$. Said another way, the unit of energy used in SNU is the unit of angular frequency so that $\hbar$, the ratio between the energy carried by a wavefunction of a given angular frequency to that angular frequency, is 1. Implicitly this defines a unit of mass. Thus, $\epsilon_0 = \hbar = 1$ in SNU; the unit of mass induced by this is $\frac{\text{s}}{\text{m}^2}$ and the unit of charge induced by this is $\sqrt{\frac{\text{m}}{\text{s}}}$. This system is well suited to describing nonrelativistic quantum mechanics. SNU can be converted down to GNU by using $\hbar$ as a conversion factor to reintroduce units of the kilogram as desired. Ultimately SNU has only time and length as independent units.

NU/HEU (Natural Units) or High Energy Units

NU or HEU is the unit system I advocate for most. It is already the most common unit system in theoretical physics (some sources set ϵ_0 to be $\frac{1}{4\pi}$, but this is on the decline outside of a few specific subfields). HEU is based on the understanding that relativity and quantum mechanics imply that $c, \hbar, \epsilon_0, k_B$ are universal and invariant with numerical values set arbitrarily by your choice of units. HEU then declutters the action/Lagrangian/Hamiltonian by setting each of these to 1: $c = \hbar = \epsilon_0 = k_B = 1$. Consequently, the only remaining free unit is the unit of time (or equivalently the unit of length or the reciprocal of the unit of mass). For the last remaining unit, if you want to keep as close to SI as possible, you should take the unit of time to be the second. Alternatively, especially for actual applications within high energy physics, it is nice to use the unit of the electronvolt eV for energy. The electronvolt is defined exactly as the energy gained by an electron when it is accelerated through an electrostatic potential difference of 1 Volt ($1 \text{ Volt} = 1 \frac{\text{kg m}^2}{\text{s}^2 \text{C}}$ in SI units). Using the SI definition of the second gives that in HEU the electronvolt and the second are exactly related by:

$$1\text{eV} = 2\pi \frac{1.602176634}{6.62607015} 10^{15} \frac{1}{\text{s}} \approx 1.51926744787862620125 \times 10^{15} \frac{1}{\text{s}}. \quad (\text{B.1.2})$$

So, for HEU we take either the eV or the second as our one defining unit and use the number presented here as a conversion factor between those two choices. Although the electronvolt naively references several SI units, all of these references drop out in this formula as we have not related it to the second, which is defined intrinsically as before in terms of cesium-133.

It is important to understand the conceptual advantage HEU has over other unit systems. In SI units, lengths and times are measured by a different unit. Relativity shows that displacements in space and durations in time are not independent of each other; they mix under a Lorentz transformation. Because of Lorentz symmetry, there is no way to separate the notions of space and time in a way consistent with the symmetries of the universe. Consequently, there is not a physics based reason to use different units for lengths and times. The reason we tend to do so in everyday contexts is social, not physical. Any duration of time which is typical for a human, such as a second, leads to a distance unit that is comically large for human purposes (a lightsecond is about 80 percent of the distance from the Earth to its moon). So, because we don't want to say "I am 6 nanolightseconds tall", we use a separate unit of length for social convenience. As well, there is a monumental historical inertia behind unit systems due to the amount of infrastructure built using historical systems. The same argument about the social inconvenience of the size of the lightsecond applies to the other eliminated units in HEU as well. In HEU a mass on the order of one kilogram would be described as having mass on the order of $10^{51} \frac{1}{\text{s}}$. The nanolightsecond situation is at least manageable. Nano is easy enough to

remember; it is too much to ask anyone to learn 50 orders of magnitude worth of unit prefixes. This problem is not lessened by using eV instead of the second. One way or the other 50 orders of magnitude have to be shuffled around. So, while HEU eliminates awkwardness in seeing and applying symmetries of our universe (and thus is best for physics), it leads to socially inconvenient numerical values for everyday quantities.

HEU can be directly converted to other unit systems which keep their redundant units by reintroducing powers of c , $\hbar$, ϵ_0 and k_B necessary to match between them. The other systems of natural units described and modern SI can be useful intermediary systems for bridging the gap between the conceptual muddiness of the old SI system and the social inconvenience of HEU.

Planck Units

Sources attempting to bring together general relativity and quantum field theory will sometimes set $G = 1$ in addition to what is done in the HEU system. Doing so removes all arbitrary reference units giving a purely numerical value to every quantity. This system is called Planck units. This might seem like the natural and inevitable endpoint of what we have been doing. However, I think this reasoning is mistaken. At the level of application, G is only known to about 1 part in 50000 but some dimensionful quantities can be currently measured to as many as 12 digits. Resting our unit definitions on G would practically destroy huge advances in precision measurement. Even if this was not an issue, there is a theoretical problem with choosing G as special to set a scale. There is a uniqueness to the choices made in HEU. c is not only *a* universal invariant speed but necessarily *the* only universal invariant speed. So, for defining a unit relationship between length and time it is the only universal physics based choice. Similarly, $\hbar$ and ϵ_0 are the only universal and invariant quantities of their respective units which appear in physics and so they can be uniquely removed and reduce a corresponding unit each. But, in HEU where the only unit left is length, there are multiple independent universal invariant length scales to choose from. There is a length scale set by G , another by the cosmological constant Λ , another for each particle mass in the standard model, and yet another for the Higgs vacuum expectation value. There is no reason to select any of these different scales as the special one to be set to 1. If there was a theory which could derive all of those scales from a single specified scale, it would be appropriate to set that special scale to define a length unit of 1. However, no such theory is known¹.

There is often significant conceptual confusion regarding the meaning of Planck units. Especially in nonacademic sources is it common to suggest that the length scale which is set to 1 by Planck units, called the Planck length, is somehow the smallest length scale that could exist. Correspondingly, it is sometimes similarly suggested that the Planck time or Planck mass (the corresponding values of those quantities which are set to 1 in PU) are physically special (representing the smallest meaningful duration, and because the unit of mass is inverse to that of length, the largest mass). For reference, the Planck length is about 10^{-35} meters, the Planck time about 10^{-44} seconds, and the Planck mass about .02 milligrams. The first two of these sound so small that one might be forgiven for thinking they are the smallest scales possible. On the other hand, .02 mg doesn't sound nearly as special. It is incorrect to say the Planck length/time is the smallest meaningful distance/duration or to suggest that somehow spacetime is discretized at that scale. All existing experimental evidence is consistent with a completely continuous universe but no experiment so far performed is able to probe anything close to the distance resolution of a Planck length. The Planck length is a very small distance currently about 15 orders of magnitude smaller than our best experimental resolution; it is silly to make metaphysical guesses about how special it might be.

There is a meaning to the Planck energy *relative to our current knowledge of physics*. However, that actual meaning is significantly weaker than the wrongheaded interpretation just discussed. The Planck energy (the Planck mass times c^2) is about 10^{19} GeV. If you attempt to make general relativity a quantum field theory (which is believed to be necessary in some way to make a theory which contains both gravity and the standard model) you will find that the quantum corrections to classical general relativity are suppressed by the ratio of the energy scale of the experiment to the Planck energy. Thus, naively assuming that Einstein's gravity is correct on all length scales before quantum effects become important, we would expect quantum contributions to gravity to become significant around an experimental energy on the order of the Planck energy. In this way the Planck energy gives an order of magnitude approximation so that certainly by that energy quantum gravity becomes important. It is very well possible that quantum gravity or other corrections to Einstein's theory could become important before that because we currently don't know of any specific theory of quantum gravity which reproduces the standard model and Einstein's gravity under appropriate

¹You might hear someone say they know of such a theory. Certainly this claim has been made before but at this time no actual derivation of the physical values in the standard model from a single scale exists, no matter what string theorists tell themselves.

limits. Said concisely: the meaning of the Planck energy is that based on our current knowledge of gravity it gives a crude approximation of the energy by which Einstein's gravity will have to be replaced by a quantum theory of gravity. The actual value at which this might happen could be many orders of magnitude lower. The Planck time and length then correspond to the scales of the period and wavelength of typical quantum corrections to Einstein's gravity, assuming that the Planck energy is around where those effects become important.

B.2 Conversion Chart

Sometimes one will hear a claim against natural units by someone saying that natural units are inconvenient for comparing to experiment. The point of this section to show that this thinking is entirely incorrect and that natural units are exactly as easy to compare to any measurement as SI units. When using HEU or any of the other natural units described, we have set a particular symbol appearing in SI units to 1 to eliminate physically redundant choices of arbitrary reference measurements. Here we will use L, T, M, Q, θ to refer to units of length, time, mass, charge, and temperature respectively².

A general quantity f will have some units $L^A T^B M^C Q^D \theta^E$ for some numbers A, B, C, D, E . We write this as:

$$[f]_{\text{SI}} = L^A T^B M^C Q^D \theta^E. \quad (\text{B.2.1})$$

All of the numbers A, B, C, D, E are determined if you know what units f should have in SI units, which if you are comparing to SI units you certainly do. The multiplier necessary to convert f from another unit system into SI is then given by the table:

Starting System	Units	Multiplier to make SI
SI	$L^A T^B M^C Q^D \theta^E$	1
GNU	$L^{A+\frac{3}{2}D+2E} T^{B-D-2E} M^{C+\frac{1}{2}D+E}$	$\epsilon_0^{\frac{D}{2}} k_B^{-E}$
LNU	$T^{A+B+\frac{1}{2}D} M^{C+\frac{1}{2}D+E}$	$c^{A+\frac{3}{2}D+2E} \epsilon_0^{\frac{D}{2}} k_B^{-E}$
SNU	$L^{A-2C+\frac{D}{2}} T^{B+C-\frac{D}{2}-E}$	$\hbar^{C+\frac{D}{2}+E} \epsilon_0^{\frac{D}{2}} k_B^{-E}$
HEU	$T^{A+B-C-E}$	$c^{A-2C+\frac{D}{2}} \hbar^{C+\frac{D}{2}+E} \epsilon_0^{\frac{D}{2}} k_B^{-E}$
PU	1	$G^{\frac{A+B-C-E}{2}} c^{-\frac{3A+5B-C-D-5E}{2}} \hbar^{-\frac{A+B+C+D+E}{2}} \epsilon_0^{-\frac{D}{2}} k_B^{-E}$

Here we have defined the exact values in SI units:

$$\begin{aligned} c &= 299792458 \frac{\text{m}}{\text{s}}, & q_e &= 1.602176634 \times 10^{-19} \text{ A s}, \\ 2\pi\hbar &= 6.62607015 \times 10^{-34} \frac{\text{kg m}^2}{\text{s}}, & k_B &= 1.380649 \times 10^{-23} \frac{\text{kg m}^2}{\text{s}^2 \text{ K}} \end{aligned} \quad (\text{B.2.2})$$

as well as the approximately measured values:

$$\begin{aligned} \alpha &= 0.0072973525693(11), & \epsilon_0 &= 8.8541878128(13) \times 10^{-12} \frac{\text{A}^2 \text{ s}^4}{\text{kg m}^3}, \\ G &= 6.67430(15) \times 10^{-11} \frac{\text{m}^3}{\text{kg s}^2}. \end{aligned} \quad (\text{B.2.3})$$

(The value of ϵ_0 is implied by the measured value of the fine structure constant $\alpha = \frac{q_e^2}{4\pi\epsilon_0\hbar c}$ and the choice of SI to define the electron charge exactly.)

With our chart here any quantity in any of the given unit systems can be converted to its associated quantity in SI units as if none of the quantities $c, \hbar, \epsilon_0, k_B, G$ had ever been set to one simply by multiplying our starting quantity by the corresponding factor in the last column of the chart. In order to convert between the unit systems here other than SI, one can simply convert to SI as an intermediary which amounts to multiplying by the factor to convert the start to SI and then dividing by the factor to convert the final to SI. Simplifying then gives a map between each of the unit systems, completely losslessly.

²We could also include units for amount of substance, but this is already a conversion which happens within SI and physicists tend to use moles less often anyway. Always, 1 mole just means $N_A = 6.02214076 \times 10^{23}$ of something and so any number of particles can be converted to a corresponding number of moles. Similarly we exclude the candela which is a specialized unit that can be eliminated this same way but is not of interest to us.

Let us do an example to see how it works. In the low velocity limit the power radiated per unit solid angular by a moving charged particle expressed in HEU is:

$$\frac{d\mathcal{P}}{d\Omega} = \frac{q^2}{16\pi^2} |\hat{r} \times \ddot{\vec{y}}|^2 \quad (\text{B.2.4})$$

The dimensionful quantities in SI units here are the power, with units of $\frac{\text{kg m}^2}{\text{s}^3}$, charge, with units of A s, and the acceleration, with units of $\frac{\text{m}}{\text{s}^2}$. In order, these have A, B, C, D, E values of 2,-3,1,0,0 then 0,0,0,1,0 and finally 1,-2,0,0,0. Using the chart then, the SI and HEU quantities are related by:

$$\mathcal{P}_{\text{SI}} = \hbar \mathcal{P}_{\text{HEU}}, \quad q_{\text{SI}} = \sqrt{c\hbar\epsilon_0} q_{\text{HEU}}, \quad \ddot{\vec{y}}_{\text{SI}} = c \ddot{\vec{y}}_{\text{HEU}}. \quad (\text{B.2.5})$$

The equation we started with was written in HEU units and so reexpressing each of the piece in it in terms of the SI counterparts leads to the SI equation:

$$\frac{d\mathcal{P}_{\text{SI}}}{d\Omega} = \frac{\mu_0 q_{\text{SI}}^2}{16\pi^2 c} |\hat{r} \times \ddot{\vec{y}}_{\text{SI}}|^2 \quad (\text{B.2.6})$$

which is in fact the correct version of this equation in SI units.

Appendix C

How to write your Lagrangian

Lagrangian (first half) and Lagrangian Density (second half) contributions	
Nonrelativistic mass m :	$+\frac{1}{2}m \dot{\vec{x}} ^2$
with a potential energy $U(t, \vec{x})$:	$-U(t, \vec{x})$
Special relativistic mass m :	$-mc^2\sqrt{1 - \frac{ \dot{\vec{x}} ^2}{c^2}} = -m\sqrt{-\eta_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}$
General relativistic mass m :	$-m\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}$
In a Newtonian gravitational potential ϕ :	$-m\phi(t, \vec{x})$
In vector potential $\vec{A}(t, \vec{x})$:	$+q\vec{A}(t, \vec{x}) \cdot \dot{\vec{x}} - q\phi(t, \vec{x}) = +qA_\mu\dot{x}^\mu$
With nonrelativistic rigid rotations by angular velocity $\vec{\omega}(t)$:	$+\frac{1}{2}\vec{\omega}^T \hat{R} \hat{I} \hat{R}^T \vec{\omega}$
Quantum System with Hamiltonian operator $\hat{H}$:	$+i\hbar\langle\psi \dot{\psi}\rangle - \langle\psi \hat{H} \psi\rangle$
Newtonian gravitational potential ϕ :	$-\frac{ \nabla\phi ^2}{8\pi G}$
Wave equation for scalar ϕ (constant A , speed v):	$\frac{A}{2}(\dot{\phi}^2 - v^2 \nabla\phi ^2)$
Diffusion equation for scalar ϕ (conjugate φ , constant κ):	$+\varphi\dot{\phi} - \kappa\varphi\nabla^2\phi$
Maxwell theory (electromagnetism):	$+\frac{\epsilon_0}{2} \vec{E} ^2 - \frac{ \vec{B} ^2}{2\mu_0} = -\frac{1}{4}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu}$
Nonrelativistic irrotational ideal fluid (density ρ , conjugate S):	$+S\dot{\rho} - \frac{\rho}{2} \nabla S ^2 - \rho u(\rho)$
Euler Fluid (in active coordinates):	$+\frac{1}{2}\rho \dot{\vec{z}} ^2 - \rho u(\rho)$
Relativistic Fluid:	$-n\mathcal{U} + qnu^\mu A_\mu$
Spin-0 Nonrelativistic Quantum Particle:	$+i\psi^*\mathcal{D}_t\psi - \frac{ \vec{\mathcal{D}}\psi ^2}{2m}$
Spin-1/2 Nonrelativistic Quantum Particle:	$+i\psi^\dagger\mathcal{D}_t\psi - \frac{ \vec{\mathcal{D}}\psi ^2}{2m} + \gamma\psi^\dagger\vec{B} \cdot \hat{\vec{S}}\psi$
Relativistic Scalar Field:	$-\mathcal{D}^\mu\phi^\dagger\mathcal{D}_\mu\phi - m^2 \phi ^2$
Dirac Field:	$+i\bar{\psi}\gamma^\mu\mathcal{D}_\mu\psi - m\bar{\psi}\psi$
Gauge Theory:	$-\frac{1}{4}\mathcal{F}_a^{\mu\nu}\mathcal{F}_{\mu\nu}^a$
Higgs Field:	$-\mathcal{D}^\mu\Phi^\dagger\mathcal{D}_\mu\Phi - \frac{m_H^2}{2v^2}\left(\Phi^\dagger\Phi - \frac{v^2}{2}\right)^2$
Up-type Yukawa Coupling:	$-2\text{Im}(\Gamma_u^{ab}u_{Ra}^\dagger\Phi^T\sigma_2q_{Lb})$
Down-type Yukawa Coupling:	$-2\text{Re}(\Gamma_d^{ab}d_{Ra}^\dagger\Phi q_{Lb})$
Einstein Gravity:	$+\frac{R}{16\pi G}$
Cosmological Constant:	$-\frac{\Lambda}{8\pi G}$

The first two lines in the first half are the right way of thinking about the common kinetic minus potential idea. Every variable and interaction in your theory adds a term to the Lagrangian and the above table lists some common contributions from common variables and interactions. In order to construct an appropriate Lagrangian for a theory one simply needs to sum the contributions from this table relevant to the theory at hand. The first half of the table represents contributions directly to the Lagrangian while the second half represents contributions to the Lagrangian density (so such contributions need to be integrated against spatial volume over the region of interest).

Appendix D

References

- [1] Allahverdyan, A. E. Balian, R. Nieuwenhuizen, T. M. *A sub-ensemble theory of ideal quantum measurement processes* (2013). Annals of Physics. Volume 376. Pages 324-352. doi:10.1016/j.aop.2016.11.001.
- [2] Arnold, V. I. *Mathematical Methods of Classical Mechanics* (1989). Springer-Verlag. 0387968903.
- [3] Ballentine, L. *Quantum Mechanics: a Modern Development* (2000). World Scientific Publishing. 9810241054.
- [4] Barlow, R. *Statistics* (1993). Wiley & Sons. 9780471922957.
- [5] Becker, A. *What Is Real?: The Unfinished Quest for the Meaning of Quantum Physics* (2018). Basic Books. 9780465096053.
- [6] Bertlmann, R. *Anomalies in Quantum Field Theory* (1996). Oxford University Press. 9780198507628.
- [7] Bevington, P. and Robinson, D. *Data Reduction and Error Analysis for the Physical Sciences* (1969). McGraw Hill. 9780072472271.
- [8] Blinder, S. M. *Canonical partition function for the hydrogen atom via the Coulomb propagator* (1995). Journal of Mathematical Physics 36(3): 1208-1216.
- [9] Bonilla, L. L. and Guinea, F. *Collapse of the wave packet and chaos in a model with classical and quantum degrees of freedom* (1992). Phys. Rev. A 45, 7718. doi:10.1103/PhysRevA.45.7718.
- [10] Boyce, W.E. and DiPrima, R.C. *Elementary Differential Equations and Boundary Value Problems* (2012). Wiley Plus Products Series. John Wiley & Sons, Incorporated. 9781118567593.
- [11] Breuer, H. P. and Petruccione, F. *The Theory of Open Quantum Systems* (2002). United Kingdom: Oxford University Press.
- [12] Breuer, H.P. and Petruccione, F. *Quantum measurement and the transformation from quantum to classical probabilities* (1996). Phys. Rev. A 54, 1146. doi:10.1103/PhysRevA.54.1146.
- [13] Callen, H. B. *Thermodynamics and an Introduction to Thermostatistics (2nd ed.)* (1991). Wiley. 9780471862567.
- [14] Carroll, S. M. *Spacetime and Geometry: An Introduction to General Relativity* (2003). Addison-Wesley. 9780805387322.
- [15] Chandrasekhar, S. *The Mathematical Theory of Black Holes* (1998). Clarendon Press. 9780198503705.
- [16] Coleman, S. Lecture delivered at Harvard University (1975).
- [17] Colley, S. J. *Vector Calculus* (2012). Pearson Education, Inc. 9780321780652.
- [18] Corral, M. *Vector Calculus* (2008). GNU Free Documentation.
- [19] Cousins, R. *Lectures on Statistics in Theory: Prelude to Statistics in Practice* (2018). arXiv:1807.05996.
- [20] Cowan, G. *Statistical Data Analysis* (1998). Oxford Science Publications. 9780198501558.
- [21] de la Cruz, R. J. and Faßbender, H. *On the diagonalizability of a matrix by a symplectic equivalence, similarity or congruence transformation* (2016). Linear Algebra and its Applications, Volume 496, Pages 288-306, ISSN 0024-3795, doi: 10.1016/j.laa.2016.01.030.
- [22] Date, G. *Lectures on Constrained Systems* (2010). arxiv:1010.2062.
- [23] Dirac, P. A. M. *Generalized Hamiltonian Dynamics* (1950). Canadian Journal of Mathematics. doi: 10.4153/CJM-1950-012-1.
- [24] Drake, S. *The Role of Music in Galileo's Experiments* (1975). Scientific American.
- [25] Ferrell, W. McKay, A. *Anchorman: The Legend of Ron Burgundy* (2004). Apatow Productions. Dreamworks Pictures.

-
- [26] Feynman, R. Lecture delivered at Cornell University (1964).
 - [27] Feynman, R. *Fun to Imagine* (1983). BBC.
 - [28] Flannery, M. R. *The Enigma of Nonholonomic Constraints* (2005). American Journal of Physics 73, 265. doi: 10.1119/1.1830501.
 - [29] Flannery, M. R. *The Elusive d'Alembert-Lagrange dynamics nonholonomic system* (2011). American Journal of Physics 79, 932. doi: 10.1119/1.3563538.
 - [30] Friedberg, S. Insel, A. and Spence, L. *Linear Algebra* (2003). Prentice Hall. 9780130084514.
 - [31] Fukagawa, H. and Fujitani, Y. *A Variational Principle for Dissipative Fluid Dynamics* (2012). Progress of Theoretical Physics, Volume 127, Issue 5, May 2012, Pages 921–935.
 - [32] Galley, Chad R. *Classical Mechanics of Nonconservative Systems* (2013). Physical Review, Vol. 110, issue 17.
 - [33] Galley, C. Tsang, D. Stein, L. C. *The principle of stationary nonconservative action for classical mechanics and field theories* (2014). arXiv:1412.3082.
 - [34] Gatland, I. R. *Nonholonomic Constraints: A test case* (2004). American Journal of Physics 72, 941. doi: 10.1119/1.1701844.
 - [35] Giles, R. *Reconstruction of gauge potentials from Wilson loops* (1981). Physical Review D, Vol. 24, no. 8.
 - [36] Glashow, S. *The Elegant Universe* NOVA Interview (2003).
 - [37] Goldstein, H. *Classical Mechanics* (2011). Pearson Education, Inc. 9788131758915.
 - [38] Götze, H.J. *International Gravity Formula* (2019). In: Gupta, H. (eds) Encyclopedia of Solid Earth Geophysics. Encyclopedia of Earth Sciences Series. Springer, Cham. 9783030104757.
 - [39] Gralla, S. Harte, A. and Wald, R. *A Rigorous Derivation of Electromagnetic Self-force* (2009). arXiv:0905.2391.
 - [40] Gustafson, J. L. *Asymptotic formulas for elliptic integrals* (1982). Retrospective Theses and Dissertations. 7501. <https://lib.dr.iastate.edu/rtd/7501>.
 - [41] Hall, B. C. *Lie Groups, Lie Algebras, and Representations* (2015). Springer Graduate Texts in Mathematics. 9783319134673.
 - [42] Hawking, S. W. Ellis, G. F. R. *The Large Scale Structure of Space-Time* (1975). Cambridge Monographs in Mathematical Physics. Cambridge University Press. 9780521099066.
 - [43] Henneaux, M. and Teitelboim, C. *Quantization of Gauge Systems* (1994). Princeton University Press. 9780691037691.
 - [44] Hermann, A. *The Genesis of Quantum Theory* (1971). In reference to a letter between Planck, M. and Wood, R. W. on October 7, 1931. English translation by C. W. Nash. Physik Verlag, Mosbach/Baden.
 - [45] Heslot, A. *Quantum mechanics as a classical theory* (1985). Phys. Rev. D. Vol. 31, issue 6. doi:10.1103/PhysRevD.31.1341.
 - [46] Horn, R.A. and Johnson, C.R. *Matrix analysis (2nd ed.)* (2013). Cambridge University Press.
 - [47] Huff, D. Prewett, O. *The nature of the physical universe: 1976 Nobel Conference* (1979). Wiley. 9780471031901
 - [48] Hydon, P. *Symmetry Methods for Differential Equations* (2005). Cambridge University Press. 9780521497039.
 - [49] Israel, W. and Stewart, J. M. *On Transient Relativistic Thermodynamics and Kinetic Theory. II* (1979). Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, 365(1720), 43–52.
 - [50] Iwinski, Z. and Turski, K. *Canonical Theories of Systems Interacting Electromagnetically* (1976). Appl. Eng Sci. 4 (3), 179-191.
 - [51] Iyer, V. and Wald, R. *Some Properties of Noether Charge and a Proposal for Dynamical Black Hole Entropy* (1994). Phys. Rev. D, Vol. 50, no. 2.
 - [52] Jackson, J. D. *Classical Electrodynamics* (1999). New York: John Wiley and Sons. 9780471309321.
 - [53] James, F. *Statistical Methods in Experimental Physics* (2006). World Scientific. 9789812705273.
 - [54] Janssen, M. et al (ed.). *The Collected Papers of Albert Einstein. Volume 7: The Berlin Years: Writings, 1918–1921* (2002). Quoting Einstein, A. *Document 31: Ideas and Methods. II. The theory of General Relativity*. Princeton University Press.
 - [55] Jones, C. and Maltese, M. *Fast and Furry-ous* (1949). Warner Bros.
 - [56] Kleppner and Kolenkow. *An Introduction to Mechanics* (2013). Cambridge University Press. 9780521198110.
 - [57] Klimontovich, Y. *Statistical Physics* (1986). Harwood Academic Publishers GmbH.

- [58] Koopman, B. *Quantum Theory and the Foundations of Probability* (1957). Applied Probability. Proceedings of the Symposia in Applied Mathematics, Volume 7. McGraw-Hill Book Company Inc.
- [59] Lamb Jr, W.E. and Scully, M.O. *The photoelectric effect without photons* (1968). 1968. No. TS-QED-68-1.
- [60] Landau, L. D. and Lifshitz, E. *Course of Theoretical Physics Volume 1: Mechanics* (1982). United Kingdom: Elsevier Science.
- [61] Landau, L. D. and Lifshitz, E. *Course of Theoretical Physics Volume 5: Statistical Physics*. (1980). Pergamon Press Ltd.
- [62] Landau, L. D. and Lifshitz, E. *Course of Theoretical Physics Volume 6: Fluid Mechanics* (1986). Pergamon Press Ltd.
- [63] Mach, E. *The Science of Mechanics* (1919). The Open Court Publishing Co.
- [64] Maclean, I. *Logic, Signs, and Nature in the Renaissance: The Case of Learned Medicine* (2007). Translates the original Latin of Kepler, J. *Concerning the More Certain Fundamentals of Astrology* (1601).
- [65] Maggiore, M. *Gravitational Waves* (2007). Oxford University Press. 9780198570745.
- [66] Mandel, L. and Wolf, E. *Optical Coherence and Quantum Optics* (1995). United Kingdom: Cambridge University Press.
- [67] Manzano, D. *A short introduction to the Lindblad master equation* (2020). AIP Advances 1 February 2020; 10 (2): 025106. doi:/10.1063/1.5115323.
- [68] Mendelev, D. Faraday Lecture, the Royal Institution, London (1889).
- [69] Merzbacher, E. *Quantum Mechanics, 3rd ed* (1998). John Wiley & Sons, Inc. 9780471887027.
- [70] Meyer, C. *Basic Electronics: An Introduction to Electronics for Science Students* (2010).
- [71] Milham, W. I. *Time and Timekeepers* (1945). New York: MacMillan. 0780800087.
- [72] Misner, C. W. Thorne, K. S. Wheeler, J. A. *Gravitation* (2017). Princeton University Press. 9780691177793.
- [73] Mostow, M. and Shnider, S. *Counterexamples to some results on the existence of field copies* (1983). Communications in Mathematical Physics, 90(4) 521-526 1983.
- [74] Mott, N. F. *The Solution of the Wave Equation for the Scattering of Particles by a Coulombian Centre of Force* (1928). Proc. R. Soc. Lond. A118542–549. doi:10.1098/rspa.1928.0067.
- [75] Mott, N. F. *The wave mechanics of Alpha-Ray tracks* (1929). Proc. R. Soc. Lond. A12679–84. doi:10.1098/rspa.1929.0205.
- [76] Neumaier, A. *Coherent Quantum Physics: A Reinterpretation of the Tradition* (2019). De Gruyter. 9783110667295.
- [77] New York Times, May 4 1935.
- [78] Newell, D. and Tiesinga, E. (Editors). *The International System of Units (SI)* (2019). National Institute of Standards and Technology. Special Publication 330.
- [79] Nieuwenhuizen, T.M. *Is the Contextuality Loophole Fatal for the Derivation of Bell Inequalities?* (2011). Found Phys 41, 580–591. doi:10.1007/s10701-010-9461-z
- [80] Olver, P. *Applications of Lie Groups to Differential Equations* (1993). Springer Graduate Texts in Mathematics. 9780387950006.
- [81] Olver, P. *Equivalence, Invariants, and Symmetry* (1995). Cambridge University Press. 9780521478113.
- [82] Olver, P. *Introduction to Partial Differential Equations* (2014). Springer Undergraduate Texts in Mathematics. 9783319020990.
- [83] Olver, P. *Symmetry and Moving Frames* (2012) online lecture notes. University of Minnesota. <http://www-users.math.umn.edu/olver/sm.html>.
- [84] Olver, P. and Shakiban, C. *Applied Linear Algebra* (2018). Springer Undergraduate Texts in Mathematics. 9783319910413.
- [85] O'Reilly, B. *The O'Reilly Factor* January 4, 2011. Fox News.
- [86] Peskin, M. and Schroeder, D. *An Introduction To Quantum Field Theory* (2015). Frontiers in Physics. Westview Press. 9780813350196.
- [87] Planck, Max K. *Scientific Autobiography and Other Papers* (1950). New York: Philosophical library.
- [88] Poisson, E. *A Relativist's Toolkit: The Mathematics of Black-Hole Mechanics* (2004). United Kingdom: Cambridge University Press.
- [89] Purcell, E. and Morin, D. *Electricity and Magnetism* (2013). Cambridge University Press. 9781107014022.
- [90] Ralston, J. P. *Emergent un-Quantum Mechanics* (2013). In (Ed.), *Advances in Quantum Mechanics*.

- IntechOpen. doi: 10.5772/55954.
- [91] Ralston, J. P. *PT and CPT Quantum Mechanics Embedded in Symplectic Quantum Mechanics* (2007). J. Phys. A: Math. Theor. 40 9883.
 - [92] Ralston, J. P. *Understanding Basic Quantum Mechanics* (2016).
 - [93] Ralston, J. P. *Quantum Probability* (2015).
 - [94] Reid, C. *Hilbert* (1970).
 - [95] Rezzolla, L. and Zanotti, O. *Relativistic Hydrodynamics* (2013). Oxford University Press. 9780198528906.
 - [96] Richeson, D. and Wiseman, J. *A Fixed Point Theorem for Bounded Dynamical Systems* (2002). Illinois Journal of Mathematics 46, no. 2 (2002): 491-495.
 - [97] Rosenbaum, D. *Proof of the Impossibility of a Classical Action Principle for Magnetic Monopoles and Charges without Subsidiary Conditions* (1965). Physical Review, Vol. 147, no. 4.
 - [98] Sakurai, J.J. and Napolitano, J. *Modern Quantum Mechanics* (2011). Pearson Education, Inc.
 - [99] Salam, A. Nobel Banquet. December 10, 1979.
 - [100] Salam, A. *Grand Unification of Fundamental Forces*. Nobel Lecture. December 8, 1979.
 - [101] Salmon, R. *Lectures on Geophysical Fluid Dynamics* (1998). Oxford University Press.
 - [102] Schilpp, P. A. (ed.). *Albert Einstein-Philosopher Scientist (2nd ed)* (1998). Autobiographical Notes of Einstein, A. (1951). New York: Tudor Publishing.
 - [103] Schonfeld, J. F. *The First Droplet in a Cloud Chamber Track* (2021). Foundations of Physics 51 (2):1-18.
 - [104] Schrödinger, E. Letter to John Lighton Synge, November 9, 1959.
 - [105] Schwinger, J. DeRaad, L. L. Milton, K. A. *Casimir effect in dielectrics* (1978). Ann. Phys. (N.Y.) 115, 1-23.
 - [106] Sethna, J. *Entropy, Order Parameters, and Complexity* (2011). Oxford University Press.
 - [107] Smith, G. *Newton's Philosophiae Naturalis Principia Mathematica in The Stanford Encyclopedia of Philosophy* (2008). <https://plato.stanford.edu/archives/win2008/entries/newton-principia/>
 - [108] Shankar, R. *Principles of Quantum Mechanics* (1994). Springer, 2nd edition. 9780306447907.
 - [109] Soper, D. *Classical Field Theory* (2008). Dover Publications. 9780486462608.
 - [110] Sparavigna, A. *The Science of Al-Biruni* (2013). International Journal of Sciences. 2 (12): 52–60. arXiv:1312.7288. doi:10.18483/ijSci.364. S2CID 119230163.
 - [111] Spivak, M. *Calculus* (2006). Cambridge University Press. 9780521867443.
 - [112] Srednicki, M. *Quantum Field Theory* (2007). Cambridge University Press. 9780521864497.
 - [113] Staley, K. *An Introduction to the Philosophy of Science (Cambridge Introductions to Philosophy)* (2014). Cambridge: Cambridge University Press. doi: 10.1017/CB09781139047760
 - [114] Stoker, B. *Dracula* (1897). Archibald Constable and Company (UK).
 - [115] Strogatz, S.H. and Dichter, M. *Nonlinear Dynamics and Chaos, 2nd ed* (2016). Studies in Nonlinearity. Avalon Publishing. 9780813350844.
 - [116] Styer, D. *Statistical Mechanics* (2014). <http://www.oberlin.edu/physics/dstyer>.
 - [117] Taylor, J. *Classical Mechanics* (2005). University Science Books. 9781891389221.
 - [118] Tolman, R. *Principles of Statistical Mechanics* (1938). Oxford University Press.
 - [119] Tong, D. *Lectures on Fluid Mechanics* (2022) online lecture notes. University of Cambridge. <http://www.damtp.cam.ac.uk/user/tong/fluids/fluids.pdf>.
 - [120] Tonti, E. *Variational Formulation of Nonlinear Differential Equations* (1969). Classe Des Sciences, Series 5, Tome 55.
 - [121] Wald, R. *Advanced Classical Electromagnetism* (2022). Princeton University Press.
 - [122] Wald, R. *General Relativity* (1984). University of Chicago Press.
 - [123] Walsh, J. *Knowing the Odds: An Introduction to Probability* (2012). American Mathematical Society. 9780821885321.
 - [124] Walton, F. R. (Translator). *Diodorus Siculus, Library of History, Volume XI: Fragments of Books 21-32* (1957). Loeb Classical Library 409. Harvard University Press.
 - [125] Weinberg, S. *The Quantum Theory of Fields, Volume 1: Foundations* (2005). Cambridge University Press. 9780521670531.
 - [126] Weinberg, S. *Dreams of a Final Theory: The Scientist's Search for the Ultimate Laws of Nature* (1994). Knopf Doubleday Publishing Group. 9780679744085.
 - [127] Weinberg, S. *Lectures on Quantum Mechanics* (2015). Cambridge University Press, 2nd edition. 9781107111660.
 - [128] Zangwill, A. *Modern Electrodynamics* (2012). Cambridge University Press. 9780521896979.
 - [129] P.A. Zyla et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020)