Quantum Theory, Groups and Representations: An Introduction (*under construction*)

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Preface

This document began as course notes prepared for a class taught at Columbia during the 2012-13 academic year. The intent was to cover the basics of quantum mechanics, up to and including basic material on relativistic quantum field theory, from a point of view emphasizing the role of unitary representations of Lie groups in the foundations of the subject. It has been significantly rewritten and extended during the past year and the intent is to continue this process based upon experience teaching the same material during 2014-5. The current state of the document is that of a first draft of a book. As changes are made, the latest version will be available at

`http://www.math.columbia.edu/~woit/QM/qmbook.pdf`

Corrections, comments, criticism, and suggestions about improvements are encouraged, with the best way to contact me email to woit@math.columbia.edu

The approach to this material is simultaneously rather advanced, using crucially some fundamental mathematical structures normally only discussed in graduate mathematics courses, while at the same time trying to do this in as elementary terms as possible. The Lie groups needed are relatively simple ones that can be described purely in terms of small matrices. Much of the representation theory will just use standard manipulations of such matrices. The only prerequisite for the course as taught was linear algebra and multi-variable calculus. My hope is that this level of presentation will simultaneously be useful to mathematics students trying to learn something about both quantum mechanics and representation theory, as well as to physics students who already have seen some quantum mechanics, but would like to know more about the mathematics underlying the subject, especially that relevant to exploiting symmetry principles.

The topics covered often intentionally avoid overlap with the material of standard physics courses in quantum mechanics and quantum field theory, for which many excellent textbooks are available. This document is best read in conjunction with such a text. Some of the main differences with standard physics presentations include:

- The role of Lie groups, Lie algebras, and their unitary representations is systematically emphasized, including not just the standard use of these to derive consequences for the theory of a "symmetry" generated by operators commuting with the Hamiltonian.

- Symplectic geometry and the role of the Lie algebra of functions on phase space in Hamiltonian mechanics is emphasized, with quantization just the passage to a unitary representation of (a subalgebra of) this Lie algebra.
- The role of the metaplectic representation and the subtleties of the projective factor involved are described in detail.
- The parallel role of the Clifford algebra and spinor representation are extensively investigated.
- Some topics usually first encountered in the context of relativistic quantum field theory are instead first developed in simpler non-relativistic or finite-dimensional contexts. Non-relativistic quantum field theory based on the Schrödinger equation is described in detail before moving on to the relativistic case. The topic of irreducible representations of space-time symmetry groups is first encountered with the case of the Euclidean group, where the implications for the non-relativistic theory are explained. The analogous problem for the relativistic case, that of the irreducible representations of the Poincaré group, is then worked out later on.
- The emphasis is on the Hamiltonian formalism and its representation-theoretical implications, with the Lagrangian formalism de-emphasized. In particular, the operators generating symmetry transformations are derived using the moment map for the action of such transformations on phase space, not by invoking Noether's theorem for transformations that leave invariant a Lagrangian.
- Care is taken to keep track of the distinction between vector spaces and their duals, as well as the distinction between real and complex vector spaces, making clear exactly where complexification and the choice of a complex structure enters the theory.
- A fully rigorous treatment of the subject is beyond the scope of what is covered here, but an attempt is made to keep clear the difference between where a rigorous treatment could be pursued relatively straight-forwardly, and where there are serious problems of principle making a rigorous treatment very hard to achieve.

Chapter 1

Introduction and Overview

1.1 Introduction

A famous quote from Richard Feynman goes "I think it is safe to say that no one understands quantum mechanics."[17]. In this book we'll pursue one possible route to such an understanding, emphasizing the deep connections of quantum mechanics to fundamental ideas and powerful techniques of modern mathematics. The strangeness inherent in quantum theory that Feynman was referring to has two rather different sources. One of them is the inherent disjunction and incommensurability between the conceptual framework of the classical physics which governs our everyday experience of the physical world, and the very different framework which governs physical reality at the atomic scale. Familiarity with the powerful formalisms of classical mechanics and electromagnetism provides deep understanding of the world at the distance scales familiar to us. Supplementing these with the more modern (but still "classical" in the sense of "not quantum") subjects of special and general relativity extends our understanding into other less accessible regimes, while still leaving atomic physics a mystery.

Read in context though, Feynman was pointing to a second source of difficulty, contrasting the mathematical formalism of quantum mechanics with that of the theory of general relativity, a supposedly equally hard to understand subject. General relativity can be a difficult subject to master, but its mathematical and conceptual structure involves a fairly straight-forward extension of structures that characterize 19th century physics. The fundamental physical laws (Einstein's equations for general relativity) are expressed as partial differential equations, a familiar if difficult mathematical subject. The state of the system is determined by the set of fields satisfying these equations, and observable quantities are functionals of these fields. The mathematics is just that of the usual calculus: differential equations and their real-valued solutions.

In quantum mechanics, the state of a system is best thought of as a different sort of mathematical object: a vector in a complex vector space, the so-called

state space. One can sometimes interpret this vector as a function, the wavefunction, although this comes with the non-classical feature that wavefunctions are complex-valued. What's truly completely different is the treatment of observable quantities, which correspond to self-adjoint linear operators on the state space. This has no parallel in classical physics, and violates our intuitions about how physics should work, with observables now often no longer commuting.

During the earliest days of quantum mechanics, the mathematician Hermann Weyl quickly recognized that the mathematical structures being used were ones he was quite familiar with from his work in the field of representation theory. From the point of view that takes representation theory as a fundamental structure, the framework of quantum mechanics looks perfectly natural. Weyl soon wrote a book expounding such ideas [72], but this got a mixed reaction from physicists unhappy with the penetration of unfamiliar mathematical structures into their subject (with some of them characterizing the situation as the "Gruppenpest", the group theory plague). One goal of this course will be to try and make some of this mathematics as accessible as possible, boiling down Weyl's exposition to its essentials while updating it in the light of many decades of progress and better understanding of the subject.

Weyl's insight that quantum mechanics crucially involves understanding the Lie groups that act on the phase space of a physical system and the unitary representations of these groups has been vindicated by later developments which dramatically expanded the scope of these ideas. The use of representation theory to exploit the symmetries of a problem has become a powerful tool that has found uses in many areas of science, not just quantum mechanics. I hope that readers whose main interest is physics will learn to appreciate the mathematical structures that lie behind the calculations of standard textbooks, helping them understand how to effectively exploit them in other contexts. Those whose main interest is mathematics will hopefully gain some understanding of fundamental physics, at the same time as seeing some crucial examples of groups and representations. These should provide a good grounding for appreciating more abstract presentations of the subject that are part of the standard mathematical curriculum. Anyone curious about the relation of fundamental physics to mathematics, and what Eugene Wigner described as "The Unreasonable Effectiveness of Mathematics in the Natural Sciences"[73] should benefit from an exposure to this remarkable story at the intersection of the two subjects.

The following sections give an overview of the fundamental ideas behind much of the material to follow. In this sketchy and abstract form they will likely seem rather mystifying to those meeting them for the first time. As we work through basic examples in coming chapters, a better understanding of the overall picture described here should start to emerge.

1.2 Basic principles of quantum mechanics

We'll divide the conventional list of basic principles of quantum mechanics into two parts, with the first covering the fundamental mathematics structures.

1.2.1 Fundamental axioms of quantum mechanics

In classical physics, the state of a system is given by a point in a "phase space", which one can think of equivalently as the space of solutions of an equation of motion, or as (parametrizing solutions by initial value data) the space of coordinates and momenta. Observable quantities are just functions on this space (i.e. functions of the coordinates and momenta). There is one distinguished observable, the energy or Hamiltonian, and it determines how states evolve in time through Hamilton's equations.

The basic structure of quantum mechanics is quite different, with the formalism built on the following simple axioms:

Axiom (States)**.** *The state of a quantum mechanical system is given by a non-zero vector in a complex vector space $\mathcal{H}$ with Hermitian inner product $\langle \cdot, \cdot \rangle$.*

We'll review in chapter 4 some linear algebra, including the properties of inner products on complex vector spaces. $\mathcal{H}$ may be finite or infinite dimensional, with further restrictions required in the infinite-dimensional case (e.g. we may want to require $\mathcal{H}$ to be a Hilbert space). Note two very important differences with classical mechanical states:

- The state space is always linear: a linear combination of states is also a state.
- The state space is a *complex* vector space: these linear combinations can and do crucially involve complex numbers, in an inescapable way. In the classical case only real numbers appear, with complex numbers used only as an inessential calculational tool.

In this course we will sometimes use the notation introduced by Dirac for vectors in the state space $\mathcal{H}$: such a vector with a label ψ is denoted

$$|\psi\rangle$$

Axiom (Observables)**.** *The observables of a quantum mechanical system are given by self-adjoint linear operators on $\mathcal{H}$.*

We'll also review the notion of self-adjointness in our review of linear algebra. When $\mathcal{H}$ is infinite-dimensional, further restrictions will be needed on the class of linear operators to be used.

Axiom (Dynamics)**.** *There is a distinguished observable, the Hamiltonian H. Time evolution of states $|\psi(t)\rangle \in \mathcal{H}$ is given by the Schrödinger equation*

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle$$

The Hamiltonian observable H will have a physical interpretation in terms of energy, and one may also want to specify some sort of positivity property on H, in order to assure the existence of a stable lowest energy state.

$\hbar$ is a dimensional constant, the value of which depends on what units one uses for time and for energy. It has the dimensions $[energy] \cdot [time]$ and its experimental values are

$$1.054571726(47) \times 10^{-34}\text{Joule} \cdot \text{seconds} = 6.58211928(15) \times 10^{-16}\text{eV} \cdot \text{seconds}$$

(eV is the unit of "electron-Volt", the energy acquired by an electron moving through a one-Volt electric potential). The most natural units to use for quantum mechanical problems would be energy and time units chosen so that $\hbar = 1$. For instance one could use seconds for time and measure energies in the very small units of 6.6×10^{-16} eV, or use eV for energies, and then the very small units of 6.6×10^{-16} seconds for time. Schrödinger's equation implies that if one is looking at a system where the typical energy scale is an eV, one's state-vector will be changing on the very short time scale of 6.6×10^{-16} seconds. When we do computations, usually we will just set $\hbar = 1$, implicitly going to a unit system natural for quantum mechanics. When we get our final result, we can insert appropriate factors of $\hbar$ to allow one to get answers in more conventional unit systems.

It is sometimes convenient however to carry along factors of $\hbar$, since this can help make clear which terms correspond to classical physics behavior, and which ones are purely quantum mechanical in nature. Typically classical physics comes about in the limit where

$$\frac{(energy\ scale)(time\ scale)}{\hbar}$$

is large. This is true for the energy and time scales encountered in everyday life, but it can also always be achieved by taking $\hbar \to 0$, and this is what will often be referred to as the "classical limit".

1.2.2 Principles of measurement theory

The above axioms characterize the mathematical structure of a quantum theory, but they don't address the "measurement problem". This is the question of how to apply this structure to a physical system interacting with some sort of macroscopic, human-scale experimental apparatus that "measures" what is going on. This is highly thorny issue, requiring in principle the study of two interacting quantum systems (the one being measured, and the measurement apparatus) in an overall state that is not just the product of the two states, but is highly "entangled" (for the meaning of this term, see chapter 9). Since a macroscopic apparatus will involve something like 10^{23} degrees of freedom, this question is extremely hard to analyze purely within the quantum mechanical framework (for one thing, one would need to solve a Schrödinger equation in 10^{23} variables).

Instead of trying to resolve in general this problem of how classical physics behavior emerges for macroscopic objects, one can adopt the following two principles as describing what will happen, and these allow one to make precise statistical predictions using quantum theory:

Principle (Observables)**.** *States where the value of an observable can be characterized by a well-defined number are the states that are eigenvectors for the corresponding self-adjoint operator. The value of the observable in such a state will be a real number, the eigenvalue of the operator.*

This principle identifies the states we have some hope of sensibly associating a label to (the eigenvalue), a label which in some contexts corresponds to an observable quantity characterizing states in classical mechanics. The observables of most use will turn out to correspond to some group action on the physical system (for instance the energy, momentum, angular momentum, or charge).

Principle (The Born rule)**.** *Given an observable O and two unit-norm states $|\psi_1\rangle$ and $|\psi_2\rangle$ that are eigenvectors of O with eigenvalues λ_1 and λ_2 (i.e. $O|\psi_1\rangle = \lambda_1|\psi_1\rangle$ and $O|\psi_2\rangle = \lambda_2|\psi_2\rangle$), the complex linear combination state*

$$c_1|\psi_1\rangle + c_2|\psi_2\rangle$$

may not have a well-defined value for the observable O. If one attempts to measure this observable, one will get either λ_1 or λ_2, with probabilities

$$\frac{|c_1^2|}{|c_1^2| + |c_2^2|}$$

and

$$\frac{|c_2^2|}{|c_1^2| + |c_2^2|}$$

respectively.

The Born rule is sometimes raised to the level of an axiom of the theory, but it is plausible to expect that, given a full understanding of how measurements work, it can be derived from the more fundamental axioms of the previous section. Such an understanding though of how classical behavior emerges in experiments is a very challenging topic, with the notion of "decoherence" playing an important role. See the end of this chapter for some references that discuss the these issues in detail.

Note that the state $c|\psi\rangle$ will have the same eigenvalues and probabilities as the state $|\psi\rangle$, for any complex number c. It is conventional to work with states of norm fixed to the value 1, which fixes the amplitude of c, leaving a remaining ambiguity which is a phase $e^{i\theta}$. By the above principles this phase will not contribute to the calculated probabilities of measurements. We will however not at all take the point of view that this phase information can be ignored. It plays an important role in the mathematical structure, and the relative phase of two different states certainly does affect measurement probabilities.

1.3 Unitary group representations

The mathematical framework of quantum mechanics is closely related to what mathematicians describe as the theory of "unitary group representations". We

will be examining this notion in great detail and working through many examples in coming chapters, but here's a quick summary of the relevant definitions, as well as an indication of the relationship to the quantum theory formalism.

Definition (Group)**.** *A group G is a set with an associative multiplication, such that the set contains an identity element, as well as the multiplicative inverse of each element.*

Many different kinds of groups are of interest in mathematics, with an example of the sort that we will be interested in the group of all rotations about a point in 3-dimensional space. Most of the groups we will consider are "matrix groups", i.e. subgroups of the group of n by n invertible matrices (with real or complex coefficients).

Definition (Representation)**.** *A (complex) representation (π, V) of a group G is a homomorphism*

$$\pi : g \in G \to \pi(g) \in GL(V)$$

where $GL(V)$ is the group of invertible linear maps $V \to V$, with V a complex vector space.

Saying the map π is a homomorphism means

$$\pi(g_1)\pi(g_2) = \pi(g_1 g_2)$$

for all $g_1, g_2 \in G$. When V is finite dimensional and we have chosen a basis of V, then we have an identification of linear maps and matrices

$$GL(V) \simeq GL(n, \mathbf{C})$$

where $GL(n, \mathbf{C})$ is the group of invertible n by n complex matrices. We will begin by studying representations that are finite dimensional and will try to make rigorous statements. Later on we will get to representations on function spaces, which are infinite dimensional, and from then on will need to consider the serious analytical difficulties that arise when one tries to make mathematically precise statements in the infinite-dimensional case.

One source of confusion is that representations (π, V) are sometimes referred to by the map π, leaving implicit the vector space V that the matrices $\pi(g)$ act on, but at other times referred to by specifying the vector space V, leaving implicit the map π. One reason for this is that the map π may be the identity map: often G is a matrix group, so a subgroup of $GL(n, \mathbf{C})$, acting on $V \simeq \mathbf{C}^n$ by the standard action of matrices on vectors. One should keep in mind though that just specifying V is generally not enough to specify the representation, since it may not be the standard one. For example, it could very well carry the trivial representation, where

$$\pi(g) = \mathbf{1}_n$$

i.e. each element of G acts on V as the identity.

It turns out that in mathematics the most interesting classes of complex representations are "unitary", i.e. preserving the notion of length given by

the standard Hermitian inner product in a complex vector space. In physical applications, the group representations under consideration typically correspond to physical symmetries, and will preserve lengths in $\mathcal{H}$, since these correspond to probabilities of various observations. We have the definition

Definition (Unitary representation)**.** *A representation (π, V) on a complex vector space V with Hermitian inner product $\langle \cdot, \cdot \rangle$ is a unitary representation if it preserves the inner product, i.e.*

$$\langle \pi(g)v_1, \pi(g)v_2 \rangle = \langle v_1, v_2 \rangle$$

for all $g \in G$ and $v_1, v_2 \in V$.

For a unitary representation, the matrices $\pi(g)$ take values in a subgroup $U(n) \subset GL(n, \mathbf{C})$. In our review of linear algebra we will see that $U(n)$ can be characterized as the group of n by n complex matrices U such that

$$U^{-1} = U^\dagger$$

where $U^\dagger$ is the conjugate-transpose of U. Note that we'll be using the notation "$\dagger$" to mean the "adjoint" or conjugate-transpose matrix. This notation is pretty universal in physics, whereas mathematicians prefer to use "$*$" instead of "$\dagger$".

1.4 Representations and quantum mechanics

The fundamental relationship between quantum mechanics and representation theory is that whenever we have a physical quantum system with a group G acting on it, the space of states $\mathcal{H}$ will carry a unitary representation of G (at least up to a phase factor). For physicists working with quantum mechanics, this implies that representation theory provides information about quantum mechanical state spaces. For mathematicians studying representation theory, this means that physics is a very fruitful source of unitary representations to study: any physical system with a symmetry group G will provide one.

For a representation π and group elements g that are close to the identity, one can use exponentiation to write $\pi(g) \in GL(n, \mathbf{C})$ as

$$\pi(g) = e^A$$

where A is also a matrix, close to the zero matrix.

We will study this situation in much more detail and work extensively with examples, showing in particular that if $\pi(g)$ is unitary (i.e. in the subgroup $U(n) \subset GL(n, \mathbf{C})$), then A will be skew-adjoint:

$$A^\dagger = -A$$

where $A^\dagger$ is the conjugate-transpose matrix. Defining $B = iA$, we find that B is self-adjoint

$$B^\dagger = B$$

We thus see that, at least in the case of finite-dimensional $\mathcal{H}$, the unitary representation π of G on $\mathcal{H}$ coming from a symmetry G of our physical system gives us not just unitary matrices $\pi(g)$, but also corresponding self-adjoint operators B on $\mathcal{H}$. Symmetries thus give us quantum mechanical observables, with the fact that these are self-adjoint linear operators corresponding to the fact that symmetries are realized as unitary representations on the state space.

In the following chapters we'll see many examples of this phenomenon. A fundamental example that we will study in detail is that of time-translation symmetry. Here the group $G = \mathbf{R}$ and we get a unitary representation of $\mathbf{R}$ on the space of states $\mathcal{H}$. The corresponding self-adjoint operator is the Hamiltonian operator H. This unitary representation gives the dynamics of the theory, with the Schrödinger equation just the statement that $\frac{i}{\hbar}H\Delta t$ is the skew-adjoint operator that gets exponentiated to give the unitary transformation that moves states $\psi(t)$ ahead in time by an amount Δt.

1.5 Symmetry groups and their representations on function spaces

It is conventional to refer to the groups that appear in this subject as "symmetry groups", which emphasizes the phenomenon of invariance of properties of objects under sets of transformations that form a group. This is a bit misleading though, since we are interested in not just invariance, but the more general phenomenon of groups acting on sets, according to the following definition:

Definition (Group action on a set)**.** *An action of a group G on a set M is given by a map*

$$(g, x) \in G \times M \to g \cdot x \in M$$

such that

$$g_1 \cdot (g_2 \cdot x) = (g_1 g_2) \cdot x$$

and

$$e \cdot x = x$$

where e is the identity element of G

A good example to keep in mind is that of 3-dimensional space $M = \mathbf{R}^3$ with the standard inner product. This comes with an action of the group $G = \mathbf{R}^3$ on $X = M$ by translations, and of the group $G' = O(3)$ of 3-dimensional orthogonal transformations (by rotations about the origin). Note that order matters: we will often be interested in non-commutative groups like G' where $g_1 g_2 \neq g_2 g_1$ for some group elements g_1, g_2

A fundamental principle of modern mathematics is that the way to understand a space X, given as some set of points, is to look at $Fun(M)$, the set of functions on this space. This "linearizes" the problem, since the function space is a vector space, no matter what the geometrical structure of the original set is. If our original set has a finite number of elements, the function space will be

a finite dimensional vector space. In general though it will be infinite dimensional and we will need to further specify the space of functions (i.e. continuous functions, differentiable functions, functions with finite integral, etc.).

Given a group action of G on M, taking complex functions on M provides a representation $(\pi, Fun(M))$ of G, with π defined on functions f by

$$(\pi(g)f)(x) = f(g^{-1} \cdot x)$$

Note the inverse that is needed to get the group homomorphism property to work since one has

$$\begin{aligned}(\pi(g_1)\pi(g_2)f)(x) &= (\pi(g_2)f)(g_1^{-1} \cdot x) \\ &= f(g_2^{-1} \cdot (g_1^{-1} \cdot x)) \\ &= f((g_2^{-1}g_1^{-1}) \cdot x) \\ &= f((g_1 g_2)^{-1} \cdot x) \\ &= \pi(g_1 g_2)f(x)\end{aligned}$$

This calculation would not work out properly for non-commutative G if one defined $(\pi(g)f)(x) = f(g \cdot x)$.

One way to construct quantum mechanical state spaces $\mathcal{H}$ is as "wavefunctions", meaning complex-valued functions on space-time. The above shows that given any group action on space-time, we get a representation π on the state space $\mathcal{H}$ of such wavefunctions.

Note that only in the case of M a finite set of points will we get a finite-dimensional representation this way, since only then will $Fun(M)$ be a finite-dimensional vector space ($\mathbf{C}^{\#\text{ of points in M}}$). A good example to consider to understand this construction is the following:

- Take M to be a set of 3 elements x_1, x_2, x_3. So $Fun(M) = \mathbf{C}^3$. For $f \in Fun(M)$, f is a vector in $\mathbf{C}^3$, with components $(f(x_1), f(x_2), f(x_3))$.
- Take $G = S_3$, the group of permutations of 3 elements. This group has $3! = 6$ elements.
- Take G to act on M by permuting the 3 elements.

  $$(g, x_i) \to g \cdot x_i$$

  where $i = 1, 2, 3$ gives the three elements of M.
- Find the representation matrices $\pi(g)$ for the representation of G on $Fun(M)$ as above

  $$(\pi(g)f)(x_i) = f(g^{-1} \cdot x_i)$$

This construction gives six 3 by 3 complex matrices, which under multiplication of matrices satisfy the same relations as the elements of the group under group multiplication. In this particular case, all the entries of the matrix will be 0 or 1, but that is special to the permutation representation.

The discussion here has been just a quick sketch of some of the ideas behind the material we will cover in later chapters. These ideas will be examined in much greater detail, beginning with the next two chapters, where they will appear very concretely when we discuss the simplest possible quantum systems, those with one and two-complex dimensional state spaces.

1.6 For further reading

We will be approaching the subject of quantum theory from a different direction than the conventional one, starting with the role of symmetry and with the simplest possible finite-dimensional quantum systems, systems which are purely quantum mechanical, with no classical analog. This means that the early discussion one finds in most physics textbooks is rather different than the one here. They will generally include the same fundamental principles described here, but often begin with the theory of motion of a quantized particle, trying to motivate it from classical mechanics. The state space is then a space of wavefunctions, which is infinite-dimensional and necessarily brings some analytical difficulties. Quantum mechanics is inherently a quite different conceptual structure than classical mechanics. The relationship of the two subjects is rather complicated, but it is clear that quantum mechanics cannot be derived from classical mechanics, so attempts to motivate it that way are of necessity unconvincing, although they correspond to the very interesting historical story of how the subject evolved. We will come to the topic of the quantized motion of a particle only in chapter 10, at which point it should become much easier to follow the standard books.

There are many good physics quantum mechanics textbooks available, aimed at a wide variety of backgrounds, and a reader of this book should look for one at an appropriate level to supplement the discussions here. One example would be [57], which is not really an introductory text, but it includes the physicist's version of many of the standard calculations we will also be considering. Some useful textbooks on the subject aimed at mathematicians are [13], [29], [30], [40], and [64]. The first few chapters of [20] provide an excellent while very concise summary of both basic physics and quantum mechanics. One important topic we won't discuss is that of the application of the representation theory of finite groups in quantum mechanics. For this as well as a discussion that overlaps quite a bit with the point of view of this course while emphasizing different areas, see [59].

For the difficult issue of how measurements work and how classical physics emerges from quantum theory, an important part of the story is the notion of "decoherence". Good places to read about this are Wojciech Zurek's updated version of his 1991 Physics Today article [80], as well as his more recent work on "quantum Darwinism" [81]. There is an excellent book on the subject by Schlosshauer [52] and for the details of what happens in real experimental setups, see the book by Haroche and Raimond [31]. For a review of how classical physics emerges from quantum written from the mathematical point of view,

see Landsman [37]. Finally, to get an idea of the wide variety of points of view available on the topic of the "interpretation" of quantum mechanics, there's a volume of interviews [53] with experts on the topic.

Chapter 2

The Group $U(1)$ and its Representations

The simplest example of a Lie group is the group of rotations of the plane, with elements parametrized by a single number, the angle of rotation θ. It is useful to identify such group elements with unit vectors in the complex plane, given by $e^{i\theta}$. The group is then denoted $U(1)$, since such complex numbers can be thought of as 1 by 1 unitary matrices . We will see in this chapter how the general picture described in chapter 1 works out in this simple case. State spaces will be unitary representations of the group $U(1)$, and we will see that any such representation decomposes into a sum of one-dimensional representations. These one-dimensional representations will be characterized by an integer q, and such integers are the eigenvalues of a self-adjoint operator we will call Q, which is an observable of the quantum theory.

One motivation for the notation Q is that this is the conventional physics notation for electric charge, and this is one of the places where a $U(1)$ group occurs in physics. Examples of $U(1)$ groups acting on physical systems include:

- Quantum particles can be described by a complex-valued "wavefunction", and $U(1)$ acts on such wavefunctions by phase transformations of the value of the function. This phenomenon can be used to understand how particles interact with electromagnetic fields, and in this case the physical interpretation of the eigenvalues of the Q operator will be the electric charge of the particle. We will discuss this in detail in chapter 42.

- If one chooses a particular direction in three-dimensional space, then the group of rotations about that axis can be identified with the group $U(1)$. The eigenvalues of Q will have a physical interpretation as the quantum version of angular momentum in the chosen direction. The fact that such eigenvalues are not continuous, but integral, shows that quantum angular momentum has quite different behavior than classical angular momentum.

- When we study the harmonic oscillator we will find that it has a $U(1)$ sym-

metry (rotations in the position-momentum plane), and that the Hamiltonian operator is a multiple of the operator Q for this case. This implies that the eigenvalues of the Hamiltonian (which give the energy of the system) will be integers times some fixed value. When one describes multi-particle systems in terms of quantum fields one finds a harmonic oscillator for each momentum mode, and then the Q for that mode counts the number of particles with that momentum.

We will sometimes refer to the operator Q as a "charge" operator, assigning a much more general meaning to the term than that of the specific example of electric charge. $U(1)$ representations are also ubiquitous in mathematics, where often the integral eigenvalues of the Q operator will be called "weights".

In a very real sense, the reason for the "quantum" in "quantum mechanics" is precisely because of the role of $U(1)$ symmetries. Such symmetries imply observables that characterize states by an integer eigenvalue of an operator Q, and it is this "quantization" of observables that motivates the name of the subject.

2.1 Some representation theory

Recall the definition of a group representation:

Definition (Representation)**.** *A (complex) representation (π, V) of a group G on a complex vector space V (with a chosen basis identifying $V \simeq \mathbf{C}^n$) is a homomorphism*

$$\pi : G \to GL(n, \mathbf{C})$$

This is just a set of n by n matrices, one for each group element, satisfying the multiplication rules of the group elements. n is called the dimension of the representation.

The groups G we are interested in will be examples of what mathematicians call "Lie groups". For those familiar with differential geometry, such groups are examples of smooth manifolds. This means one can define derivatives of functions on G and more generally the derivative of maps between Lie groups. We will assume that our representations are given by differentiable maps π. Some difficult general theory shows that considering the more general case of continuous maps gives nothing new since the homomorphism property of these maps is highly constraining. In any case, our goal in this course will be to study quite explicitly certain specific groups and representations which are central in quantum mechanics, and these representations will always be easily seen to be differentiable.

Given two representations one can form their direct sum:

Definition (Direct sum representation)**.** *Given representations π_1 and π_2 of dimensions n_1 and n_2, one can define another representation, of dimension $n_1 + n_2$ called the direct sum of the two representations, denoted by $\pi_1 \oplus \pi_2$.*

This representation is given by the homomorphism

$$(\pi_1 \oplus \pi_2) : g \in G \to \begin{pmatrix} \pi_1(g) & \mathbf{0} \\ \mathbf{0} & \pi_2(g) \end{pmatrix}$$

In other words, one just takes as representation matrices block-diagonal matrices with π_1 and π_2 giving the blocks.

To understand the representations of a group G, one proceeds by first identifying the irreducible ones, those that cannot be decomposed into two representations of lower dimension:

Definition (Irreducible representation)**.** *A representation π is called irreducible if it is not of the form $\pi_1 \oplus \pi_2$, for π_1 and π_2 representations of dimension greater than zero.*

This criterion is not so easy to check, and the decomposition of an arbitrary reducible representation into irreducible components can be a very non-trivial problem. Recall that one gets explicit matrices for the $\pi(g)$ of a representation (π, V) only when a basis for V is chosen. To see if the representation is reducible, one can't just look to see if the $\pi(g)$ are all in block-diagonal form. One needs to find out whether there is some basis for V with respect to which they are all in such form, something very non-obvious from just looking at the matrices themselves.

Digression. *Another approach to this would be to check to see if the representation has no proper non-trivial sub-representations (subspaces of V preserved by the $\pi(g)$). This is not necessarily equivalent to our definition of irreducibility (which is often called "indecomposability"), since a sub-representation may have no complement that is also a sub-representation. A simple example of this occurs for the action of upper triangular matrices on column vectors. Such representations are however non-unitary. In the unitary case indecomposability and irreducibility are equivalent. In these notes unless otherwise specified, one should assume that all representations are unitary, so the distinction between irreducibility and indecomposability will generally not arise.*

The following theorem provides a criterion for determining if a representation is irreducible or not:

Theorem (Schur's lemma)**.** *If a complex representation (π, V) is irreducible, then the only linear maps $M : V \to V$ commuting with all the $\pi(g)$ are $\lambda \mathbf{1}$, multiplication by a scalar $\lambda \in \mathbf{C}$.*

Proof. Since we are working over the field $\mathbf{C}$ (this doesn't work for $\mathbf{R}$), we can always solve the eigenvalue equation

$$det(M - \lambda \mathbf{1}) = 0$$

to find the eigenvalues λ of M. The eigenspaces

$$V_\lambda = \{v \in V : Mv = \lambda v\}$$

are non-zero vector subspaces of V and can also be described as $ker(M - \lambda \mathbf{1})$, the kernel of the operator $M - \lambda \mathbf{1}$. Since this operator and all the $\pi(g)$ commute, we have

$$v \in ker(M - \lambda \mathbf{1}) \implies \pi(g)v \in ker(M - \lambda \mathbf{1})$$

so $ker(M - \lambda \mathbf{1}) \subset V$ is a representation of G. If V is irreducible, we must have either $ker(M - \lambda \mathbf{1}) = V$ or $ker(M - \lambda \mathbf{1}) = 0$. Since λ is an eigenvalue, $ker(M - \lambda \mathbf{1}) \neq 0$, so $ker(M - \lambda \mathbf{1}) = V$ and thus $M = \lambda \mathbf{1}$ as a linear operator on V. □

More concretely Schur's lemma says that for an irreducible representation, if a matrix M commutes with all the representation matrices $\pi(g)$, then M must be a scalar multiple of the unit matrix.

Note that the proof crucially uses the fact that one can solve the eigenvalue equation. This will only be true in general if one works with $\mathbf{C}$ and thus with complex representations. For the theory of representations on real vector spaces, Schur's lemma is no longer true.

An important corollary of Schur's lemma is the following characterization of irreducible representations of G when G is commutative.

Theorem. *If G is commutative, all of its irreducible representations are one-dimensional.*

Proof. For G commutative, $g \in G$, any representation will satisfy

$$\pi(g)\pi(h) = \pi(h)\pi(g)$$

for all $h \in G$. If π is irreducible, Schur's lemma implies that, since they commute with all the $\pi(g)$, the matrices $\pi(h)$ are all scalar matrices, i.e. $\pi(h) = \lambda_h \mathbf{1}$ for some $\lambda_h \in \mathbf{C}$. π is then irreducible exactly when it is the one-dimensional representation given by $\pi(h) = \lambda_h$. □

2.2 The group $U(1)$ and its representations

One can think of the group $U(1)$ as the unit circle, with the multiplication rule on its points given by addition of angles. More explicitly:

Definition (The group $U(1)$)**.** *The elements of the group $U(1)$ are points on the unit circle, which can be labeled by the unit complex number $e^{i\theta}$, for $\theta \in \mathbf{R}$. Note that θ and $\theta + N2\pi$ label the same group element for $N \in \mathbf{Z}$. Multiplication of group elements is just complex multiplication, which by the properties of the exponential satisfies*

$$e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1 + \theta_2)}$$

so in terms of angles the group law is just addition (mod 2π).

By our theorem from the last section, since $U(1)$ is a commutative group, all irreducible representations will be one-dimensional. Such an irreducible representation will be given by a map

$$\pi : U(1) \to GL(1, \mathbf{C})$$

but an invertible 1 by 1 matrix is just an invertible complex number, and we will denote the group of these as $\mathbf{C}^*$. We will always assume that our representations are given by differentiable maps, since we will often want to study them in terms of their derivatives. A differentiable map π that is a representation of $U(1)$ must satisfy homomorphism and periodicity properties which can be used to show:

Theorem 2.1. *All irreducible representations of the group $U(1)$ are unitary, and given by*

$$\pi_k : \theta \in U(1) \to \pi_k(\theta) = e^{ik\theta} \in U(1) \subset GL(1, \mathbf{C}) \simeq \mathbf{C}^*$$

for $k \in \mathbf{Z}$.

Proof. The given π_k satisfy the homomorphism property

$$\pi_k(\theta_1 + \theta_2) = \pi_k(\theta_1)\pi_k(\theta_2)$$

and periodicity property

$$\pi_k(2\pi) = \pi_k(0) = 1$$

We just need to show that any differentiable map

$$f : U(1) \to \mathbf{C}^*$$

satisfying the homomorphism and periodicity properties is of this form. Computing the derivative $f'(\theta) = \frac{df}{d\theta}$ we find

$$\begin{aligned} f'(\theta) &= \lim_{\Delta\theta \to 0} \frac{f(\theta + \Delta\theta) - f(\theta)}{\Delta\theta} \\ &= f(\theta) \lim_{\Delta\theta \to 0} \frac{(f(\Delta\theta) - 1)}{\Delta\theta} \quad \text{(using the homomorphism property)} \\ &= f(\theta) f'(0) \end{aligned}$$

Denoting the constant $f'(0)$ by C, the only solutions to this differential equation satisfying $f(0) = 1$ are

$$f(\theta) = e^{C\theta}$$

Requiring periodicity we find

$$f(2\pi) = e^{C2\pi} = f(0) = 1$$

which implies $C = ik$ for $k \in \mathbf{Z}$, and $f = \pi_k$ for some integer k. □

The representations we have found are all unitary, with π_k taking values not just in $\mathbf{C}^*$, but in $U(1) \subset \mathbf{C}^*$. One can check that the complex numbers $e^{ik\theta}$ satisfy the condition to be a unitary 1 by 1 matrix, since

$$(e^{ik\theta})^{-1} = e^{-ik\theta} = \overline{e^{ik\theta}}$$

These representations are restrictions to the unit circle $U(1)$ of the irreducible representations of the group $\mathbf{C}^*$, which are given by

$$\pi_k : z \in \mathbf{C}^* \to \pi_k(z) = z^k \in \mathbf{C}^*$$

Such representations are not unitary, but they have an extremely simple form, so it sometimes is convenient to work with them, later restricting to the unit circle, where the representation is unitary.

Digression (Fourier analysis of periodic functions)**.** *We'll discuss Fourier analysis more seriously in chapter 10 when we come to the case of the translation groups and of state-spaces that are spaces of "wavefunctions" on space-time. For now though, it might be worth pointing out an important example of a representation of $U(1)$: the space $Fun(S^1)$ of complex-valued functions on the circle S^1. We will evade discussion here of the very non-trivial analysis involved, by not specifying what class of functions we are talking about (e.g. continuous, integrable, differentiable, etc.). Periodic functions can be studied by rescaling the period to 2π, thus looking at complex-valued functions of a real variable ϕ satisfying*

$$f(\phi + N2\pi) = f(\phi)$$

for integer N, which we can think of as functions on a circle, parametrized by angle ϕ. We have an action of the group $U(1)$ on the circle by rotation, with the group element $e^{i\theta}$ acting as:

$$\phi \to \phi + \theta$$

where ϕ is the angle parametrizing the circle S^1.

In chapter 1 we saw that given an action of a group on a space X, we can "linearize" and get a representation $(\pi, Fun(X))$ of the group on the functions on the space, by taking

$$(\pi(g)f)(x) = f(g^{-1} \cdot x)$$

for $f \in Fun(X), x \in X$. Here $X = S^1$, the action is the rotation action and we find

$$(\pi(\theta)f)(\phi) = f(\phi - \theta)$$

since the inverse of a rotation by θ is a rotation by $-\theta$.

This representation $(\pi, Fun(S^1))$ is infinite-dimensional, but one can still ask how it decomposes into the one-dimensional irreducible representations $(\pi_k, \mathbf{C})$ of $U(1)$. What we learn from the subject of Fourier analysis is that each $(\pi_k, \mathbf{C})$ occurs exactly once in the decomposition of $Fun(S^1)$ into irreducibles, i.e.

$$(\pi, Fun(S^1)) = \widehat{\bigoplus}_{k \in \mathbf{Z}} (\pi_k, \mathbf{C})$$

where we have matched the sin of not specifying the class of functions in $Fun(S^1)$ on the left-hand side with the sin of not explaining how to handle the infinite direct sum $\widehat{\oplus}$ on the right-hand side. What can be specified precisely is how the irreducible sub-representation $(\pi_k, \mathbf{C})$ sits inside $Fun(S^1)$. It is the set of functions f satisfying

$$(\pi(\theta)f)(\phi) = f(\phi - \theta) = e^{ik\theta}f(\phi)$$

so explicitly given by the one-complex dimensional space of functions proportional to $e^{-ik\phi}$.

One part of the relevance of representation theory to Fourier analysis is that the representation theory of $U(1)$ picks out a distinguished basis of the infinite-dimensional space of periodic functions by using the decomposition of the function space into irreducible representations. One can then effectively study functions by expanding them in terms of their components in this special basis, writing an $f \in Fun(S^1)$ as

$$f(\phi) = \sum_{k \in Z} c_k e^{ik\phi}$$

for some complex coefficients c_k, with analytical difficulties then appearing as questions about the convergence of this series.

2.3 The charge operator

Recall from chapter 1 the claim of a general principle that, since the state space $\mathcal{H}$ is a unitary representation of a Lie group, we get an associated self-adjoint operator on $\mathcal{H}$. We'll now illustrate this for the simple case of $G = U(1)$. For $\mathcal{H}$ irreducible, the representation is one-dimensional, of the form $(\pi_q, \mathbf{C})$ for some $q \in \mathbf{Z}$, and the self-adjoint operator will just be multiplication by the integer q. In general, we have

$$\mathcal{H} = \mathcal{H}_{q_1} \oplus \mathcal{H}_{q_2} \oplus \cdots \oplus \mathcal{H}_{q_n}$$

for some set of integers $q_1, q_2, \ldots, q_n$ (n is the dimension of $\mathcal{H}$, the q_i may not be distinct) and can define:

Definition. *The charge operator Q for the $U(1)$ representation $(\pi, \mathcal{H})$ is the self-adjoint linear operator on $\mathcal{H}$ that acts by multiplication by q_j on the irreducible representation $\mathcal{H}_{q_j}$. Taking basis elements in $\mathcal{H}_{q_j}$ it acts on $\mathcal{H}$ as the matrix*

$$\begin{pmatrix} q_1 & 0 & \cdots & 0 \\ 0 & q_2 & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & q_n \end{pmatrix}$$

Q is our first example of a quantum mechanical observable, a self-adjoint operator on $\mathcal{H}$. States in the subspaces $\mathcal{H}_{q_j}$ will be eigenvectors for Q and will

have a well-defined numerical value for this observable, the integer q_j. A general state will be a linear superposition of state vectors from different $\mathcal{H}_{q_j}$ and there will not be a well-defined numerical value for the observable Q on such a state.

From the action of Q on $\mathcal{H}$, one can recover the representation, i.e. the action of the symmetry group $U(1)$ on $\mathcal{H}$, by multiplying by i and exponentiating, to get

$$\pi(\theta) = e^{iQ\theta} = \begin{pmatrix} e^{iq_1\theta} & 0 & \cdots & 0 \\ 0 & e^{iq_2\theta} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & e^{iq_n\theta} \end{pmatrix} \in U(n) \subset GL(n, \mathbf{C})$$

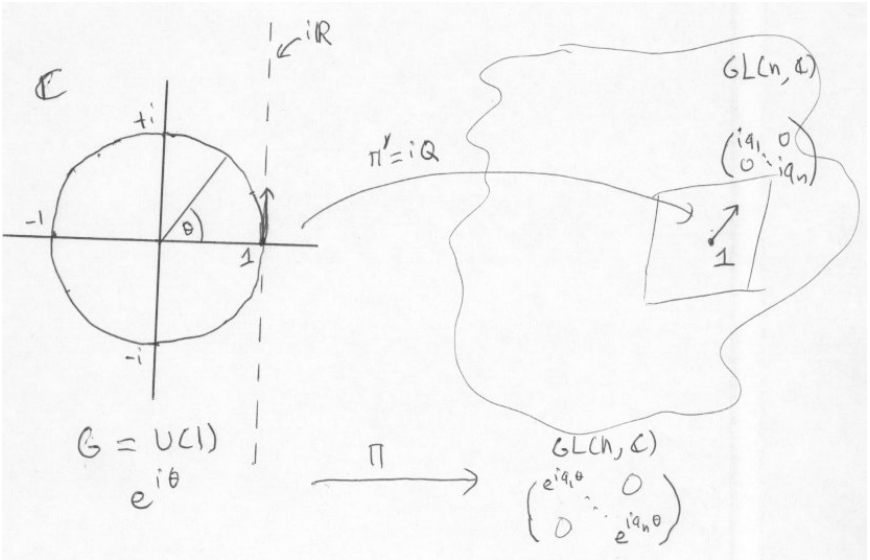
The standard physics terminology is that "Q generates the $U(1)$ symmetry transformations".

The general abstract mathematical point of view (which we will discuss in more detail later) is that the representation π is a map between manifolds, from the Lie group $U(1)$ to the Lie group $GL(n, \mathbf{C})$ that takes the identity of $U(1)$ to the identity of $GL(n, \mathbf{C})$. As such it has a differential π', which is a map from the tangent space at the identity of $U(1)$ (which here is $i\mathbf{R}$) to the tangent space at the identity of $GL(n, \mathbf{C})$ (which is the space $M(n, \mathbf{C})$ of n by n complex matrices). The tangent space at the identity of a Lie group is called a "Lie algebra". We will later study these in detail in many examples to come, including their role in specifying a representation.

Here the relation between the differential of π and the operator Q is

$$\pi' : i\theta \in i\mathbf{R} \to \pi'(i\theta) = iQ\theta$$

One can sketch the situation like this:



The right-hand side of the picture is supposed to somehow represent $GL(n, \mathbf{C})$, which is the $2n^2$ dimensional real vector space of n by n complex matrices, minus the locus of matrices with zero determinant, which are those that can't be inverted. It has a distinguished point, the identity. The derivative π' of the representation map π is the linear operator iQ.

In this very simple example, this abstract picture is over-kill and likely confusing. We will see the same picture though occurring in many other examples in later chapters, examples where the abstract technology is increasingly useful. Keep in mind that, just like in this $U(1)$ case, the maps π will just be exponential maps in the examples we care about, with very concrete incarnations given by exponentiating matrices.

2.4 Conservation of charge and $U(1)$ symmetry

The way we have defined observable operators in terms a group representation on $\mathcal{H}$, the action of these operators has nothing to do with the dynamics. If we start at time $t = 0$ in a state in $\mathcal{H}_{q_j}$, with definite numerical value q_j for the observable, there is no reason that time evolution should preserve this. Recall from one of our basic axioms that time evolution of states is given by the Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle$$

(we have set $\hbar = 1$). We will later more carefully study the relation of this equation to the symmetry of time translation (basically the Hamiltonian operator H generates an action of the group $\mathbf{R}$ of time translations, just as the operator Q generates an action of the group $U(1)$). For now though, note that for time-independent Hamiltonian operators H, the solution to this equation is given by exponentiating H, with

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

for

$$U(t) = e^{-itH}$$

The commutator of two operators O_1, O_2 is defined by

$$[O_1, O_2] := O_1O_2 - O_2O_1$$

and such operators are said to commute if $[O_1, O_2] = 0$. If the Hamiltonian operator H and the charge operator Q commute then Q will also commute with all powers of H

$$[H^k, Q] = 0$$

and thus with the exponential of H, so

$$[U(t), Q] = 0$$

This condition

$$U(t)Q = QU(t) \tag{2.1}$$

implies that if a state has a well-defined value q_j for the observable Q at time $t = 0$, it will continue to have the same value at any other time t, since

$$Q|\psi(t)\rangle = QU(t)|\psi(0)\rangle = U(t)Q|\psi(0)\rangle = U(t)q_j|\psi(0)\rangle = q_j|\psi(t)\rangle$$

This will be a general phenomenon: if an observable commutes with the Hamiltonian observable, we get a conservation law. This conservation law says that if we start in a state with a well-defined numerical value for the observable (an eigenvector for the observable operator), we will remain in such a state, with the value not changing, i.e. "conserved".

In this situation, the group $U(1)$ is said to act as a "symmetry group" of the system. Equation 2.1 implies that

$$U(t)e^{iQ\theta} = e^{iQ\theta}U(t)$$

so the action of the $U(1)$ group on the state space of the system commutes with the time evolution law determined by the choice of Hamiltonian. We see that this notion of symmetry implies a corresponding conservation law.

2.5 Summary

To summarize the situation for $G = U(1)$, we have found

- Irreducible representations π are one-dimensional and characterized by their derivative π' at the identity. If $G = \mathbf{R}$, π' could be any complex number. If $G = U(1)$, periodicity requires that π' must be $iq, q \in \mathbf{Z}$, so irreducible representations are labeled by an integer.

- An arbitrary representation π of $U(1)$ is of the form

  $$\pi(e^{i\theta}) = e^{i\theta Q}$$

  where Q is a matrix with eigenvalues a set of integers q_j. For a quantum system, Q is the self-adjoint observable corresponding to the $U(1)$ symmetry of the system, and is said to be a "generator" of the symmetry.

- If $[Q, H] = 0$, the $U(1)$ group acts on the state space as "symmetries". In this case the q_j will be "conserved quantities", numbers that characterize the quantum states, and do not change as the states evolve in time.

2.6 For further reading

I've had trouble finding another source that covers the material here. Most quantum mechanics books consider it somehow too trivial to mention, starting their discussion of symmetries with more complicated examples.

Chapter 3

Two-state Systems and $SU(2)$

The simplest truly non-trivial quantum systems have state spaces that are inherently two-complex dimensional. This provides a great deal more structure than that seen in chapter 2, which could be analyzed by breaking up the space of states into one-dimensional subspaces of given charge. We'll study these two-state systems in this section, encountering for the first time the implications of working with representations of non-commutative groups. Since they give the simplest non-trivial realization of many quantum phenomena, such systems are the fundamental objects of quantum information theory (the "qubit") and the focus of attempts to build a quantum computer (which would be built out of multiple copies of this sort of fundamental object). Many different possible two-state quantum systems could potentially be used as the physical implementation of a qubit.

One of the simplest possibilities to take would be the idealized situation of a single electron, somehow fixed so that its spatial motion could be ignored, leaving its quantum state described just by its so-called "spin degree of freedom", which takes values in $\mathcal{H} = \mathbf{C}^2$. The term "spin" is supposed to call to mind the angular momentum of an object spinning about about some axis, but such classical physics has nothing to do with the qubit, which is a purely quantum system.

In this chapter we will analyze what happens for general quantum systems with $\mathcal{H} = \mathbf{C}^2$ by first finding the possible observables. Exponentiating these will give the group $U(2)$ of unitary 2 by 2 matrices acting on $\mathcal{H} = \mathbf{C}^2$. This is a specific representation of $U(2)$, the "defining" representation. By restricting to the subgroup $SU(2) \subset U(2)$ of elements of determinant one, we get a representation of $SU(2)$ on $\mathbf{C}^2$ often called the "spin 1/2" representation.

Later on, in chapter 8, we will find all the irreducible representations of $SU(2)$. These are labeled by a natural number

$$N = 0, 1, 2, 3, \dots$$

and have dimension $N+1$. The corresponding quantum systes are said to have "spin $N/2$". The case $N=0$ is the trivial representation on $\mathbf{C}$ and the case $N=1$ is the case of this chapter. In the limit $N \to \infty$ one can make contact with classical notions of spinning objects and angular momentum, but the spin $1/2$ case is at the other limit, where the behavior is purely quantum-mechanical.

3.1 The two-state quantum system

3.1.1 The Pauli matrices: observables of the two-state quantum system

For a quantum system with two-dimensional state space $\mathcal{H} = \mathbf{C}^2$, observables are self-adjoint linear operators on $\mathbf{C}^2$. With respect to a chosen basis of $\mathbf{C}^2$, these are 2 by 2 complex matrices M satisfying the condition $M = M^\dagger$ ($M^\dagger$ is the conjugate transpose of M). Any such matrix will be a (real) linear combination of four matrices:

$$M = c_0\mathbf{1} + c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3$$

with $c_j \in \mathbf{R}$ and the standard choice of basis elements given by

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The σ_j are called the "Pauli matrices" and are a pretty universal choice of basis in this subject. This choice of basis is a convention, with one aspect of this convention that of taking the basis element in the 3-direction to be diagonal. In common physical situations and conventions, the third direction is the distinguished "up-down" direction in space, so often chosen when a distinguished direction in $\mathbf{R}^3$ is needed.

Recall that the basic principle of how measurements are supposed to work in quantum theory says that the only states that have well-defined values for these four observables are the eigenvectors for these matrices. The first matrix gives a trivial observable (the identity on every state), whereas the last one, σ_3, has the two eigenvectors

$$\sigma_3 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$\sigma_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = - \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

with eigenvalues $+1$ and -1. In quantum information theory, where this is the qubit system, these two eigenstates are labeled $|0\rangle$ and $|1\rangle$ because of the analogy with a classical bit of information. Later on when we get to the theory of spin, we will see that $\frac{1}{2}\sigma_3$ is the observable corresponding to the $SO(2) = U(1)$ symmetry group of rotations about the third spatial axis, and the eigenvalues

$-\frac{1}{2}, +\frac{1}{2}$ of this operator will be used to label the two eigenstates

$$|+\frac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The two eigenstates $|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ provide a basis for C^2, so an arbitrary vector in $\mathcal{H}$ can be written as

$$|\psi\rangle = \alpha|+\frac{1}{2}\rangle + \beta|-\frac{1}{2}\rangle$$

for $\alpha, \beta \in \mathbf{C}$. Only if α or β is 0 does the observable σ_3 correspond to a well-defined number that characterizes the state and can be measured. This will be either $\frac{1}{2}$ (if $\beta = 0$ so the state is an eigenvector $|+\frac{1}{2}\rangle$), or $-\frac{1}{2}$ (if $\alpha = 0$ so the state is an eigenvector $|-\frac{1}{2}\rangle$).

An easy to check fact is that $|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ are NOT eigenvectors for the operators σ_1 and σ_2. One can also check that no pair of the three σ_j commute, which implies that one cannot find vectors that are simultaneous eigenvectors for more than one σ_j. This non-commutativity of the operators is responsible for the characteristic classically paradoxical property of quantum observables: one can find states with a well defined number for the measured value of one observable σ_j, but such states will not have a well-defined number for the measured value of the other two non-commuting observables. The physical description of this phenomenon in the realization of this system as a spin $\frac{1}{2}$ particle is that if one prepares states with a well-defined spin component in the j-direction, the two other components of the spin can't be assigned a numerical value in such a state. Any attempt to prepare states that simultaneously have specific chosen numerical values for the 3 observables corresponding to the σ_j is doomed. So is any attempt to simultaneously measure such values: if one measures the value for a particular observable σ_j, then going on to measure one of the other two will ensure that the first measurement is no longer valid (repeating it will not necessarily give the same thing). There are many subtleties in the theory of measurement for quantum systems, but this simple two-state example already shows some of the main features of how the behavior of observables is quite different than in classical physics.

The choice we have made for the σ_j corresponds to a choice of basis for $\mathcal{H}$ such that the basis vectors are eigenvectors of σ_3. σ_1 and σ_2 take these basis vectors to non-trivial linear combinations of basis vectors. It turns out that there are two specific linear combinations of σ_1 and σ_2 that do something very simple to the basis vectors, since

$$(\sigma_1 + i\sigma_2) = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad (\sigma_1 - i\sigma_2) = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$

we have

$$(\sigma_1 + i\sigma_2)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\sigma_1 + i\sigma_2)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and

$$(\sigma_1 - i\sigma_2)\begin{pmatrix}1\\0\end{pmatrix} = 2\begin{pmatrix}0\\1\end{pmatrix} \quad (\sigma_1 - i\sigma_2)\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$$

$(\sigma_1 + i\sigma_2)$ is called a "raising operator": on eigenvectors of σ_3 it either increases the eigenvalue by 2, or annihilates the vector. $(\sigma_1 - i\sigma_2)$ is called a "lowering operator": on eigenvectors of σ_3 it either decreases the eigenvalue by 2, or annihilates the vector. Note that these linear combinations are not self-adjoint, $(\sigma_1 + i\sigma_2)$ is the adjoint of $(\sigma_1 - i\sigma_2)$ and vice-versa.

3.1.2 Exponentials of Pauli matrices: unitary transformations of the two-state system

We saw in chapter 2 that in the $U(1)$ case, knowing the observable operator Q on $\mathcal{H}$ determined the representation of $U(1)$, with the representation matrices found by exponentiating $i\theta Q$. Here we will find the representation corresponding to the two-state system observables by exponentiating the observables in a similar way.

Taking the the identity matrix first, multiplication by $i\theta$ and exponentiation gives the diagonal unitary matrix

$$e^{i\theta\mathbf{1}} = \begin{pmatrix}e^{i\theta} & 0\\ 0 & e^{i\theta}\end{pmatrix}$$

This is just exactly the case studied in chapter 2, for a $U(1)$ group acting on $\mathcal{H} = \mathbf{C}^2$, with

$$Q = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

This matrix commutes with any other 2 by 2 matrix, so we can treat its action on $\mathcal{H}$ independently of the action of the σ_j.

Turning to the other three basis elements of the space of observables, the Pauli matrices, it turns out that since all the σ_j satisfy $\sigma_j^2 = \mathbf{1}$, their exponentials also take a simple form.

$$\begin{aligned} e^{i\theta\sigma_j} &= \mathbf{1} + i\theta\sigma_j + \frac{1}{2}(i\theta)^2\sigma_j^2 + \frac{1}{3!}(i\theta)^3\sigma_j^3 + \cdots \\ &= \mathbf{1} + i\theta\sigma_j - \frac{1}{2}\theta^2\mathbf{1} - i\frac{1}{3!}\theta^3\sigma_j + \cdots \\ &= (1 - \frac{1}{2!}\theta^2 + \cdots)\mathbf{1} + i(\theta - \frac{1}{3!}\theta^3 + \cdots)\sigma_j \\ &= (\cos\theta)\mathbf{1} + i\sigma_j(\sin\theta) \end{aligned} \tag{3.1}$$

As θ goes from $\theta = 0$ to $\theta = 2\pi$, this exponential traces out a circle in the space of unitary 2 by 2 matrices, starting and ending at the unit matrix. This circle is a group, isomorphic to $U(1)$. So, we have found three different $U(1)$

subgroups inside the unitary 2 by 2 matrices, but only one of them (the case $j = 3$) will act diagonally on $\mathcal{H}$, with the $U(1)$ representation determined by

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For the other two cases $j = 1$ and $j = 2$, by a change of basis one could put either one in the same diagonal form, but doing this for one value of j makes the other two no longer diagonal. All three values of j need to be treated simultaneously, and one needs to consider not just the $U(1)$s but the group one gets by exponentiating general linear combinations of Pauli matrices.

To compute such exponentials, one can check that these matrices satisfy the following relations, useful in general for doing calculations with them instead of multiplying out explicitly the 2 by 2 matrices:

$$[\sigma_j, \sigma_k]_+ = \sigma_j\sigma_k + \sigma_k\sigma_j = 2\delta_{jk}\mathbf{1}$$

Here $[\cdot, \cdot]_+$ is the anticommutator. This relation says that all σ_j satisfy $\sigma_j^2 = \mathbf{1}$ and distinct σ_j anticommute (e.g. $\sigma_j\sigma_k = -\sigma_k\sigma_j$ for $j \neq k$).

Notice that the anticommutation relations imply that, if we take a vector $\mathbf{v} = (v_1, v_2, v_3) \in \mathbf{R}^3$ and define a 2 by 2 matrix by

$$\mathbf{v} \cdot \sigma = v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3 = \begin{pmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{pmatrix}$$

then taking powers of this matrix we find

$$(\mathbf{v} \cdot \sigma)^2 = (v_1^2 + v_2^2 + v_3^2)\mathbf{1} = |\mathbf{v}|^2\mathbf{1}$$

If $\mathbf{v}$ is a unit vector, we have

$$(\mathbf{v} \cdot \sigma)^n = \begin{cases} \mathbf{1} & n \text{ even} \\ (\mathbf{v} \cdot \sigma) & n \text{ odd} \end{cases}$$

Replacing σ_j by $\mathbf{v} \cdot \sigma$, the same calculation as for equation 3.1 gives (for $\mathbf{v}$ a unit vector)

$$e^{i\theta\mathbf{v}\cdot\sigma} = (\cos\theta)\mathbf{1} + i(\sin\theta)\mathbf{v} \cdot \sigma$$

Notice that one can easily compute the inverse of this matrix:

$$(e^{i\theta\mathbf{v}\cdot\sigma})^{-1} = (\cos\theta)\mathbf{1} - i(\sin\theta)\mathbf{v} \cdot \sigma$$

since

$$((\cos\theta)\mathbf{1} + i(\sin\theta)\mathbf{v} \cdot \sigma)((\cos\theta)\mathbf{1} - i(\sin\theta)\mathbf{v} \cdot \sigma) = (\cos^2\theta + \sin^2\theta)\mathbf{1} = \mathbf{1}$$

We'll review linear algebra and the notion of a unitary matrix in chapter 4, but one form of the condition for a matrix M to be unitary is

$$M^\dagger = M^{-1}$$

so the self-adjointness of the σ_j implies unitarity of $e^{i\theta\mathbf{v}\cdot\sigma}$ since

$$\begin{aligned}(e^{i\theta\mathbf{v}\cdot\sigma})^\dagger &= ((\cos\theta)\mathbf{1} + i(\sin\theta)\mathbf{v}\cdot\sigma)^\dagger \\ &= ((\cos\theta)\mathbf{1} - i(\sin\theta)\mathbf{v}\cdot\sigma^\dagger) \\ &= ((\cos\theta)\mathbf{1} - i(\sin\theta)\mathbf{v}\cdot\sigma) \\ &= (e^{i\theta\mathbf{v}\cdot\sigma})^{-1}\end{aligned}$$

One can also easily compute the determinant of $e^{i\theta\mathbf{v}\cdot\sigma}$, finding

$$\begin{aligned}det(e^{i\theta\mathbf{v}\cdot\sigma}) &= det((\cos\theta)\mathbf{1} + i(\sin\theta)\mathbf{v}\cdot\sigma) \\ &= det\begin{pmatrix}\cos\theta + i\sin\theta v_3 & i\sin\theta(v_1 - iv_2) \\ i\sin\theta(v_1 + iv_2) & \cos\theta - i\sin\theta v_3\end{pmatrix} \\ &= \cos^2\theta + \sin^2\theta(v_1^2 + v_2^2 + v_3^2) \\ &= 1\end{aligned}$$

So, we see that by exponentiating i times linear combinations of the self-adjoint Pauli matrices (which all have trace zero), we get unitary matrices of determinant one. These are invertible, and form the group named $SU(2)$, the group of unitary 2 by 2 matrices of determinant one. If we exponentiated not just $i\theta\mathbf{v}\cdot\sigma$, but $i(\phi\mathbf{1} + \theta\mathbf{v}\cdot\sigma)$ for some real constant ϕ (such matrices will not have trace zero unless $\phi = 0$), we would get a unitary matrix with determinant $e^{i2\phi}$. The group of unitary 2 by 2 matrices with arbitrary determinant is called $U(2)$. It contains as subgroups $SU(2)$ as well as the $U(1)$ described at the beginning of this section. $U(2)$ is slightly different than the product of these two subgroups, since the group element

$$\begin{pmatrix}-1 & 0 \\ 0 & -1\end{pmatrix}$$

is in both subgroups. In our review of linear algebra to come we will encounter the generalization to $SU(n)$ and $U(n)$, groups of unitary n by n complex matrices.

To get some more insight into the structure of the group $SU(2)$, consider an arbitrary 2 by 2 complex matrix

$$\begin{pmatrix}\alpha & \beta \\ \gamma & \delta\end{pmatrix}$$

Unitarity implies that the rows are orthonormal. One can see this explicitly from the condition that the matrix times its conjugate-transpose is the identity

$$\begin{pmatrix}\alpha & \beta \\ \gamma & \delta\end{pmatrix}\begin{pmatrix}\overline{\alpha} & \overline{\gamma} \\ \overline{\beta} & \overline{\delta}\end{pmatrix} = \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}$$

Orthogonality of the two rows gives the relation

$$\gamma\overline{\alpha} + \delta\overline{\beta} = 0 \implies \delta = -\frac{\gamma\overline{\alpha}}{\overline{\beta}}$$

The condition that the first row has length one gives

$$\alpha\overline{\alpha} + \beta\overline{\beta} = |\alpha|^2 + |\beta|^2 = 1$$

Using these two relations and computing the determinant (which has to be 1) gives

$$\alpha\delta - \beta\gamma = -\frac{\alpha\overline{\alpha}\gamma}{\overline{\beta}} - \beta\gamma = -\frac{\gamma}{\overline{\beta}}(\alpha\overline{\alpha} + \beta\overline{\beta}) = -\frac{\gamma}{\overline{\beta}} = 1$$

so one must have

$$\gamma = -\overline{\beta},\ \delta = \overline{\alpha}$$

and an $SU(2)$ matrix will have the form

$$\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

where $(\alpha, \beta) \in \mathbf{C}^2$ and

$$|\alpha|^2 + |\beta|^2 = 1$$

So, the elements of $SU(2)$ are parametrized by two complex numbers, with the sum of their length-squareds equal to one. Identifying $\mathbf{C}^2 = \mathbf{R}^4$, these are just vectors of length one in $\mathbf{R}^4$. Just as $U(1)$ could be identified as a space with the unit circle S^1 in $\mathbf{C} = \mathbf{R}^2$, $SU(2)$ can be identified with the unit three-sphere S^3 in $\mathbf{R}^4$.

3.2 Commutation relations for Pauli matrices

An important set of relations satisfied by Pauli matrices are their commutation relations:

$$[\sigma_j, \sigma_k] = \sigma_j\sigma_k - \sigma_k\sigma_j = 2i\sum_{l=1}^{3}\epsilon_{jkl}\sigma_l$$

where ϵ_{jkl} satisfies $\epsilon_{123} = 1$, is antisymmetric under permutation of two of its subscripts, and vanishes if two of the subscripts take the same value. More explicitly, this says:

$$[\sigma_1, \sigma_2] = 2i\sigma_3,\ [\sigma_2, \sigma_3] = 2i\sigma_1,\ [\sigma_3, \sigma_1] = 2i\sigma_2$$

One can easily check these relations by explicitly computing with the matrices. Putting together the anticommutation and commutation relations, one gets a formula for the product of two Pauli matrices:

$$\sigma_j\sigma_k = \delta_{jk}\mathbf{1} + i\sum_{l=1}^{3}\epsilon_{jkl}\sigma_l$$

While physicists prefer to work with self-adjoint Pauli matrices and their real eigenvalues, one can work instead with the following skew-adjoint matrices

$$X_j = -i\frac{\sigma_j}{2}$$

which satisfy the slightly simpler commutation relations

$$[X_j, X_k] = \sum_{l=1}^{3} \epsilon_{jkl} X_l$$

or more explicitly

$$[X_1, X_2] = X_3, \ [X_2, X_3] = X_1, \ [X_3, X_1] = X_2$$

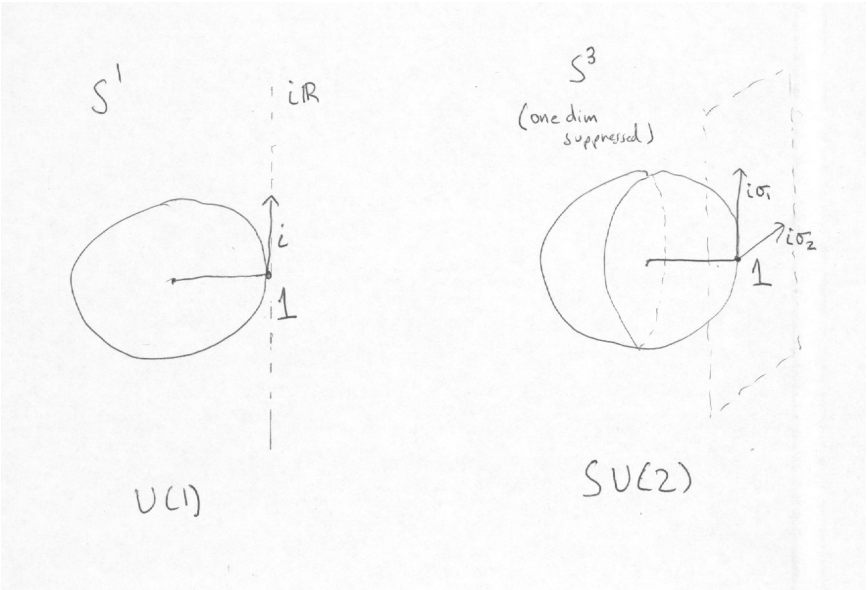
If these commutators were zero, the $SU(2)$ elements one gets by exponentiating linear combinations of the X_j would be commuting group elements. The non-triviality of the commutators reflects the non-commutativity of the group. Group elements $U \in SU(2)$ near the identity satisfy

$$U \simeq \mathbf{1} + \epsilon_1 X_1 + \epsilon_2 X_2 + \epsilon_3 X_2$$

for ϵ_j small and real, just as group elements $z \in U(1)$ near the identity satisfy

$$z \simeq 1 + i\epsilon$$

One can think of the X_j and their commutation relations as an infinitesimal version of the full group and its group multiplication law, valid near the identity. In terms of the geometry of manifolds, recall that $SU(2)$ is the space S^3. The X_j give a basis of the tangent space $\mathbf{R}^3$ to the identity of $SU(2)$, just as i gives a basis of the tangent space to the identity of $U(1)$.



3.3 Dynamics of a two-state system

Recall that the time dependence of states in quantum mechanics is given by the Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle$$

where H is a particular self-adjoint linear operator on $\mathcal{H}$, the Hamiltonian operator. The most general such operator on $\mathbf{C}^2$ will be given by

$$H = h_0\mathbf{1} + h_1\sigma_1 + h_2\sigma_2 + h_3\sigma_3$$

for four real parameters h_0, h_1, h_2, h_3. The solution to the Schrödinger equation is just given by exponentiation:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

where

$$U(t) = e^{-itH}$$

The $h_0\mathbf{1}$ term in H just contributes an overall phase factor e^{-ih_0t}, with the remaining factor of $U(t)$ an element of the group $SU(2)$ rather than the larger group $U(2)$ of all 2 by 2 unitaries.

Using our earlier equation

$$e^{i\theta\mathbf{v}\cdot\sigma} = (\cos\theta)\mathbf{1} + i(\sin\theta)\mathbf{v}\cdot\sigma$$

valid for a unit vector $\mathbf{v}$, our $U(t)$ is given by taking $\mathbf{h} = (h_1, h_2, h_3)$, $\mathbf{v} = \frac{\mathbf{h}}{|\mathbf{h}|}$ and $\theta = -t|\mathbf{h}|$, so we find

$$\begin{aligned}
U(t) =& e^{-ih_0t}(\cos(-t|\mathbf{h}|)\mathbf{1} + i\sin(-t|\mathbf{h}|)\frac{h_1\sigma_1 + h_2\sigma_2 + h_3\sigma_3}{|\mathbf{h}|}) \\
=& e^{-ih_0t}(\cos(t|\mathbf{h}|)\mathbf{1} - i\sin(t|\mathbf{h}|)\frac{h_1\sigma_1 + h_2\sigma_2 + h_3\sigma_3}{|\mathbf{h}|}) \\
=& \begin{pmatrix} e^{-ih_0t}(\cos(t|\mathbf{h}|) - i\frac{h_3}{|\mathbf{h}|}\sin(t|\mathbf{h}|)) & -i\sin(t|\mathbf{h}|)\frac{h_1 - ih_2}{|\mathbf{h}|} \\ -i\sin(t|\mathbf{h}|)\frac{h_1 + ih_2}{|\mathbf{h}|} & e^{-ih_0t}(\cos(t|\mathbf{h}|) + i\frac{h_3}{|\mathbf{h}|}\sin(t|\mathbf{h}|)) \end{pmatrix}
\end{aligned}$$

In the special case $\mathbf{h} = (0, 0, h_3)$ we have

$$U(t) = \begin{pmatrix} e^{-it(h_0+h_3)} & 0 \\ 0 & e^{-it(h_0-h_3)} \end{pmatrix}$$

so if our initial state is

$$|\psi(0)\rangle = \alpha|+\frac{1}{2}\rangle + \beta|-\frac{1}{2}\rangle$$

for $\alpha, \beta \in \mathbf{C}$, at later times the state will be

$$|\psi(t)\rangle = \alpha e^{-it(h_0+h_3)}|+\frac{1}{2}\rangle + \beta e^{-it(h_0-h_3)}|-\frac{1}{2}\rangle$$

In this special case, one can see that the eigenvalues of the Hamiltonian are $h_0 \pm h_3$.

In the physical realization of this system by a spin 1/2 particle (ignoring its spatial motion), the Hamiltonian is given by

$$H = \frac{ge}{4mc}(B_1\sigma_1 + B_2\sigma_2 + B_3\sigma_3)$$

where the B_j are the components of the magnetic field, and the physical constants are the gyromagnetic ratio (g), the electric charge (e), the mass (m) and the speed of light (c), so we have solved the problem of the time evolution of such a system, setting $h_j = \frac{ge}{4mc}B_j$. For magnetic fields of size $|B|$ in the 3-direction, we see that the two different states with well-defined energy ($|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$) will have an energy difference between them of

$$\frac{ge}{2mc}|B|$$

This is known as the Zeeman effect and is readily visible in the spectra of atoms subjected to a magnetic field. We will consider this example in more detail in chapter 7, seeing how the group of rotations of $\mathbf{R}^3$ appears. Much later, in chapter 42, we will derive this Hamiltonian term from general principles of how electromagnetic fields couple to such spin 1/2 particles.

3.4 For further reading

Many quantum mechanics textbooks now begin with the two-state system, giving a much more detailed treatment than the one given here, including much more about the physical interpretation of such systems (see for example [68]). Volume III of Feynman's *Lectures on Physics* [16] is a quantum mechanics text with much of the first half devoted to two-state systems. The field of "Quantum Information Theory" gives a perspective on quantum theory that puts such systems (in this context called the "qubit") front and center. One possible reference for this material is John Preskill's notes on quantum computation [48].

Chapter 4

Linear Algebra Review, Unitary and Orthogonal Groups

A significant background in linear algebra will be assumed in later chapters, and we'll need a range of specific facts from that subject. These will include some aspects of linear algebra not emphasized in a typical linear algebra course, such as the role of the dual space and the consideration of various classes of invertible matrices as defining a group. For now our vector spaces will be finite-dimensional. Later on we will come to state spaces that are infinite dimensional, and will address the various issues that this raises at that time.

4.1 Vector spaces and linear maps

A vector space V over a field k is just a set such that one can consistently take linear combinations of elements with coefficients in k. We will only be using the cases $k = \mathbf{R}$ and $k = \mathbf{C}$, so such finite-dimensional V will just be $\mathbf{R}^n$ or $\mathbf{C}^n$. Choosing a basis (set of n linearly independent vectors) $\{\mathbf{e}_j\}$, an arbitrary vector $v \in V$ can be written as

$$v = v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + \cdots + v_n\mathbf{e}_n$$

giving an explicit identification of V with n-tuples v_j of real or complex numbers which we will usually write as column vectors

$$v = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

The choice of a basis $\{\mathbf{e}_j\}$ also allows us to express the action of a linear operator Ω on V

$$\Omega : v \in V \to \Omega v \in V$$

as multiplication by an n by n matrix:

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \to \begin{pmatrix} \Omega_{11} & \Omega_{12} & \dots & \Omega_{1n} \\ \Omega_{21} & \Omega_{22} & \dots & \Omega_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \Omega_{n1} & \Omega_{n2} & \dots & \Omega_{nn} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

The invertible linear operators on V form a group under composition, a group we will sometimes denote $GL(V)$. Choosing a basis identifies this group with the group of invertible matrices, with group law matrix multiplication. For V n-dimensional, we will denote this group by $GL(n, \mathbf{R})$ in the real case, $GL(n, \mathbf{C})$ in the complex case.

Note that when working with vectors as linear combinations of basis vectors, we can use matrix notation to write a linear transformation as

$$v \to \Omega v = \begin{pmatrix} \mathbf{e}_1 & \cdots & \mathbf{e}_n \end{pmatrix} \begin{pmatrix} \Omega_{11} & \Omega_{12} & \dots & \Omega_{1n} \\ \Omega_{21} & \Omega_{22} & \dots & \Omega_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \Omega_{n1} & \Omega_{n2} & \dots & \Omega_{nn} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

One sees from this that we can think of the transformed vector as we did above in terms of transformed coefficients v_j with respect to fixed basis vectors, but also could leave the v_j unchanged and transform the basis vectors. At times we will want to use matrix notation to write formulas for how the basis vectors transform in this way, and then will write

$$\begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \vdots \\ \mathbf{e}_n \end{pmatrix} \to \begin{pmatrix} \Omega_{11} & \Omega_{21} & \dots & \Omega_{n1} \\ \Omega_{12} & \Omega_{22} & \dots & \Omega_{n2} \\ \vdots & \vdots & \vdots & \vdots \\ \Omega_{1n} & \Omega_{2n} & \dots & \Omega_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \vdots \\ \mathbf{e}_n \end{pmatrix}$$

Note that putting the basis vectors $\mathbf{e}_j$ in a column vector like this causes the matrix for Ω to act on them by the transposed matrix. This is not a group action since in general the product of two transposed matrices is not the transpose of the product.

4.2 Dual vector spaces

To any vector space V one can associate a new vector space, its dual:

Definition (Dual vector space)**.** *Given a vector space V over a field k, the dual vector space V^* is the set of all linear maps $V \to k$, i.e.*

$$V^* = \{l : V \to k \text{ such that } l(\alpha v + \beta w) = \alpha l(v) + \beta l(w)\}$$

for $\alpha, \beta \in k,\ v, w \in V$.

Given a linear transformation Ω acting on V, one can define:

Definition (Transpose transformation)**.** *The transpose of* Ω *is the linear transformation*

$$\Omega^T : V^* \to V^*$$

that satisfies

$$(\Omega^T l)(v) = l(\Omega v)$$

for $l \in V^*, v \in V$.

For any representation (π, V) of a group G on V, one can define a corresponding representation on V^*

Definition (Dual or contragredient representation)**.** *The dual or contragredient representation on* V^* *is given by taking as linear operators*

$$(\pi^T)^{-1}(g) : V^* \to V^*$$

These satisfy the homomorphism property since

$$(\pi^T(g_1))^{-1}(\pi^T(g_2))^{-1} = (\pi^T(g_2)\pi^T(g_1))^{-1} = ((\pi(g_1)\pi(g_2))^T)^{-1}$$

For any choice of basis $\{\mathbf{e}_j\}$ of V, one has a dual basis $\{\mathbf{e}_j^*\}$ of V^* that satisfies

$$\mathbf{e}_j^*(\mathbf{e}_k) = \delta_{jk}$$

Coordinates on V with respect to a basis are linear functions, and thus elements of V^*. One can identify the coordinate function v_j with the dual basis vector $\mathbf{e}_j^*$ since

$$\mathbf{e}_j^*(v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + \cdots + v_n\mathbf{e}_n) = v_j$$

One can easily show that the elements of the matrix for Ω in the basis $\mathbf{e}_j$ are given by

$$\Omega_{jk} = \mathbf{e}_j^*(\Omega\mathbf{e}_k)$$

and that the matrix for the transpose map (with respect to the dual basis) is just the matrix transpose

$$(\Omega^T)_{jk} = \Omega_{kj}$$

One can use matrix notation to write elements

$$l = l_1\mathbf{e}_1^* + l_2\mathbf{e}_2^* + \cdots + l_n\mathbf{e}_n^* \in V^*$$

of V^* as row vectors

$$\begin{pmatrix} l_1 & l_2 & \cdots & l_n \end{pmatrix}$$

of coordinates on V^*. Then evaluation of l on a vector v given by matrix multiplication

$$l(v) = \begin{pmatrix} l_1 & l_2 & \cdots & l_n \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = l_1v_1 + l_2v_2 + \cdots + l_nv_n$$

4.3 Change of basis

Any invertible transformation A on V can be used to change the basis $\mathbf{e}_j$ of V to a new basis $\mathbf{e}'_j$ by taking

$$\mathbf{e}_j \to \mathbf{e}'_j = A\mathbf{e}_j$$

The matrix for a linear transformation Ω transforms under this change of basis as

$$\begin{aligned}\Omega_{jk} = \mathbf{e}_j^*(\Omega\mathbf{e}_k) \to (\mathbf{e}'_j)^*(\Omega\mathbf{e}'_k) =& (A\mathbf{e}_j)^*(\Omega A\mathbf{e}_k) \\ =& (A^T)^{-1}(\mathbf{e}_j^*)(\Omega A\mathbf{e}_k) \\ =& \mathbf{e}_j^*(A^{-1}\Omega A\mathbf{e}_k) \\ =& (A^{-1}\Omega A)_{jk}\end{aligned}$$

In the second step we are using the fact that elements of the dual basis transform as the dual representation. One can check that this is what is needed to ensure the relation

$$(\mathbf{e}'_j)^*(\mathbf{e}'_k) = \delta_{jk}$$

The change of basis formula shows that if two matrices Ω_1 and Ω_2 are related by conjugation by a third matrix A

$$\Omega_2 = A^{-1}\Omega_1 A$$

then one can think of them as both representing the same linear transformation, just with respect to two different choices of basis. Recall that a finite-dimensional representation is given by a set of matrices $\pi(g)$, one for each group element. If two representations are related by

$$\pi_2(g) = A^{-1}\pi_1(g)A$$

(for all g, A does not depend on g), then we can think of them as being the same representation, with different choices of basis. In such a case the representations π_1 and π_2 are called "equivalent", and we will often implicitly identify representations that are equivalent.

4.4 Inner products

An inner product on a vector space V is an additional structure that provides a notion of length for vectors, of angle between vectors, and identifies $V^* \simeq V$. One has, in the real case:

Definition (Inner Product, real case)**.** *An inner product on a real vector space V is a map*

$$\langle\cdot,\cdot\rangle : V \times V \to \mathbf{R}$$

that is linear in both variables and symmetric ($\langle v, w\rangle = \langle w, v\rangle$).

Our inner products will usually be positive-definite ($\langle v, v\rangle \geq 0$ and $\langle v, v\rangle = 0 \implies v = 0$), with indefinite inner products only appearing in the context of special or general relativity, where an indefinite inner product on four-dimensional space-time is used.

In the complex case, one has

Definition (Inner Product, complex case)**.** *An Hermitian inner product on a complex vector space V is a map*

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbf{C}$$

that is conjugate symmetric

$$\langle v, w\rangle = \overline{\langle w, v\rangle}$$

as well as linear in the second variable, and antilinear in the first variable: for $\alpha \in \mathbf{C}$ and $u, v, w \in V$

$$\langle u + v, w\rangle = \langle u, w\rangle + \langle v, w\rangle, \quad \langle \alpha u, v\rangle = \overline{\alpha}\langle u, v\rangle$$

An inner product gives a notion of length $||\cdot||$ for vectors, with

$$||v||^2 = \langle v, v\rangle$$

Note that whether to specify antilinearity in the first or second variable is a matter of convention. The choice we are making is universal among physicists, with the opposite choice common among mathematicians.

An inner product also provides an (antilinear in the complex case) isomorphism $V \simeq V^*$ by the map

$$v \in V \to l_v \in V^*$$

where l_v is defined by

$$l_v(w) = \langle v, w\rangle$$

Physicists have a useful notation for elements of vector space and their duals, for the case when V is a complex vector space with an Hermitian inner product (such as the state space for a quantum theory). An element of such a vector space V is written as a "ket vector"

$$|v\rangle$$

where v is a label for a vector. An element of the dual vector space V^* is written as a "bra vector"

$$\langle l|$$

Evaluating $l \in V^*$ on $v \in V$ gives an element of $\mathbf{C}$, written

$$\langle l|v\rangle$$

If $\Omega : V \to V$ is a linear map

$$\langle l|\Omega|v\rangle = \langle l|\Omega v\rangle = l(\Omega v)$$

In the bra-ket notation, one denotes the dual vector l_v by $\langle v|$. Note that in the inner product the angle bracket notation means something different than in the bra-ket notation. The similarity is intentional though, since in the bra-ket notation one has

$$\langle v|w\rangle = \langle v, w\rangle$$

Note that our convention of linearity in the second variable of the inner product, antilinearity in the first, implies

$$|\alpha v\rangle = \alpha|v\rangle, \quad \langle \alpha v| = \overline{\alpha}\langle v|$$

for $\alpha \in \mathbf{C}$.

For a choice of orthonormal basis $\{\mathbf{e}_j\}$, i.e. satisfying

$$\langle \mathbf{e}_j, \mathbf{e}_k\rangle = \delta_{jk}$$

a useful notation is

$$|j\rangle = \mathbf{e}_j$$

Because of orthonormality, coefficients of vectors can be calculated as

$$v_j = \langle \mathbf{e}_j, v\rangle$$

In bra-ket notation we have

$$v_j = \langle j|v\rangle$$

and

$$|v\rangle = \sum_{j=1}^{n} |j\rangle\langle j|v\rangle$$

For corresponding elements of V^*, one has (using antilinearity)

$$\langle v| = \sum_{j=1}^{n} \overline{v_j}\langle j| = \sum_{j=1}^{n} \langle v|j\rangle\langle j|$$

With respect to the chosen orthonormal basis $\{\mathbf{e}_j\}$, one can represent vectors v as column vectors and the operation of taking a vector $|v\rangle$ to a dual vector $\langle v|$ corresponds to taking a column vector to the row vector that is its conjugate-transpose.

$$\langle v| = \begin{pmatrix} \overline{v_1} & \overline{v_2} & \cdots & \overline{v_n} \end{pmatrix}$$

Then one has

$$\langle v|w\rangle = \begin{pmatrix} \overline{v_1} & \overline{v_2} & \cdots & \overline{v_n} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \overline{v_1}w_1 + \overline{v_2}w_2 + \cdots + \overline{v_n}w_n$$

If Ω is a linear operator $\Omega : V \to V$, then with respect to the chosen basis it becomes a matrix with matrix elements

$$\Omega_{kj} = \langle k|\Omega j\rangle$$

The decomposition of a vector v in terms of coefficients

$$|v\rangle = \sum_{j=1}^{n} |j\rangle\langle j|v\rangle$$

can be interpreted as a matrix multiplication by the identity matrix

$$\mathbf{1} = \sum_{j=1}^{n} |j\rangle\langle j|$$

and this kind of expression is referred to by physicists as a "completeness relation", since it requires that the set of $|j\rangle$ be a basis with no missing elements. The operator

$$P_j = |j\rangle\langle j|$$

is called the projection operator onto the j'th basis vector, it corresponds to the matrix that has 0s everywhere except in the jj component.

Digression. *In this course, all our indices will be lower indices. One way to keep straight the difference between vectors and dual vectors is to use upper indices for components of vectors, lower indices for components of dual vectors. This is quite useful in Riemannian geometry and general relativity, where the inner product is given by a metric that can vary from point to point, causing the isomorphism between vectors and dual vectors to also vary. For quantum mechanical state spaces, we will be using a single, standard, fixed inner product, so there will be a single isomorphism between vectors and dual vectors. The bra-ket notation will take care of the notational distinction between vectors and dual vectors as necessary.*

4.5 Adjoint operators

When V is a vector space with inner product, one can define the adjoint of Ω by

Definition (Adjoint Operator)**.** *The adjoint of a linear operator $\Omega : V \to V$ is the operator $\Omega^\dagger$ satisfying*

$$\langle \Omega v, w\rangle = \langle v, \Omega^\dagger w\rangle$$

or, in bra-ket notation

$$\langle \Omega v|w\rangle = \langle v|\Omega^\dagger w\rangle$$

for all $v, w \in V$.

Generalizing the fact that

$$\langle \alpha v| = \overline{\alpha}\langle v|$$

for $\alpha \in \mathbf{C}$, one can write

$$\langle \Omega v| = \langle v|\Omega^\dagger$$

Note that mathematicians tend to favor Ω^* as notation for the adjoint of Ω, as opposed to the physicist's notation $\Omega^\dagger$ that we are using.

In terms of explicit matrices, since $\langle \Omega v|$ is the conjugate-transpose of $|\Omega v\rangle$, the matrix for $\Omega^\dagger$ will be given by the conjugate transpose $\overline{\Omega^T}$ of the matrix for Ω:

$$\Omega^\dagger_{jk} = \overline{\Omega_{kj}}$$

In the real case, the matrix for the adjoint is just the transpose matrix. We will say that a linear transformation is self-adjoint if $\Omega^\dagger = \Omega$, skew-adjoint if $\Omega^\dagger = -\Omega$.

4.6 Orthogonal and unitary transformations

A special class of linear transformations will be invertible transformations that preserve the inner product, i.e. satisfying

$$\langle \Omega v, \Omega w\rangle = \langle \Omega v|\Omega w\rangle = \langle v, w\rangle = \langle v|w\rangle$$

for all $v, w \in V$. Such transformations take orthonormal bases to orthonormal bases, so they will appear in one role as change of basis transformations.

In terms of adjoints, this condition becomes

$$\langle \Omega v, \Omega w\rangle = \langle v, \Omega^\dagger \Omega w\rangle = \langle v, w\rangle$$

so

$$\Omega^\dagger \Omega = \mathbf{1}$$

or equivalently

$$\Omega^\dagger = \Omega^{-1}$$

In matrix notation this first condition becomes

$$\sum_{k=1}^{n} (\Omega^\dagger)_{jk}\Omega_{kl} = \sum_{k=1}^{n} \overline{\Omega_{kj}}\Omega_{kl} = \delta_{jl}$$

which says that the column vectors of the matrix for Ω are orthonormal vectors. Using instead the equivalent condition

$$\Omega\Omega^\dagger = \mathbf{1}$$

one finds that the row vectors of the matrix for Ω are also orthornormal.

Since such linear transformations preserving the inner product can be composed and are invertible, they form a group, and some of the basic examples of Lie groups are given by these groups for the cases of real and complex vector spaces.

4.6.1 Orthogonal groups

We'll begin with the real case, where these groups are called orthogonal groups:

Definition (Orthogonal group)**.** *The orthogonal group $O(n)$ in n-dimensions is the group of invertible transformations preserving an inner product on a real n-dimensional vector space V. This is isomorphic to the group of n by n real invertible matrices Ω satisfying*

$$\Omega^{-1} = \Omega^T$$

The subgroup of $O(n)$ of matrices with determinant 1 (equivalently, the subgroup preserving orientation of orthonormal bases) is called $SO(n)$.

Recall that for a representation π of a group G on V, one has a dual representation on V^* given by taking the transpose-inverse of π. If G is an orthogonal group, then π and its dual are the same matrices, with V identified by V^* by the inner product.

Since the determinant of the transpose of a matrix is the same as the determinant of the matrix, we have

$$\Omega^{-1}\Omega = \mathbf{1} \implies det(\Omega^{-1})det(\Omega) = det(\Omega^T)det(\Omega) = (det(\Omega))^2 = 1$$

so

$$det(\Omega) = \pm 1$$

$O(n)$ is a continuous Lie group, with two components: $SO(n)$, the subgroup of orientation-preserving transformations, which include the identity, and a component of orientation-changing transformations.

The simplest non-trivial example is for $n = 2$, where all elements of $SO(2)$ are given by matrices of the form

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

These matrices give counter-clockwise rotations in $\mathbf{R}^2$ by an angle θ. The other component of $O(2)$ will be given by matrices of the form

$$\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

Note that the group $SO(2)$ is isomorphic to the group $U(1)$ by

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \Leftrightarrow e^{i\theta}$$

so the representation theory of $SO(2)$ is just as for $U(1)$, with irreducible complex representations one-dimensional and classified by an integer.

In chapter 6 we will consider in detail the case of $SO(3)$, which is crucial for physical applications because it is the group of rotations in the physical three-dimensional space.

4.6.2 Unitary groups

In the complex case, groups of invertible transformations preserving the Hermitian inner product are called unitary groups:

Definition (Unitary group)**.** *The unitary group $U(n)$ in n-dimensions is the group of invertible transformations preserving an Hermitian inner product on a complex n-dimensional vector space V. This is isomorphic to the group of n by n complex invertible matrices satisfying*

$$\Omega^{-1} = \overline{\Omega}^T = \Omega^\dagger$$

The subgroup of $U(n)$ of matrices with determinant 1 is called $SU(n)$.

In the unitary case, the dual of a representation π has representation matrices that are transpose-inverses of those for π, but

$$(\pi(g)^T)^{-1} = \overline{\pi(g)}$$

so the dual representation is given by conjugating all elements of the matrix.

The same calculation as in the real case here gives

$$det(\Omega^{-1})det(\Omega) = det(\Omega^\dagger)det(\Omega) = \overline{det(\Omega)}det(\Omega) = |det(\Omega)|^2 = 1$$

so $det(\Omega)$ is a complex number of modulus one. The map

$$\Omega \in U(n) \to det(\Omega) \in U(1)$$

is a group homomorphism.

We have already seen the examples $U(1)$, $U(2)$ and $SU(2)$. For general values of n, the case of $U(n)$ can be split into the study of its determinant, which lies in $U(1)$ so is easy to deal with, and the subgroup $SU(n)$, which is a much more complicated story.

Digression. *Note that is not quite true that the group $U(n)$ is the product group $SU(n) \times U(1)$. If one tries to identify the $U(1)$ as the subgroup of $U(n)$ of elements of the form $e^{i\theta}\mathbf{1}$, then matrices of the form*

$$e^{i\frac{m}{n}2\pi}\mathbf{1}$$

for m an integer will lie in both $SU(n)$ and $U(1)$, so $U(n)$ is not a product of those two groups.

We saw at the end of section 3.1.2 that $SU(2)$ can be identified with the three-sphere S^3, since an arbitrary group element can be constructed by specifying one row (or one column), which must be a vector of length one in $\mathbf{C}^2$. For the case $n = 3$, the same sort of construction starts by picking a row of length one in $\mathbf{C}^3$, which will be a point in S^5. The second row must be orthornormal, and one can show that the possibilities lie in a three-sphere S^3. Once the first two rows are specified, the third row is uniquely determined. So as a manifold, $SU(3)$ is eight-dimensional, and one might think it could be identified with $S^5 \times S^3$. It turns out

that this is not the case, since the S^3 varies in a topologically non-trivial way as one varies the point in S^5. As spaces, the $SU(n)$ are topologically "twisted" products of odd-dimensional spheres, providing some of the basic examples of quite non-trivial topological manifolds.

4.7 Eigenvalues and eigenvectors

We have seen that that the matrix for a linear transformation Ω of a vector space V changes by conjugation when we change our choice of basis of V. To get basis-independent information about Ω, one considers the eigenvalues of the matrix. Complex matrices behave in a much simpler fashion than real matrices, since in the complex case the eigenvalue equation

$$det(\lambda \mathbf{1} - \Omega) = 0$$

can always be factored into linear factors, and solved for the eigenvalues λ. For an arbitrary n by n complex matrix there will be n solutions (counting repeated eigenvalues with multiplicity). One can always find a basis for which the matrix will be in upper triangular form.

The case of self-adjoint matrices Ω is much more constrained, since transposition relates matrix elements. One has:

Theorem (Spectral theorem for self-adjoint matrices)**.** *Given a self-adjoint complex n by n matrix Ω, one can always find a unitary matrix U such that*

$$U\Omega U^{-1} = D$$

where D is a diagonal matrix with entries $D_{jj} = \lambda_j, \lambda_j \in \mathbf{R}$.

Given Ω, one finds the eigenvalues λ_j by solving the eigenvalue equation. One can then go on to solve for the eigenvectors and use these to find U. For distinct eigenvalues one finds that the corresponding eigenvectors are orthogonal.

This theorem is of crucial importance in quantum mechanics, where for Ω an observable, the eigenvectors are the states in the state space with well-defined numerical values characterizing the state, and these numerical values are the eigenvalues. The theorem also tells us that given an observable, we can use it to choose distinguished orthonormal bases for the state space by picking a basis of eigenvectors, normalized to length one. This is a theorem about finite-dimensional vector spaces, but later on in the course we will see that something similar will be true even in the case of infinite-dimensional state spaces.

One can also diagonalize unitary matrices themselves by conjugation by another unitary. The diagonal entries will all be complex numbers of unit length, so of the form $e^{i\lambda_j}, \lambda_j \in \mathbf{R}$.

For the simplest examples, consider the cases of the groups $SU(2)$ and $U(2)$. Any matrix in $U(2)$ can be conjugated by a unitary matrix to the diagonal matrix

$$\begin{pmatrix} e^{i\lambda_1} & 0 \\ 0 & e^{i\lambda_2} \end{pmatrix}$$

which is the exponential of a corresponding diagonalized skew-adjoint matrix

$$\begin{pmatrix} i\lambda_1 & 0 \\ 0 & i\lambda_2 \end{pmatrix}$$

For matrices in the subgroup $SU(2)$, one has $\lambda_2 = -\lambda_1 = \lambda$ so in diagonal form an $SU(2)$ matrix will be

$$\begin{pmatrix} e^{i\lambda} & 0 \\ 0 & e^{-i\lambda} \end{pmatrix}$$

which is the exponential of a corresponding diagonalized skew-adjoint matrix that has trace zero

$$\begin{pmatrix} i\lambda & 0 \\ 0 & -i\lambda \end{pmatrix}$$

4.8 For further reading

Almost any of the more advanced linear algebra textbooks should cover the material of this chapter.

Chapter 5

Lie Algebras and Lie Algebra Representations

For a group G we have defined unitary representations (π, V) for finite-dimensional vector spaces V of complex dimension n as homomorphisms

$$\pi : G \to U(n)$$

Recall that in the case of $G = U(1)$, we could use the homomorphism property of π to determine π in terms of its derivative at the identity. This turns out to be a general phenomenon for Lie groups G: we can study their representations by considering the derivative of π at the identity, which we will call π'. Because of the homomorphism property, knowing π' is often sufficient to characterize the representation π it comes from. π' is a linear map from the tangent space to G at the identity to the tangent space of $U(n)$ at the identity. The tangent space to G at the identity will carry some extra structure coming from the group multiplication, and this vector space with this structure will be called the Lie algebra of G.

The subject of differential geometry gives many equivalent ways of defining the tangent space at a point of manifolds like G, but we do not want to enter here into the subject of differential geometry in general. One of the standard definitions of the tangent space is as the space of tangent vectors, with tangent vectors defined as the possible velocity vectors of parametrized curves $g(t)$ in the group G.

More advanced treatments of Lie group theory develop this point of view (see for example [70]) which applies to arbitrary Lie groups, whether or not they are groups of matrices. In our case though, since we are interested in specific groups that are explicitly given as groups of matrices, we can give a more concrete definition, just using the exponential map on matrices. For a more detailed exposition of this subject, using the same concrete definition of the Lie algebra in terms of matrices, see Brian Hall's book [27] or the abbreviated on-line version [28].

Note that the material of this chapter is quite general, and may be hard to make sense of until one has some experience with basic examples. The next chapter will discuss in detail the groups $SU(2)$ and $SO(3)$ and their Lie algebras, as well as giving some examples of their representations, and this may be helpful in making sense of the general theory of this chapter.

5.1 Lie algebras

We'll work with the following definition of a Lie algebra:

Definition (Lie algebra)**.** *For G a Lie group of n by n invertible matrices, the Lie algebra of G (written Lie(G) or $\mathfrak{g}$) is the space of n by n matrices X such that $e^{tX} \in G$ for $t \in \mathbf{R}$.*

Notice that while the group G determines the Lie algebra $\mathfrak{g}$, the Lie algebra does not determine the group. For example, $O(n)$ and $SO(n)$ have the same tangent space at the identity, and thus the same Lie algebra, but elements in $O(n)$ not in the component of the identity can't be written in the form e^{tX} (since then you could make a path of matrices connecting such an element to the identity by shrinking t to zero). Note also that, for a given X, different values of t may give the same group element, and this may happen in different ways for different groups sharing the same Lie algebra. For example, consider $G = U(1)$ and $G = (\mathbf{R}, +)$, which both have the same Lie algebra $\mathfrak{g} = \mathbf{R}$. In the first case an infinity of values of t give the same group element, in the second, only one does. In the next chapter we'll see a more subtle example of this: $SU(2)$ and $SO(3)$ are different groups with the same Lie algebra.

We have $G \subset GL(n, \mathbf{C})$, and $X \in M(n, \mathbf{C})$, the space of n by n complex matrices. For all $t \in \mathbf{R}$, the exponential e^{tX} is an invertible matrix (with inverse e^{-tX}), so in $GL(n, \mathbf{C})$. For each X, we thus have a path of elements of $GL(n, \mathbf{C})$ going through the identity matrix at $t = 0$, with velocity vector

$$\frac{d}{dt} e^{tX} = X e^{tX}$$

which takes the value X at $t = 0$:

$$\frac{d}{dt}(e^{tX})_{|t=0} = X$$

To calculate this derivative, just use the power series expansion for the exponential, and differentiate term-by-term.

For the case $G = GL(n, \mathbf{C})$, we just have $\mathfrak{gl}(n, \mathbf{C}) = M(n, \mathbf{C})$, which is a linear space of the right dimension to be the tangent space to G at the identity, so this definition is consistent with our general motivation. For subgroups $G \subset GL(n, \mathbf{C})$ given by some condition (for example that of preserving an inner product), we will need to identify the corresponding condition on $X \in M(n, \mathbf{C})$ and check that this defines a linear space.

The existence of such a linear space $\mathfrak{g} \subset M(n, \mathbf{C})$ will provide us with a distinguished representation, called the "adjoint representation"

Definition (Adjoint representation)**.** *The adjoint representation* $(Ad, \mathfrak{g})$ *is given by the homomorphism*

$$Ad : g \in G \to Ad(g) \in GL(\mathfrak{g})$$

where $Ad(g)$ *acts on* $X \in \mathfrak{g}$ *by*

$$(Ad(g))(X) = gXg^{-1}$$

To show that this is well-defined, one needs to check that $gXg^{-1} \in \mathfrak{g}$ when $X \in \mathfrak{g}$, but this can be shown using the identity

$$e^{tgXg^{-1}} = ge^{tX}g^{-1}$$

which implies that $e^{tgXg^{-1}} \in G$ if $e^{tX} \in G$. To check this, just expand the exponential and use

$$(gXg^{-1})^k = (gXg^{-1})(gXg^{-1}) \cdots (gXg^{-1}) = gX^kg^{-1}$$

It is also easy to check that this is a homomorphism, with

$$Ad(g_1)Ad(g_2) = Ad(g_1g_2)$$

A Lie algebra $\mathfrak{g}$ is not just a real vector space, but comes with an extra structure on the vector space

Definition (Lie bracket)**.** *The Lie bracket operation on* $\mathfrak{g}$ *is the bilinear anti-symmetric map given by the commutator of matrices*

$$[\cdot, \cdot] : (X, Y) \in \mathfrak{g} \times \mathfrak{g} \to [X, Y] = XY - YX \in \mathfrak{g}$$

We need to check that this is well-defined, i.e. that it takes values in $\mathfrak{g}$.

Theorem. *If* $X, Y \in \mathfrak{g}$, $[X, Y] = XY - YX \in \mathfrak{g}$.

Proof. Since $X \in \mathfrak{g}$, we have $e^{tX} \in G$ and we can act on $Y \in \mathfrak{g}$ by the adjoint representation

$$Ad(e^{tX})Y = e^{tX}Ye^{-tX} \in \mathfrak{g}$$

As t varies this gives us a parametrized curve in $\mathfrak{g}$. Its velocity vector will also be in $\mathfrak{g}$, so

$$\frac{d}{dt}(e^{tX}Ye^{-tX}) \in \mathfrak{g}$$

One has (by the product rule, which can easily be shown to apply in this case)

$$\begin{aligned}\frac{d}{dt}(e^{tX}Ye^{-tX}) &= (\frac{d}{dt}(e^{tX}Y))e^{-tX} + e^{tX}Y(\frac{d}{dt}e^{-tX}) \\ &= Xe^{tX}Ye^{-tX} - e^{tX}YXe^{-tX}\end{aligned}$$

Evaluating this at $t = 0$ gives

$$XY - YX$$

which is thus shown to be in $\mathfrak{g}$. □

The relation

$$\frac{d}{dt}(e^{tX}Ye^{-tX})_{|t=0} = [X, Y] \tag{5.1}$$

used in this proof will be continually useful in relating Lie groups and Lie algebras.

To do calculations with a Lie algebra, one can just choose a basis $X_1, X_2, \ldots, X_n$ for the vector space $\mathfrak{g}$, and use the fact that the Lie bracket can be written in terms of this basis as

$$[X_j, X_k] = \sum_{l=1}^{n} c_{jkl} X_l$$

where c_{jkl} is a set of constants known as the "structure constants" of the Lie algebra. For example, in the case of $\mathfrak{su}(2)$, the Lie algebra of $SU(2)$ one has a basis X_1, X_2, X_3 satisfying

$$[X_j, X_k] = \sum_{l=1}^{3} \epsilon_{jkl} X_l$$

so the structure constants of $\mathfrak{su}(2)$ are just the totally antisymmetric ϵ_{jkl}.

5.2 Lie algebras of the orthogonal and unitary groups

The groups we are most interested in are the groups of linear transformations preserving an inner product: the orthogonal and unitary groups. We have seen that these are subgroups of $GL(n, \mathbf{R})$ or $GL(n, \mathbf{C})$, consisting of those elements Ω satisfying the condition

$$\Omega\Omega^\dagger = \mathbf{1}$$

In order to see what this condition becomes on the Lie algebra, write $\Omega = e^{tX}$, for some parameter t, and X a matrix in the Lie algebra. Since the transpose of a product of matrices is the product (order-reversed) of the transposed matrices, i.e.

$$(XY)^T = Y^T X^T$$

and the complex conjugate of a product of matrices is the product of the complex conjugates of the matrices, one has

$$(e^{tX})^\dagger = e^{tX^\dagger}$$

The condition

$$\Omega\Omega^\dagger = \mathbf{1}$$

thus becomes

$$e^{tX}(e^{tX})^\dagger = e^{tX}e^{tX^\dagger} = \mathbf{1}$$

Taking the derivative of this equation gives

$$e^{tX}X^\dagger e^{tX^\dagger} + Xe^{tX}e^{tX^\dagger} = 0$$

Evaluating this at $t = 0$ one finds

$$X + X^\dagger = 0$$

so the matrices we want to exponentiate are skew-adjoint, satisfying

$$X^\dagger = -X$$

Note that physicists often choose to define the Lie algebra in these cases as self-adjoint matrices, then multiplying by i before exponentiating to get a group element. We will not use this definition, with one reason that we want to think of the Lie algebra as a real vector space, so want to avoid an unnecessary introduction of complex numbers at this point.

5.2.1 Lie algebra of the orthogonal group

Recall that the orthogonal group $O(n)$ is the subgroup of $GL(n, \mathbf{R})$ of matrices Ω satisfying $\Omega^T = \Omega^{-1}$. We will restrict attention to the subgroup $SO(n)$ of matrices with determinant 1 which is the component of the group containing the identity, and thus elements that can be written as

$$\Omega = e^{tX}$$

These give a path connecting Ω to the identity (taking $e^{sX}, s \in [0, t]$). We saw above that the condition $\Omega^T = \Omega^{-1}$ corresponds to skew-symmetry of the matrix X

$$X^T = -X$$

So in the case of $G = SO(n)$, we see that the Lie algebra $\mathfrak{so}(n)$ is the space of skew-symmetric ($X^T = -X$) n by n real matrices, together with the bilinear, antisymmetric product given by the commutator:

$$(X, Y) \in \mathfrak{so}(n) \times \mathfrak{so}(n) \to [X, Y] \in \mathfrak{so}(n)$$

The dimension of the space of such matrices will be

$$1 + 2 + \cdots + (n-1) = \frac{n^2 - n}{2}$$

and a basis will be given by the matrices ϵ_{jk}, with $j, k = 1, \ldots, n, j < k$ defined as

$$(\epsilon_{jk})_{lm} = \begin{cases} -1 & \text{if } j = l, k = m \\ +1 & \text{if } j = m, k = l \\ 0 & \text{otherwise} \end{cases} \tag{5.2}$$

In chapter 6 we will examine in detail the $n = 3$ case, where the Lie algebra $\mathfrak{so}(3)$ is $\mathbf{R}^3$, realized as the space of antisymmetric real 3 by 3 matrices.

5.2.2 Lie algebra of the unitary group

For the case of the group $U(n)$, the group is connected and one can write all group elements as e^{tX}, where now X is a complex n by n matrix. The unitarity condition implies that X is skew-adjoint (also called skew-Hermitian), satisfying

$$X^\dagger = -X$$

So the Lie algebra $\mathfrak{u}(n)$ is the space of skew-adjoint n by n complex matrices, together with the bilinear, antisymmetric product given by the commutator:

$$(X, Y) \in \mathfrak{u}(n) \times \mathfrak{u}(n) \to [X, Y] \in \mathfrak{u}(n)$$

Note that these matrices form a subspace of $\mathbf{C}^{n^2}$ of half the dimension, so of real dimension n^2. $\mathfrak{u}(n)$ is a real vector space of dimension n^2, but it is NOT a space of real n by n matrices. It is the space of skew-Hermitian matrices, which in general are complex. While the matrices are complex, only real linear combinations of skew-Hermitian matrices are skew-Hermitian (recall that multiplication by i changes a skew-Hermitian matrix into a Hermitian matrix). Within this space of complex matrices, if one looks at the subspace of real matrices one gets the sub-Lie algebra $\mathfrak{so}(n)$ of antisymmetric matrices (the Lie algebra of $SO(n) \subset U(n)$).

Given any complex matrix $Z \in M(n, \mathbf{C})$, one can write it as a sum of

$$Z = \frac{1}{2}(Z + Z^\dagger) + \frac{1}{2}(Z - Z^\dagger)$$

where the first term is self-adjoint, the second skew-Hermitian. This second term can also be written as i times a self-adjoint matrix

$$\frac{1}{2}(Z - Z^\dagger) = i(\frac{1}{2i}(Z - Z^\dagger))$$

so we see that we can get all of $M(n, \mathbf{C})$ by taking all complex linear combinations of self-adjoint matrices..

There is an identity relating the determinant and the trace of a matrix

$$det(e^X) = e^{trace(X)}$$

which can be proved by conjugating the matrix to upper-triangular form and using the fact that the trace and the determinant of a matrix are conjugation-invariant. Since the determinant of an $SU(n)$ matrix is 1, this shows that the Lie algebra $\mathfrak{su}(n)$ of $SU(n)$ will consist of matrices that are not only skew-Hermitian, but also of trace zero. So in this case $\mathfrak{su}(n)$ is again a real vector space, of dimension $n^2 - 1$.

One can show that $U(n)$ and $\mathfrak{u}(n)$ matrices can be diagonalized by conjugation by a unitary matrix to show that any $U(n)$ matrix can be written as an exponential of something in the Lie algebra. The corresponding theorem is also true for $SO(n)$ but requires looking at diagonalization into 2 by 2 blocks. It is not true for $O(n)$ (you can't reach the disconnected component of the identity by exponentiation). It also turns out to not be true for the groups $GL(n, \mathbf{R})$ and $GL(n, \mathbf{C})$ for $n \geq 2$.

5.3 Lie algebra representations

We have defined a group representation as a homomorphism (a map of groups preserving group multiplication)

$$\pi : G \to GL(n, \mathbf{C})$$

We can similarly define a Lie algebra representation as a map of Lie algebras preserving the Lie bracket:

Definition (Lie algebra representation)**.** *A (complex) Lie algebra representation (ϕ, V) of a Lie algebra $\mathfrak{g}$ on an n-dimensional complex vector space V is given by a linear map*

$$\phi : X \in \mathfrak{g} \to \phi(X) \in \mathfrak{gl}(n, \mathbf{C}) = M(n, \mathbf{C})$$

satisfying

$$\phi([X, Y]) = [\phi(X), \phi(Y)]$$

Such a representation is called unitary if its image is in $\mathfrak{u}(n)$, i.e. it satisfies

$$\phi(X)^\dagger = -\phi(X)$$

More concretely, given a basis $X_1, X_2, \ldots, X_d$ of a Lie algebra $\mathfrak{g}$ of dimension d with structure constants c_{jkl}, a representation is given by a choice of d complex n-dimensional matrices $\phi(X_j)$ satisfying the commutation relations

$$[\phi(X_j), \phi(X_k)] = \sum_{l=1}^{d} c_{jkl}\phi(X_l)$$

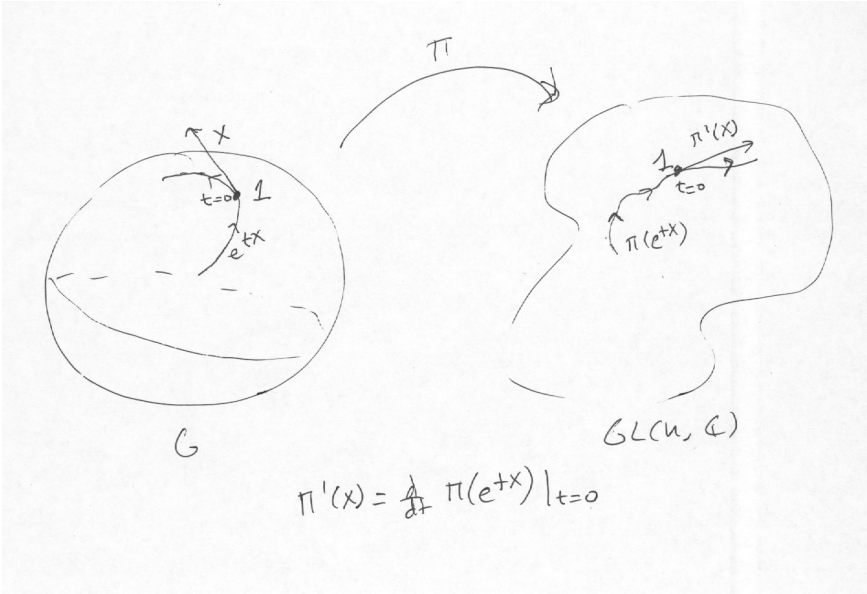
The representation is unitary when the matrices are skew-adjoint.

The notion of a Lie algebra is motivated by the fact that the homomorphism property causes the map π to be largely determined by its behavior infinitesimally near the identity, and thus by the derivative π'. One way to define the derivative of such a map is in terms of velocity vectors of paths, and this sort of definition in this case associates to a representation $\pi : G \to GL(n, \mathbf{C})$ a linear map

$$\pi' : \mathfrak{g} \to M(n, \mathbf{C})$$

where

$$\pi'(X) = \frac{d}{dt}(\pi(e^{tX}))_{|t=0}$$



In the case of $U(1)$ we classified all irreducible representations (homomorphisms $U(1) \to GL(1, \mathbf{C}) = \mathbf{C}^*$) by looking at the derivative of the map at the identity. For general Lie groups G, one can do something similar, showing that a representation π of G gives a representation of the Lie algebra (by taking the derivative at the identity), and then trying to classify Lie algebra representations.

Theorem. *If $\pi : G \to GL(n, \mathbf{C})$ is a group homomorphism, then*

$$\pi' : X \in \mathfrak{g} \to \pi'(X) = \frac{d}{dt}(\pi(e^{tX}))_{|t=0} \in \mathfrak{gl}(n, \mathbf{C}) = M(n, \mathbf{C})$$

satisfies

1. $$\pi(e^{tX}) = e^{t\pi'(X)}$$

2. *For $g \in G$*
$$\pi'(gXg^{-1}) = \pi(g)\pi'(X)(\pi(g))^{-1}$$

3. *π' is a Lie algebra homomorphism:*
$$\pi'([X, Y]) = [\pi'(X), \pi'(Y)]$$

Proof. 1. We have

$$\begin{aligned}\frac{d}{dt}\pi(e^{tX}) &= \frac{d}{ds}\pi(e^{(t+s)X})_{|s=0} \\ &= \frac{d}{ds}\pi(e^{tX}e^{sX})_{|s=0} \\ &= \pi(e^{tX})\frac{d}{ds}\pi(e^{sX})_{|s=0} \\ &= \pi(e^{tX})\pi'(X)\end{aligned}$$

So $f(t) = \pi(e^{tX})$ satisfies the differential equation $\frac{d}{dt}f = f\pi'(X)$ with initial condition $f(0) = 1$. This has the unique solution $f(t) = e^{t\pi'(X)}$

2. We have

$$\begin{aligned}e^{t\pi'(gXg^{-1})} &= \pi(e^{tgXg^{-1}}) \\ &= \pi(ge^{tX}g^{-1}) \\ &= \pi(g)\pi(e^{tX})\pi(g)^{-1} \\ &= \pi(g)e^{t\pi'(X)}\pi(g)^{-1}\end{aligned}$$

Differentiating with respect to t at $t = 0$ gives

$$\pi'(gXg^{-1}) = \pi(g)\pi'(X)(\pi(g))^{-1}$$

3. Recall that (5.1)

$$[X, Y] = \frac{d}{dt}(e^{tX}Ye^{-tX})_{|t=0}$$

so

$$\begin{aligned}\pi'([X, Y]) &= \pi'(\frac{d}{dt}(e^{tX}Ye^{-tX})_{|t=0}) \\ &= \frac{d}{dt}\pi'(e^{tX}Ye^{-tX})_{|t=0} \quad \text{(by linearity)} \\ &= \frac{d}{dt}(\pi(e^{tX})\pi'(Y)\pi(e^{-tX}))_{|t=0} \quad \text{(by 2.)} \\ &= \frac{d}{dt}(e^{t\pi'(X)}\pi'(Y)e^{-t\pi'(X)})_{|t=0} \quad \text{(by 1.)} \\ &= [\pi'(X), \pi'(Y)]\end{aligned}$$

□

This theorem shows that we can study Lie group representations (π, V) by studying the corresponding Lie algebra representation (π', V). This will generally be much easier since the $\pi'(X)$ are just linear maps. We will proceed in this manner in chapter 8 when we construct and classify all $SU(2)$ and $SO(3)$ representations, finding that the corresponding Lie algebra representations are much simpler to analyze.

For any Lie group G, we have seen that there is a distinguished representation, the adjoint representation $(Ad, \mathfrak{g})$. The corresponding Lie algebra representation is also called the adjoint representation, but written as $(Ad', \mathfrak{g}) = (ad, \mathfrak{g})$. From the fact that

$$Ad(e^{tX})(Y) = e^{tX}Ye^{-tX}$$

we can differentiate with respect to t to get the Lie algebra representation

$$ad(X)(Y) = \frac{d}{dt}(e^{tX}Ye^{-tX})_{|t=0} = [X, Y] \tag{5.3}$$

From this we see that one can define

Definition (Adjoint Lie algebra representation)**.** *ad is the Lie algebra representation given by*

$$X \in \mathfrak{g} \to ad(X)$$

where $ad(X)$ is defined as the linear map from $\mathfrak{g}$ to itself given by

$$Y \to [X, Y]$$

Note that this linear map $ad(X)$, which one can write as $[X, \cdot]$, can be thought of as the infinitesimal version of the conjugation action

$$(\cdot) \to e^{tX}(\cdot)e^{-tX}$$

The Lie algebra homomorphism property of ad says that

$$ad([X, Y]) = ad(X) \circ ad(Y) - ad(Y) \circ ad(X)$$

where these are linear maps on $\mathfrak{g}$, with $\circ$ composition of linear maps, so operating on $Z \in \mathfrak{g}$ we have

$$ad([X, Y])(Z) = (ad(X) \circ ad(Y)((Z) - (ad(Y) \circ ad(X))(Z)$$

Using our expression for ad as a commutator, we find

$$[[X, Y], Z] = [X, [Y, Z]] - [Y, [X, Z]]$$

This is called the Jacobi identity. It could have been more simply derived as an identity about matrix multiplication, but here we see that it is true for a more abstract reason, reflecting the existence of the adjoint representation. It can be written in other forms, rearranging terms using antisymmetry of the commutator, with one example the sum of cyclic permutations

$$[[X, Y], Z] + [[Z, X], Y] + [[Y, Z], X] = 0$$

One can define Lie algebras much more abstractly as follows

Definition (Abstract Lie algebra)**.** *An abstract Lie algebra over a field k is a vector space A over k, with a bilinear operation*

$$[\cdot,\cdot] : (X, Y) \in A \times A \to [X, Y] \in A$$

satisfying

1. *Antisymmetry:*
$$[X, Y] = -[Y, X]$$
2. *Jacobi identity:*
$$[[X, Y], Z] + [[Z, X], Y] + [[Y, Z], X] = 0$$

Such Lie algebras do not need to be defined as matrices, and their Lie bracket operation does not need to be defined in terms of a matrix commutator (although the same notation continues to be used). Later on in this course we will encounter important examples of Lie algebras that are defined in this more abstract way.

5.4 Complexification

The way we have defined a Lie algebra $\mathfrak{g}$, it is a real vector space, not a complex vector space. Even if G is a group of complex matrices, when it is not $GL(n, \mathbf{C})$ itself but some subgroup, its tangent space at the identity will not necessarily be a complex vector space. Consider for example the cases $G = U(1)$ and $G = SU(2)$, where $\mathfrak{u}(1) = \mathbf{R}$ and $\mathfrak{su}(2) = \mathbf{R}^3$. While the tangent space to the group of all invertible complex matrices is a complex vector space, imposing some condition such as unitarity picks out a subspace which generally is just a real vector space, not a complex one. So the adjoint representation $(Ad, \mathfrak{g})$ is in general not a complex representation, but a real representation, with

$$Ad(g) \in GL(\mathfrak{g}) = GL(dim\ \mathfrak{g}, \mathbf{R})$$

The derivative of this is the Lie algebra representation

$$ad : X \in \mathfrak{g} \to ad(X) \in \mathfrak{gl}(dim\ \mathfrak{g}, \mathbf{R})$$

and once we pick a basis of $\mathfrak{g}$, we can identify $\mathfrak{gl}(dim\ \mathfrak{g}, \mathbf{R}) = M(dim\ \mathfrak{g}, \mathbf{R})$. So, for each $X \in \mathfrak{g}$ we get a real linear operator on a real vector space.

We would however often like to work with not real representations, but complex representations, since it is for these that Schur's lemma applies, and representation operators can be diagonalized. To get from a real Lie algebra representation to a complex one, we can "complexify", extending the action of real scalars to complex scalars. If we are working with real matrices, complexification is nothing but allowing complex entries and using the same rules for multiplying scalars as before.

More generally, for any real vector space we can define:

Definition. *The complexification $V_{\mathbf{C}}$ of a real vector space V is the space of pairs (v_1, v_2) of elements of V with multiplication by $a + bi \in \mathbf{C}$ given by*

$$(a + ib)(v_1, v_2) = (av_1 - bv_2, av_2 + bv_1)$$

One should think of the complexification of V as

$$V_{\mathbf{C}} = V + iV$$

with v_1 in the first copy of V, v_2 in the second copy. Then the rule for multiplication by a complex number comes from the standard rules for complex multiplication. In the cases we will be interested in this level of abstraction is not really needed, since V will be given as a subspace of a complex space, and $V_{\mathbf{C}}$ will just be the larger subspace you get by taking complex linear combinations of elements of V.

Given a real Lie algebra $\mathfrak{g}$, the complexification $\mathfrak{g}_{\mathbf{C}}$ is pairs of elements (X_1, X_2) of $\mathfrak{g}$, with the above rule for multiplication by complex scalars. The Lie bracket on $\mathfrak{g}$ extends to a Lie bracket on $\mathfrak{g}_{\mathbf{C}}$ by the rule

$$[(X_1, X_2), (Y_1, Y_2)] = ([X_1, X_2] - [Y_1, Y_2], [X_1, Y_2] + [X_2, Y_1])$$

and $\mathfrak{g}_{\mathbf{C}}$ is a Lie algebra over the complex numbers. In many cases this definition is isomorphic to something just defined in terms of complex matrices, with the simplest case

$$\mathfrak{gl}(n, \mathbf{R})_{\mathbf{C}} = \mathfrak{gl}(n, \mathbf{C})$$

Recalling our discussion from section 5.2.2 of $\mathfrak{u}(n)$, a real Lie algebra, with elements certain (skew-Hermitian) complex matrices, one can see that complexifying will just give all complex matrices so

$$\mathfrak{u}(n)_{\mathbf{C}} = \mathfrak{gl}(n, \mathbf{C})$$

This example shows that two different real Lie algebras may have the same complexification. For yet another example, since $\mathfrak{so}(n)$ is the Lie algebra of all real antisymmetric matrices, $\mathfrak{so}(n)_{\mathbf{C}}$ is the Lie algebra of all complex antisymmetric matrices.

We can extend the operators $ad(X)$ on $\mathfrak{g}$ by complex linearity to turn ad into a complex representation of $\mathfrak{g}_{\mathbf{C}}$ on the vector space $\mathfrak{g}_{\mathbf{C}}$ itself

$$ad : Z \in \mathfrak{g}_{\mathbf{C}} \to ad(Z)$$

Here Z is now a complex linear combination of elements of $X_j \in \mathfrak{g}$, and $ad(Z)$ is the corresponding complex linear combination of the real matrices $ad(X_j)$.

5.5 For further reading

The material of this section is quite conventional mathematics, with many good expositions, although most aimed at a higher level than this course. An example

at the level of this course is the book *Naive Lie Theory* [60]. It covers basics of Lie groups and Lie algebras, but without representations. The notes [28] and book [27] of Brian Hall are a good source to study from. Some parts of the proofs given here are drawn from those notes.

Chapter 6

The Rotation and Spin Groups in 3 and 4 Dimensions

Among the basic symmetry groups of the physical world is the orthogonal group $SO(3)$ of rotations about a point in three-dimensional space. The observables one gets from this group are the components of angular momentum, and understanding how the state space of a quantum system behaves as a representation of this group is a crucial part of the analysis of atomic physics examples and many others. This is a topic one will find in some version or other in every quantum mechanics textbook.

Remarkably, it turns out that the quantum systems in nature are often representations not of $SO(3)$, but of a larger group called $Spin(3)$, one that has two elements corresponding to every element of $SO(3)$. Such a group exists in any dimension n, always as a "doubled" version of the orthogonal group $SO(n)$, one that is needed to understand some of the more subtle aspects of geometry in n dimensions. In the $n = 3$ case it turns out that $Spin(3) \simeq SU(2)$ and we will study in detail the relationship of $SO(3)$ and $SU(2)$. This appearance of the unitary group $SU(2)$ is special to geometry in 3 and 4 dimensions, and we will see that quaternions provide an explanation for this.

6.1 The rotation group in three dimensions

In $\mathbf{R}^2$ rotations about the origin are given by elements of $SO(2)$, with a counterclockwise rotation by an angle θ given by the matrix

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

This can be written as an exponential, $R(\theta) = e^{\theta L} = \cos\theta \mathbf{1} + L \sin\theta$ for

$$L = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

Here $SO(2)$ is a commutative Lie group with Lie algebra $\mathfrak{so}(2) = \mathbf{R}$ (it is one-dimensional, with trivial Lie bracket, all elements of the Lie algebra commute). Note that we have a representation on $V = \mathbf{R}^2$ here, but it is a real representation, not one of the complex ones we have when we have a representation on a quantum mechanical state space.

In three dimensions the group $SO(3)$ is 3-dimensional and non-commutative. Choosing a unit vector $\mathbf{w}$ and angle θ, one gets an element $R(\theta, \mathbf{w})$ of $SO(3)$, rotation by θ about the $\mathbf{w}$ axis. Using standard basis vectors $\mathbf{e}_j$, rotations about the coordinate axes are given by

$$R(\theta, \mathbf{e}_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad R(\theta, \mathbf{e}_2) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

$$R(\theta, \mathbf{e}_3) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

A standard parametrization for elements of $SO(3)$ is in terms of 3 "Euler angles" ϕ, θ, ψ with a general rotation given by

$$R(\phi, \theta, \psi) = R(\psi, \mathbf{e}_3) R(\theta, \mathbf{e}_1) R(\phi, \mathbf{e}_3) \tag{6.1}$$

i.e. first a rotation about the z-axis by an angle ϕ, then a rotation by an angle θ about the new x-axis, followed by a rotation by ψ about the new z-axis. Multiplying out the matrices gives a rather complicated expression for a rotation in terms of the three angles, and one needs to figure out what range to choose for the angles to avoid multiple counting.

The infinitesimal picture near the identity of the group, given by the Lie algebra structure on $\mathfrak{so}(3)$, is much easier to understand. Recall that for orthogonal groups the Lie algebra can be identified with the space of antisymmetric matrices, so one in this case has a basis

$$l_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad l_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad l_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

which satisfy the commutation relations

$$[l_1, l_2] = l_3, \ [l_2, l_3] = l_1, \ [l_3, l_1] = l_2$$

Note that these are exactly the same commutation relations satisfied by the basis vectors X_1, X_2, X_3 of the Lie algebra $\mathfrak{su}(2)$, so $\mathfrak{so}(3)$ and $\mathfrak{su}(2)$ are

isomorphic Lie algebras. They both are the vector space $\mathbf{R}^3$ with the same Lie bracket operation on pairs of vectors. This operation is familiar in yet another context, that of the cross-product of standard basis vectors $\mathbf{e}_j$ in $\mathbf{R}^3$:

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3,\ \mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1,\ \mathbf{e}_3 \times \mathbf{e}_1 = \mathbf{e}_2$$

We see that the Lie bracket operation

$$(X, Y) \in \mathbf{R}^3 \times \mathbf{R}^3 \to [X, Y] \in \mathbf{R}^3$$

that makes $\mathbf{R}^3$ a Lie algebra $\mathfrak{so}(3)$ is just the cross-product on vectors in $\mathbf{R}^3$.

So far we have three different isomorphic ways of putting a Lie bracket on $\mathbf{R}^3$, making it into a Lie algebra:

1. Identify $\mathbf{R}^3$ with antisymmetric real 3 by 3 matrices and take the matrix commutator as Lie bracket.

2. Identify $\mathbf{R}^3$ with skew-adjoint, traceless, complex 2 by 2 matrices and take the matrix commutator as Lie bracket.

3. Use the vector cross-product on $\mathbf{R}^3$ to get a Lie bracket, i.e. define

$$[\mathbf{v}, \mathbf{w}] = \mathbf{v} \times \mathbf{w}$$

Something very special that happens for orthogonal groups only in three dimensions is that the vector representation (the defining representation of $SO(n)$ matrices on $\mathbf{R}^n$) is isomorphic to the adjoint representation. Recall that any Lie group G has a representation $(Ad, \mathfrak{g})$ on its Lie algebra $\mathfrak{g}$. $\mathfrak{so}(n)$ can be identified with the antisymmetric n by n matrices, so is of (real) dimension $\frac{n^2-n}{2}$. Only for $n = 3$ is this equal to n, the dimension of the representation on vectors in $\mathbf{R}^n$. This corresponds to the geometrical fact that only in 3 dimensions is a plane (in all dimensions rotations are built out of rotations in various planes) determined uniquely by a vector (the vector perpendicular to the plane). Equivalently, only in 3 dimensions is there a cross-product $\mathbf{v} \times \mathbf{w}$ which takes two vectors determining a plane to a unique vector perpendicular to the plane.

The isomorphism between the vector representation $(\pi_{vector}, \mathbf{R}^3)$ on column vectors and the adjoint representation $(Ad, \mathfrak{so}(3))$ on antisymmetric matrices is given by

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \leftrightarrow v_1 l_1 + v_2 l_2 + v_3 l_3 = \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}$$

or in terms of bases by

$$\mathbf{e}_j \leftrightarrow l_j$$

For the vector representation on column vectors, $\pi_{vector}(g) = g$ and $\pi'_{vector}(X) = X$, where X is an antisymmetric 3 by 3 matrix, and $g = e^X$ is an orthogonal 3 by 3 matrix. Both act on column vectors by the usual multiplication.

For the adjoint representation on antisymmetric matrices, one has

$$Ad(g)\begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix} = g\begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix} g^{-1}$$

The corresponding Lie algebra representation is given by

$$ad(X)\begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix} = [X, \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}]$$

where X is a 3 by 3 antisymmetric matrix.

One can explicitly check that these representations are isomorphic, for instance by calculating how basis elements $l_j \in \mathfrak{so}(3)$ act. On vectors, these l_j act by matrix multiplication, giving for instance, for $j = 1$

$$l_1\mathbf{e}_1 = 0,\ l_1\mathbf{e}_2 = \mathbf{e}_3,\ l_1\mathbf{e}_3 = -\mathbf{e}_2$$

On antisymmetric matrices one has instead the isomorphic relations

$$(ad(l_1))(l_1) = 0,\ (ad(l_1))(l_2) = l_3,\ (ad(l_1))(l_3) = -l_2$$

6.2 Spin groups in three and four dimensions

A remarkable property of the orthogonal groups $SO(n)$ is that they come with an associated group, called $Spin(n)$, with every element of $SO(n)$ corresponding to two distinct elements of $Spin(n)$. If you have seen some topology, what is at work here is that (for $n > 2$) the fundamental group of $SO(n)$ is non-trivial, with $\pi_1(SO(n)) = \mathbf{Z}_2$ (this means there is a non-contractible loop in $SO(n)$, contractible if you go around it twice). $Spin(n)$ is topologically the simply-connected double-cover of $SO(n)$, and one can choose the covering map $\Phi : Spin(n) \to SO(n)$ to be a group homomorphism. $Spin(n)$ is a Lie group of the same dimension as $SO(n)$, with an isomorphic tangent space at the identity, so the Lie algebras of the two groups are isomorphic: $\mathfrak{so}(n) \simeq \mathfrak{spin}(n)$.

In chapter 26 we will explicitly construct the groups $Spin(n)$ for any n but here we will just do this for $n = 3$ and $n = 4$, using methods specific to these two cases. In the cases $n = 5$ (where $Spin(5) = Sp(2)$, the 2 by 2 norm-preserving quaternionic matrices) and $n = 6$ (where $Spin(6) = SU(4)$) one can also use special methods to identify $Spin(n)$ with other matrix groups. For $n > 6$ the group $Spin(n)$ will be something truly distinct.

Given such a construction of $Spin(n)$, we also need to explicitly construct the homomorphism Φ, and show that its derivative Φ' is an isomorphism of Lie algebras. We will see that the simplest construction of the spin groups here uses the group $Sp(1)$ of unit-length quaternions, with $Spin(3) = Sp(1)$ and $Spin(4) = Sp(1) \times Sp(1)$. By identifying quaternions and pairs of complex numbers, we can show that $Sp(1) = SU(2)$ and thus work with these spin groups as either 2 by 2 complex matrices (for $Spin(3)$), or pairs of such matrices (for $Spin(4)$).

6.2.1 Quaternions

The quaternions are a number system (denoted by $\mathbf{H}$) generalizing the complex number system, with elements $q \in \mathbf{H}$ that can be written as

$$q = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k},\ q_i \in \mathbf{R}$$

with $\mathbf{i}, \mathbf{j}, \mathbf{k} \in \mathbf{H}$ satisfying

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \mathbf{ij} = -\mathbf{ji} = \mathbf{k}, \mathbf{ki} = -\mathbf{ik} = \mathbf{j}, \mathbf{jk} = -\mathbf{kj} = \mathbf{i}$$

and a conjugation operation that takes

$$q \to \bar{q} = q_0 - q_1\mathbf{i} - q_2\mathbf{j} - q_3\mathbf{k}$$

This operation satisfies (for $u, v \in \mathbf{H}$)

$$\overline{uv} = \bar{v}\bar{u}$$

As a vector space over $\mathbf{R}$, $\mathbf{H}$ is isomorphic with $\mathbf{R}^4$. The length-squared function on this $\mathbf{R}^4$ can be written in terms of quaternions as

$$|q|^2 = q\bar{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

and is multiplicative since

$$|uv|^2 = uv\overline{uv} = uv\bar{v}\bar{u} = |u|^2|v|^2$$

Using

$$\frac{q\bar{q}}{|q|^2} = 1$$

one has a formula for the inverse of a quaternion

$$q^{-1} = \frac{\bar{q}}{|q|^2}$$

The length one quaternions thus form a group under multiplication, called $Sp(1)$. There are also Lie groups called $Sp(n)$ for larger values of n, consisting of invertible matrices with quaternionic entries that act on quaternionic vectors preserving the quaternionic length-squared, but these play no significant role in quantum mechanics so we won't study them further. $Sp(1)$ can be identified with the three-dimensional sphere since the length one condition on q is

$$q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$$

the equation of the unit sphere $S^3 \subset \mathbf{R}^4$.

6.2.2 Rotations and spin groups in four dimensions

Pairs (u, v) of unit quaternions give the product group $Sp(1) \times Sp(1)$. An element of this group acts on $\mathbf{H} = \mathbf{R}^4$ by

$$q \to uqv$$

This action preserves lengths of vectors and is linear in q, so it must correspond to an element of the group $SO(4)$. One can easily see that pairs (u, v) and $(-u, -v)$ give the same linear transformation of $\mathbf{R}^4$, so the same element of $SO(4)$. One can show that $SO(4)$ is the group $Sp(1) \times Sp(1)$, with the two elements (u, v) and $(-u, -v)$ identified. The name $Spin(4)$ is given to the Lie group $Sp(1) \times Sp(1)$ that "double covers" $SO(4)$ in this manner.

6.2.3 Rotations and spin groups in three dimensions

Later on in the course we'll encounter $Spin(4)$ and $SO(4)$ again, but for now we're interested in the subgroup $Spin(3)$ that only acts non-trivially on 3 of the dimensions, and double-covers not $SO(4)$ but $SO(3)$. To find this, consider the subgroup of $Spin(4)$ consisting of pairs (u, v) of the form (u, u^{-1}) (a subgroup isomorphic to $Sp(1)$, since elements correspond to a single unit length quaternion u). This subgroup acts on quaternions by conjugation

$$q \to uqu^{-1}$$

an action which is trivial on the real quaternions, but nontrivial on the "pure imaginary" quaternions of the form

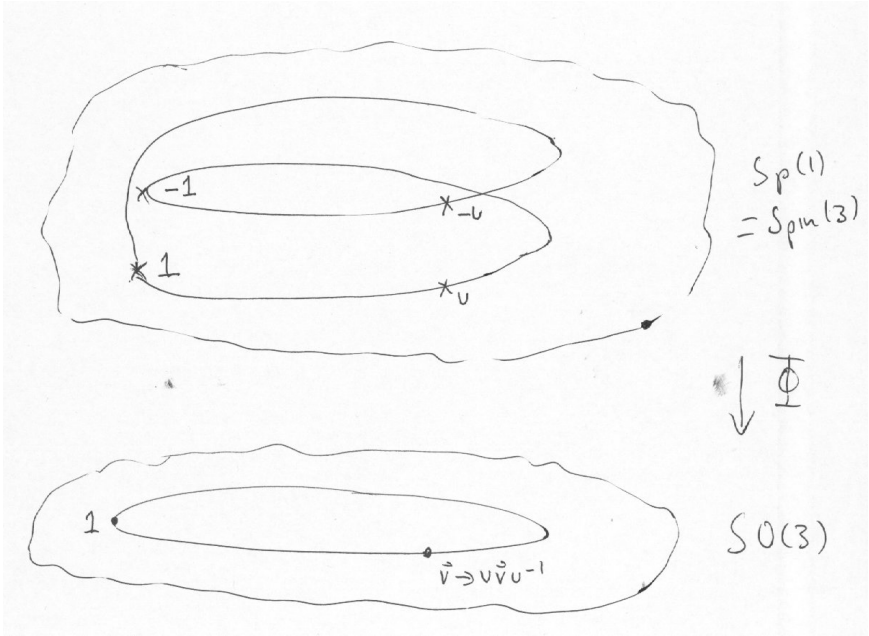
$$q = \vec{v} = v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k}$$

An element $u \in Sp(1)$ acts on $\vec{v} \in \mathbf{R}^3 \subset \mathbf{H}$ as

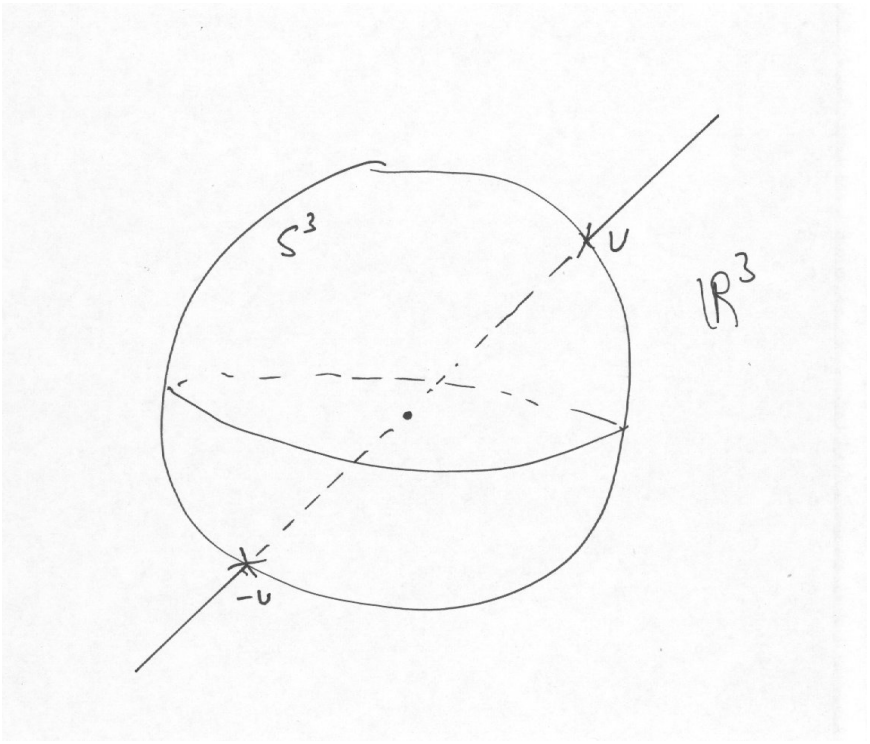
$$\vec{v} \to u\vec{v}u^{-1}$$

This is a linear action, preserving the length $|\vec{v}|$, so corresponds to an element of $SO(3)$. We thus have a map (which can easily be checked to be a homomorphism)

$$\Phi : u \in Sp(1) \to \{\vec{v} \to u\vec{v}u^{-1}\} \in SO(3)$$



Both u and $-u$ act in the same way on $\vec{v}$, so we have two elements in $Sp(1)$ corresponding to the same element in $SO(3)$. One can show that Φ is a surjective map (one can get any element of $SO(3)$ this way), so it is what is called a "covering" map, specifically a two-fold cover. It makes $Sp(1)$ a double-cover of $SO(3)$, and we give this the name "Spin(3)". This also allows us to characterize more simply $SO(3)$ as a geometrical space. It is $S^3 = Sp(1) = Spin(3)$ with opposite points on the three-sphere identified. This space is known as $\mathbf{RP}(3)$, real projective 3-space, which can also be thought of as the space of lines through the origin in $\mathbf{R}^4$ (each such line intersects S^3 in two opposite points).



For those who have seen some topology, note that the covering map Φ is an example of a topologically non-trivial cover. It is just not true that topologically $S^3 \simeq \mathbf{R}\mathbf{P}^3 \times (+1, -1)$. S^3 is a connected space, not two disconnected pieces. This topological non-triviality implies that globally there is no possible homomorphism going in the opposite direction from Φ (i.e. $SO(3) \to Spin(3)$). One can do this locally, picking a local patch in $SO(3)$ and taking the inverse of Φ to a local patch in $Spin(3)$, but this won't work if we try and extend it globally to all of $SO(3)$.

The identification $\mathbf{R}^2 = \mathbf{C}$ allowed us to represent elements of the unit circle group $U(1)$ as exponentials $e^{i\theta}$, where $i\theta$ was in the Lie algebra $\mathfrak{u}(1) = \mathbf{R}$ of $U(1)$. For $Sp(1)$ one can do much the same thing, with the Lie algebra $\mathfrak{sp}(1)$ now the space of all pure imaginary quaternions, which one can identify with $\mathbf{R}^3$ by

$$\mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \in \mathbf{R}^3 \leftrightarrow \vec{w} = w_1\mathbf{i} + w_2\mathbf{j} + w_3\mathbf{k} \in \mathbf{H}$$

Unlike the $U(1)$ case, there's a non-trivial Lie bracket, just the commutator of quaternions.

Elements of the group $Sp(1)$ are given by exponentiating such Lie algebra elements, which we will write in the form

$$u(\theta, \mathbf{w}) = e^{\theta\vec{w}} = \cos\theta + \vec{w}\sin\theta$$

where $\theta \in \mathbf{R}$ and $\vec{w}$ is a purely imaginary quaternion of unit length. Taking θ as a parameter, these give paths in $Sp(1)$ going through the identity at $\theta = 0$, with velocity vector $\vec{w}$ since

$$\frac{d}{d\theta} u(\theta, \mathbf{w})_{|\theta=0} = (-\sin\theta + \vec{w}\cos\theta)_{|\theta=0} = \vec{w}$$

We can explicitly evaluate the homomorphism Φ on such elements $u(\theta, \mathbf{w}) \in Sp(1)$, with the result that Φ takes $u(\theta, \mathbf{w})$ to a rotation by an angle 2θ around the axis $\mathbf{w}$:

Theorem 6.1.

$$\Phi(u(\theta, \mathbf{w})) = R(2\theta, \mathbf{w})$$

Proof. First consider the special case $\mathbf{w} = \mathbf{e}_3$ of rotations about the 3-axis.

$$u(\theta, \mathbf{e}_3) = e^{\theta \mathbf{k}} = \cos\theta + \mathbf{k}\sin\theta$$

and

$$u(\theta, \mathbf{e}_3)^{-1} = e^{-\theta \mathbf{k}} = \cos\theta - \mathbf{k}\sin\theta$$

so $\Phi(u(\theta, \mathbf{e}_3))$ is the rotation that takes $\mathbf{v}$ (identified with the quaternion $\vec{v} = v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k}$) to

$$\begin{aligned} u(\theta, \mathbf{e}_3)\vec{v}u(\theta, \mathbf{e}_3)^{-1} =& (\cos\theta + \mathbf{k}\sin\theta)(v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k})(\cos\theta - \mathbf{k}\sin\theta) \\ =& (v_1(\cos^2\theta - \sin^2\theta) - v_2(2\sin\theta\cos\theta))\mathbf{i} \\ & + (2v_1\sin\theta\cos\theta + v_2(\cos^2\theta - \sin^2\theta))\mathbf{j} + v_3\mathbf{k} \\ =& (v_1\cos 2\theta - v_2\sin 2\theta)\mathbf{i} + (v_1\sin 2\theta + v_2\cos 2\theta)\mathbf{j} + v_3\mathbf{k} \end{aligned}$$

This is the orthogonal transformation of $\mathbf{R}^3$ given by

$$\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \to \begin{pmatrix} \cos 2\theta & -\sin 2\theta & 0 \\ \sin 2\theta & \cos 2\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \tag{6.2}$$

One can readily do the same calculation for the case of $\mathbf{e}_1$, then use the Euler angle parametrization of equation 6.1 to show that a general $u(\theta, \mathbf{w})$ can be written as a product of the cases already worked out. □

Notice that as θ goes from 0 to 2π, $u(\theta, \mathbf{w})$ traces out a circle in $Sp(1)$. The homomorphism Φ takes this to a circle in $SO(3)$, one that gets traced out twice as θ goes from 0 to 2π, explicitly showing the nature of the double covering above that particular circle in $SO(3)$.

The derivative of the map Φ will be a Lie algebra homomorphism, a linear map

$$\Phi' : \mathfrak{sp}(1) \to \mathfrak{so}(3)$$

It takes the Lie algebra $\mathfrak{sp}(1)$ of pure imaginary quaternions to the Lie algebra $\mathfrak{so}(3)$ of 3 by 3 antisymmetric real matrices. One can compute it easily on basis vectors, using for instance equation 6.2 above to find for the case $\vec{w} = \mathbf{k}$

$$\begin{aligned}\Phi'(\mathbf{k}) =& \frac{d}{d\theta}\Phi(\cos\theta + \mathbf{k}\sin\theta)_{|\theta=0} \\ =& \begin{pmatrix} -2\sin 2\theta & -2\cos 2\theta & 0 \\ 2\cos 2\theta & -2\sin 2\theta & 0 \\ 0 & 0 & 0 \end{pmatrix}_{|\theta=0} \\ =& \begin{pmatrix} 0 & -2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 2l_3\end{aligned}$$

Repeating this on other basis vectors one finds that

$$\Phi'(\mathbf{i}) = 2l_1, \Phi'(\mathbf{j}) = 2l_2, \Phi'(\mathbf{k}) = 2l_3$$

Thus Φ' is an isomorphism of $\mathfrak{sp}(1)$ and $\mathfrak{so}(3)$ identifying the bases

$$\frac{\mathbf{i}}{2}, \frac{\mathbf{j}}{2}, \frac{\mathbf{k}}{2} \text{ and } l_1, l_2, l_3$$

Note that it is the $\frac{\mathbf{i}}{2}, \frac{\mathbf{j}}{2}, \frac{\mathbf{k}}{2}$ that satisfy simple commutation relations

$$[\frac{\mathbf{i}}{2}, \frac{\mathbf{j}}{2}] = \frac{\mathbf{k}}{2}, \ [\frac{\mathbf{j}}{2}, \frac{\mathbf{k}}{2}] = \frac{\mathbf{i}}{2}, \ [\frac{\mathbf{k}}{2}, \frac{\mathbf{i}}{2}] = \frac{\mathbf{j}}{2}$$

6.2.4 The spin group and $SU(2)$

Instead of doing calculations using quaternions with their non-commutativity and special multiplication laws, it is more conventional to choose an isomorphism between quaternions $\mathbf{H}$ and a space of 2 by 2 complex matrices, and work just with matrix multiplication and complex numbers. The Pauli matrices can be used to gives such an isomorphism, taking

$$1 \to \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \ \mathbf{i} \to -i\sigma_1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \ \ \mathbf{j} \to -i\sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{k} \to -i\sigma_3 = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

The correspondence between $\mathbf{H}$ and 2 by 2 complex matrices is then given by

$$q = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \leftrightarrow \begin{pmatrix} q_0 - iq_3 & -q_2 - iq_1 \\ q_2 - iq_1 & q_0 + iq_3 \end{pmatrix}$$

Since

$$det \begin{pmatrix} q_0 - iq_3 & -q_2 - iq_1 \\ q_2 - iq_1 & q_0 + iq_3 \end{pmatrix} = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

we see that the length-squared function on quaternions corresponds to the determinant function on 2 by 2 complex matrices. Taking $q \in Sp(1)$, so of length one, the corresponding complex matrix is in $SU(2)$.

Under this identification of $\mathbf{H}$ with 2 by 2 complex matrices, we have an identification of Lie algebras $\mathfrak{sp}(1) = \mathfrak{su}(2)$ between pure imaginary quaternions and skew-Hermitian trace-zero 2 by 2 complex matrices

$$\vec{w} = w_1\mathbf{i} + w_2\mathbf{j} + w_3\mathbf{k} \leftrightarrow \begin{pmatrix} -iw_3 & -w_2 - iw_1 \\ w_2 - iw_1 & iw_3 \end{pmatrix} = -i\mathbf{w} \cdot \sigma$$

The basis $\frac{\mathbf{i}}{2}, \frac{\mathbf{j}}{2}, \frac{\mathbf{k}}{2}$ gets identified with a basis for the Lie algebra $\mathfrak{su}(2)$ which written in terms of the Pauli matrices is

$$X_j = -i\frac{\sigma_j}{2}$$

with the X_j satisfying the commutation relations

$$[X_1, X_2] = X_3,\ [X_2, X_3] = X_1,\ [X_3, X_1] = X_2$$

which are precisely the same commutation relations as for $\mathfrak{so}(3)$

$$[l_1, l_2] = l_3,\ [l_2, l_3] = l_1,\ [l_3, l_1] = l_2$$

We now have no less than three isomorphic Lie algebras $\mathfrak{sp}(1) = \mathfrak{su}(2) = \mathfrak{so}(3)$, with elements that get identified as follows

$$\left(w_1\tfrac{\mathbf{i}}{2} + w_2\tfrac{\mathbf{j}}{2} + w_3\tfrac{\mathbf{k}}{2}\right) \leftrightarrow -\frac{i}{2}\begin{pmatrix} w_3 & w_1 - iw_2 \\ w_1 + iw_2 & -w_3 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}$$

This isomorphism identifies basis vectors by

$$\frac{\mathbf{i}}{2} \leftrightarrow -i\frac{\sigma_1}{2} \leftrightarrow l_1$$

etc. The first of these identifications comes from the way we chose to identify $\mathbf{H}$ with 2 by 2 complex matrices. The second identification is Φ', the derivative at the identity of the covering map Φ.

On each of these isomorphic Lie algebras we have adjoint Lie group (Ad) and Lie algebra (ad) representations. Ad si given by conjugation with the corresponding group elements in $Sp(1), SU(2)$ and $SO(3)$. ad is given by taking commutators in the respective Lie algebras of pure imaginary quaternions, skew-Hermitian trace-zero 2 by 2 complex matrices and 3 by 3 real antisymmetric matrices.

Note that these three Lie algebras are all three-dimensional real vector spaces, so these are real representations. If one wants a complex representation, one can complexify and take complex linear combinations of elements. This is less confusing in the case of $\mathfrak{su}(2)$ than for $\mathfrak{sp}(1)$ since taking complex

linear combinations of skew-Hermitian trace-zero 2 by 2 complex matrices just gives all trace-zero 2 by 2 matrices (the Lie algebra $\mathfrak{sl}(2, \mathbf{C})$).

In addition, recall that there is a fourth isomorphic version of this representation, the representation of $SO(3)$ on column vectors. This is also a real representation, but can straightforwardly be complexified. Since $\mathfrak{so}(3)$ and $\mathfrak{su}(2)$ are isomorphic Lie algebras, their complexifications $\mathfrak{so}(3)_{\mathbf{C}}$ and $\mathfrak{sl}(2, \mathbf{C})$ will also be isomorphic.

In terms of 2 by 2 complex matrices, one can exponentiate Lie algebra elements to get group elements in $SU(2)$ and define

$$\Omega(\theta, \mathbf{w}) = e^{\theta(w_1 X_1 + w_2 X_2 + w_3 X_3)} = e^{-i\frac{\theta}{2}\mathbf{w}\cdot\sigma} \tag{6.3}$$

$$= \cos(\frac{\theta}{2})\mathbf{1} - i(\mathbf{w}\cdot\sigma)\sin(\frac{\theta}{2}) \tag{6.4}$$

Transposing the argument of theorem 6.1 from $\mathbf{H}$ to complex matrices, one finds that, identifying

$$\mathbf{v} \leftrightarrow \mathbf{v}\cdot\sigma = \begin{pmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{pmatrix}$$

one has

$$\Phi(\Omega(\theta, \mathbf{w})) = R(\theta, \mathbf{w})$$

with $\Omega(\theta, \mathbf{w})$ acting by conjugation, taking

$$\mathbf{v}\cdot\sigma \to \Omega(\theta, \mathbf{w})(\mathbf{v}\cdot\sigma)\Omega(\theta, \mathbf{w})^{-1} = (R(\theta, \mathbf{w})\mathbf{v})\cdot\sigma \tag{6.5}$$

Note that in changing from the quaternionic to complex case, we are treating the factor of 2 differently, since in the future we will want to use $\Omega(\theta, \mathbf{w})$ to perform rotations by an angle θ. In terms of the identification $SU(2) = Sp(1)$, we have $\Omega(\theta, \mathbf{w}) = u(\frac{\theta}{2}, \mathbf{w})$.

Recall that any $SU(2)$ matrix can be written in the form

$$\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

$$\alpha = q_0 - iq_3, \quad \beta = -q_2 - iq_1$$

with $\alpha, \beta \in \mathbf{C}$ arbitrary complex numbers satisfying $|\alpha|^2 + |\beta|^2 = 1$. One can also write down a somewhat unenlightening formula for the map $\Phi : SU(2) \to SO(3)$ in terms of such explicit $SU(2)$ matrices, getting

$$\Phi(\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}) = \begin{pmatrix} \mathrm{Im}(\beta^2 - \alpha^2) & \mathrm{Re}(\alpha^2 + \beta^2) & 2\,\mathrm{Im}(\alpha\beta) \\ \mathrm{Re}(\beta^2 - \alpha^2) & \mathrm{Im}(\alpha^2 + \beta^2) & 2\,\mathrm{Re}(\alpha\beta) \\ 2\,\mathrm{Re}(\alpha\overline{\beta}) & -2\,\mathrm{Im}(\alpha\overline{\beta}) & |\alpha|^2 - |\beta|^2 \end{pmatrix}$$

See [58], page 123-4, for a derivation.

6.3 A summary

To summarize, we have shown that for three dimensions we have two distinct Lie groups:

- $Spin(3)$, which geometrically is the space S^3. Its Lie algebra is $\mathbf{R}^3$ with Lie bracket the cross-product. We have seen two different explicit constructions of $Spin(3)$, in terms of unit quaternions ($Sp(1)$), and in terms of 2 by 2 unitary matrices of determinant 1 ($SU(2)$).
- $SO(3)$, with the same Lie algebra $\mathbf{R}^3$ with the same Lie bracket.

There is a group homomorphism Φ that takes the first group to the second, which is a two-fold covering map. Its derivative Φ' is an isomorphism of the Lie algebras of the two groups.

We can see from these constructions two interesting irreducible representations of these groups:

- A representation on $\mathbf{R}^3$ which can be constructed in two different ways: as the adjoint representation of either of the two groups, or as the defining representation of $SO(3)$. This is known to physicists as the "spin 1" representation.
- A representation of the first group on $\mathbf{C}^2$, which is most easily seen as the defining representation of $SU(2)$. It is not a representation of $SO(3)$, since going once around a non-contractible loop starting at the identity takes one to minus the identity, not back to the identity as required. This is called the "spin 1/2 or "spinor" representation and will be studied in more detail in chapter 7.

6.4 For further reading

For another discussion of the relationship of $SO(3)$ and $SU(2)$ as well as a construction of the map Φ, see [58], sections 4.2 and 4.3, as well as [3], chapter 8, and [60] Chapters 2 and 4.

Chapter 7

Rotations and the Spin $\frac{1}{2}$ Particle in a Magnetic Field

The existence of a non-trivial double-cover $Spin(3)$ of the three-dimensional rotation group may seem to be a somewhat obscure mathematical fact. Remarkably though, the existence of fundamental spin-$\frac{1}{2}$ particles shows that it is $Spin(3)$ rather than $SO(3)$ that is the symmetry group corresponding to rotations of fundamental quantum systems. Ignoring the degrees of freedom describing their motion in space, which we will examine in later chapters, states of elementary particles such as the electron are described by a state space $\mathcal{H} = \mathbf{C}^2$, with rotations acting on this space by the two-dimensional irreducible representation of $SU(2) = Spin(3)$.

This is the same two-state system studied in chapter 3, with the $SU(2)$ action found there now acquiring an interpretation as corresponding to the double-cover of rotations of physical space. In this chapter we will revisit that example, emphasizing the relation to rotations.

7.1 The spinor representation

In chapter 6 we examined in great detail various ways of looking at a particular three-dimensional irreducible real representation of the groups $SO(3), SU(2)$ and $Sp(1)$. This was the adjoint representation for those three groups, and isomorphic to the vector representation for $SO(3)$. In the $SU(2)$ and $Sp(1)$ cases, there is an even simpler non-trivial irreducible representation than the adjoint: the representation of 2 by 2 complex matrices in $SU(2)$ on column vectors $\mathbf{C}^2$ by matrix multiplication or the representation of unit quaternions in $Sp(1)$ on $\mathbf{H}$ by scalar multiplication. Choosing an identification $\mathbf{C}^2 = \mathbf{H}$ these are isomorphic representations on $\mathbf{C}^2$ of isomorphic groups, and for calculational convenience we will use $SU(2)$ and its complex matrices rather than dealing with quaternions. This irreducible representation is known as the "spinor" or "spin"

representation of $Spin(3) = SU(2)$. The homomorphism π_{spinor} defining the representation is just the identity map from $SU(2)$ to itself.

The spin representation of $SU(2)$ is not a representation of $SO(3)$. The double cover map $\Phi : SU(2) \to SO(3)$ is a homomorphism, so given a representation (π, V) of $SO(3)$ one gets a representation $(\pi \circ \Phi, V)$ of $SU(2)$ by composition. One cannot go in the other direction: there is no homomorphism $SO(3) \to SU(2)$ that would allow us to make the standard representation of $SU(2)$ on $\mathbf{C}^2$ into an $SO(3)$ representation.

One could try and define a representation of $SO(3)$ by

$$\pi : g \in SO(3) \to \pi(g) = \pi_{spinor}(\tilde{g}) \in SU(2)$$

where $\tilde{g}$ is some choice of one of the elements $\tilde{g} \in SU(2)$ satisfying $\Phi(\tilde{g}) = g$. The problem with this is that we won't quite get a homomorphism. Changing our choice of $\tilde{g}$ will introduce a minus sign, so π will only be a homomorphism up to sign

$$\pi(g_1)\pi(g_2) = \pm\pi(g_1 g_2)$$

The nontrivial nature of the double-covering ensures that there is no way to completely eliminate all minus signs, no matter how we choose $\tilde{g}$. Examples like this, which satisfy the representation property only one up to a sign ambiguity, are known as "projective representations". So, the spinor representation of $SU(2) = Spin(3)$ is only a projective representation of $SO(3)$, not a true representation of $SO(3)$.

Quantum mechanics texts sometimes deal with this phenomenon by noting that physically there is an ambiguity in how one specifies the space of states $\mathcal{H}$, with multiplication by an overall scalar not changing the eigenvalues of operators or the relative probabilities of observing these eigenvalues. As a result, the sign ambiguity has no physical effect. It seems more straightforward though to not try and work with projective representations, but just use the larger group $Spin(3)$, accepting that this is the correct symmetry group reflecting the action of rotations on three-dimensional quantum systems.

The spin representation is more fundamental than the vector representation, in the sense that the spin representation cannot be found just knowing the vector representation, but the vector representation of $SO(3)$ can be constructed knowing the spin representation of $SU(2)$. We have seen this in the identification of $\mathbf{R}^3$ with 2 by 2 complex matrices, where rotations become conjugation by spin representation matrices. Another way of seeing this uses the tensor product, and is explained in section 9.4.3. Note that taking spinors as fundamental entails abandoning the descriptions of three-dimensional geometry purely in terms of real numbers. While the vector representation is a real representation of $SO(3)$ or $Spin(3)$, the spinor representation is a complex representation.

7.2 The spin 1/2 particle in a magnetic field

In chapter 3 we saw that a general quantum system with $\mathcal{H} = \mathbf{C}^2$ could be understood in terms of the action of $U(2)$ on $\mathbf{C}^2$. The self-adjoint observables

correspond (up to a factor of i) to the corresponding Lie algebra representation. The $U(1) \subset U(2)$ subgroup commutes with everything else and can be analyzed separately, so we will just consider the $SU(2)$ subgroup. For an arbitrary such system, the group $SU(2)$ has no particular geometric significance. When it occurs in its role as double-cover of the rotational group, the quantum system is said to carry "spin", in particular "spin one-half" (in chapter 8 will discuss state spaces of higher spin values).

As before, we take as a standard basis for the Lie algebra $\mathfrak{su}(2)$ the operators $X_j, j = 1, 2, 3$, where

$$X_j = -i\frac{\sigma_j}{2}$$

which satisfy the commutation relations

$$[X_1, X_2] = X_3,\ [X_2, X_3] = X_1,\ [X_3, X_1] = X_2$$

To make contact with the physics formalism, we'll define self-adjoint operators

$$S_j = iX_j = \frac{\sigma_j}{2}$$

We could have chosen the other sign, but this is the standard convention of the physics literature. In general, to a skew-adjoint operator (which is what one gets from a unitary Lie algebra representation and what exponentiates to unitary operators) we will associate a self-adjoint operator by multiplying by i. These self-adjoint operators have real eigenvalues (in this case $\pm\frac{1}{2}$), so are favored by physicists as observables since such eigenvalues will be related to experimental results. In the other direction, given a physicist's observable self-adjoint operator, we will multiply by $-i$ to get a skew-adjoint operator that can be exponentiated to get a unitary representation.

Note that the conventional definition of these operators in physics texts includes a factor of $\hbar$:

$$S_j^{phys} = i\hbar X_j = \frac{\hbar\sigma_j}{2}$$

A compensating factor of $1/\hbar$ is then introduced when exponentiating to get group elements

$$\Omega(\theta, \mathbf{w}) = e^{-i\frac{\theta}{\hbar}\mathbf{w}\cdot\mathbf{S}^{phys}} \in SU(2)$$

which do not depend on $\hbar$. The reason for this convention has to do with the action of rotations on functions on $\mathbf{R}^3$ (see chapter 17) and the appearance of $\hbar$ in the definition of the momentum operator. Our definitions of S_j and of rotations using (see equation 6.3)

$$\Omega(\theta, \mathbf{w}) = e^{-i\theta\mathbf{w}\cdot\mathbf{S}} = e^{\theta\mathbf{w}\cdot\mathbf{X}}$$

will not include these factors of $\hbar$, but in any case they will be equivalent to the physics text definitions when we make our standard choice of working with units such that $\hbar = 1$.

States in $\mathcal{H} = \mathbf{C}^2$ that have a well-defined value of the observable S_j will be the eigenvectors of S_j, with value for the observable the corresponding eigenvalue, which will be $\pm\frac{1}{2}$. Measurement theory postulates that if we perform the measurement corresponding to S_j on an arbitrary state $|\psi\rangle$, then we will

- with probability c_+ get a value of $+\frac{1}{2}$ and leave the state in an eigenvector $|j, +\frac{1}{2}\rangle$ of S_j with eigenvalue $+\frac{1}{2}$
- with probability c_- get a value of $-\frac{1}{2}$ and leave the state in an eigenvector $|j, -\frac{1}{2}\rangle$ of S_j with eigenvalue $-\frac{1}{2}$

where if

$$|\psi\rangle = \alpha|j, +\frac{1}{2}\rangle + \beta|j, -\frac{1}{2}\rangle$$

we have

$$c_+ = \frac{|\alpha|^2}{|\alpha|^2 + |\beta|^2}, \quad c_- = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2}$$

After such a measurement, any attempt to measure another $S_k, k \neq j$ will give $\pm\frac{1}{2}$ with equal probability and put the system in a corresponding eigenvector of S_k.

If a quantum system is in an arbitrary state $|\psi\rangle$ it may not have a well-defined value for some observable A, but one can calculate the "expected value" of A. This is the sum over a basis of $\mathcal{H}$ consisting of eigenvectors (which will all be orthogonal) of the corresponding eigenvalues, weighted by the probability of their occurrence. The calculation of this sum in this case ($A = S_j$) using expansion in eigenvectors of S_j gives

$$\begin{aligned}
\frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle} =& \frac{(\overline{\alpha}\langle j, +\frac{1}{2}| + \overline{\beta}\langle j, -\frac{1}{2}|)A(\alpha|j, +\frac{1}{2}\rangle + \beta|j, -\frac{1}{2}\rangle)}{(\overline{\alpha}\langle j, +\frac{1}{2}| + \overline{\beta}\langle j, -\frac{1}{2}|)(\alpha|j, +\frac{1}{2}\rangle + \beta|j, -\frac{1}{2}\rangle)} \\
=& \frac{|\alpha|^2(+\frac{1}{2}) + |\beta|^2(-\frac{1}{2})}{|\alpha|^2 + |\beta|^2} \\
=& c_+(+\frac{1}{2}) + c_-(-\frac{1}{2})
\end{aligned}$$

One often chooses to simplify such calculations by normalizing states so that the denominator $\langle\psi|\psi\rangle$ is 1. Note that the same calculation works in general for the probability of measuring the various eigenvalues of an observable A, as long as one has orthogonality and completeness of eigenvectors.

In the case of a spin one-half particle, the group $Spin(3) = SU(2)$ acts on states by the spinor representation with the element $\Omega(\theta, \mathbf{w}) \in SU(2)$ acting as

$$|\psi\rangle \to \Omega(\theta, \mathbf{w})|\psi\rangle$$

As we saw in chapter 6, the $\Omega(\theta, \mathbf{w})$ also act on self-adjoint matrices by conjugation, an action that corresponds to rotation of vectors when one makes the identification

$$\mathbf{v} \leftrightarrow \mathbf{v} \cdot \sigma$$

(see equation 6.5). Under this identification the S_j correspond (up to a factor of 2) to the basis vectors $\mathbf{e}_j$. One can write their transformation rule as

$$S_j \to S'_j = \Omega(\theta, \mathbf{w}) S_j \Omega(\theta, \mathbf{w})^{-1}$$

and

$$\begin{pmatrix} S'_1 \\ S'_2 \\ S'_3 \end{pmatrix} = R(\theta, \mathbf{w})^T \begin{pmatrix} S_1 \\ S_2 \\ S_3 \end{pmatrix}$$

Note that, recalling the discussion in section 4.1, rotations on sets of basis vectors like this involve the transpose $R(\theta, \mathbf{w})^T$ of the matrix $R(\theta, \mathbf{w})$ that acts on coordinates.

In chapter 42 we will get to the physics of electromagnetic fields and how particles interact with them in quantum mechanics, but for now all we need to know is that for a spin one-half particle, the spin degree of freedom that we are describing by $\mathcal{H} = \mathbf{C}^2$ has a dynamics described by the Hamiltonian

$$H = -\boldsymbol{\mu} \cdot \mathbf{B}$$

Here $\mathbf{B}$ is the vector describing the magnetic field, and

$$\boldsymbol{\mu} = g \frac{-e}{2mc} \mathbf{S}$$

is an operator called the magnetic moment operator. The constants that appear are: $-e$ the electric charge, c the speed of light, m the mass of the particle, and g, a dimensionless number called the "gyromagnetic ratio", which is approximately 2 for an electron, about 5.6 for a proton.

The Schrödinger equation is

$$\frac{d}{dt}|\psi(t)\rangle = -i(-\boldsymbol{\mu} \cdot \mathbf{B})|\psi(t)\rangle$$

with solution

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

where

$$U(t) = e^{it\boldsymbol{\mu}\cdot\mathbf{B}} = e^{it\frac{-ge}{2mc}\mathbf{S}\cdot\mathbf{B}} = e^{t\frac{ge}{2mc}\mathbf{X}\cdot\mathbf{B}} = e^{t\frac{ge|\mathbf{B}|}{2mc}\mathbf{X}\cdot\frac{\mathbf{B}}{|\mathbf{B}|}}$$

The time evolution of a state is thus given at time t by the same $SU(2)$ element that, acting on vectors, gives a rotation about the axis $\mathbf{w} = \frac{\mathbf{B}}{|\mathbf{B}|}$ by an angle

$$\frac{ge|\mathbf{B}|t}{2mc}$$

so is a rotation about $\mathbf{w}$ taking place with angular velocity $\frac{ge|\mathbf{B}|}{2mc}$.

The amount of non-trivial physics that is described by this simple system is impressive, including:

- The Zeeman effect: this is the splitting of atomic energy levels that occurs when an atom is put in a constant magnetic field. With respect to the energy levels for no magnetic field, where both states in $\mathcal{H} = \mathbf{C}^2$ have the same energy, the term in the Hamiltonian given above adds

$$\pm \frac{ge|\mathbf{B}|}{4mc}$$

to the two energy levels, giving a splitting between them proportional to the size of the magnetic field.

- The Stern-Gerlach experiment: here one passes a beam of spin one-half quantum systems through an inhomogeneous magnetic field. We have not yet discussed particle motion, so more is involved here than the simple two-state system. However, it turns out that one can arrange this in such a way as to pick out a specific direction $\mathbf{w}$, and split the beam into two components, of eigenvalue $+\frac{1}{2}$ and $-\frac{1}{2}$ for the operator $\mathbf{w} \cdot \mathbf{S}$.

- Nuclear magnetic resonance spectroscopy: one can subject a spin one-half system to a time-varying magnetic field $\mathbf{B}(t)$, and such a system will be described by the same Schrödinger equation, although now the solution cannot be found just by exponentiating a matrix. Nuclei of atoms provide spin one-half systems that can be probed with time and space-varying magnetic fields, allowing imaging of the material that they make up.

- Quantum computing: attempts to build a quantum computer involve trying to put together multiple systems of this kind (qubits), keeping them isolated from perturbations by the environment, but still allowing interaction with the system in a way that preserves its quantum behavior. The 2012 Physics Nobel prize was awarded for experimental work making progress in this direction.

7.3 The Heisenberg picture

So far in this course we've been describing what is known as the Schrödinger picture of quantum mechanics. States in $\mathcal{H}$ are functions of time, obeying the Schrödinger equation determined by a Hamiltonian observable H, while observable self-adjoint operators A are time-independent. Time evolution is given by a unitary transformation

$$U(t) = e^{-itH}, \quad |\psi(t)\rangle = U(t)|\psi(0)\rangle$$

One can instead use $U(t)$ to make a unitary transformation that puts the time-dependence in the observables, removing it from the states, as follows:

$$|\psi(t)\rangle \to |\psi(t)\rangle_H = U^{-1}(t)|\psi(t)\rangle = |\psi(0)\rangle, \quad A \to A_H(t) = U^{-1}(t)AU(t)$$

where the "H" subscripts for "Heisenberg" indicate that we are dealing with "Heisenberg picture" observables and states. One can easily see that the physically observable quantities given by eigenvalues and expectations values remain the same:

$$_H\langle\psi(t)|A_H|\psi(t)\rangle_H = \langle\psi(t)|U(t)(U^{-1}(t)AU(t))U^{-1}(t)|\psi(t)\rangle = \langle\psi(t)|A|\psi(t)\rangle$$

In the Heisenberg picture the dynamics is given by a differential equation not for the states but for the operators. Recall from our discussion of the adjoint representation (see equation 5.1) the formula

$$\begin{aligned}\frac{d}{dt}(e^{tX}Ye^{-tX}) &= (\frac{d}{dt}(e^{tX}Y))e^{-tX} + e^{tX}Y(\frac{d}{dt}e^{-tX}) \\ &= Xe^{tX}Ye^{-tX} - e^{tX}Ye^{-tX}X\end{aligned}$$

Using this with

$$Y = A, \quad X = iH$$

we find

$$\frac{d}{dt}A_H(t) = [iH, A_H(t)] = i[H, A_H(t)]$$

and this equation determines the time evolution of the observables in the Heisenberg picture.

Applying this to the case of the spin one-half system in a magnetic field, and taking for our observable $\mathbf{S}$ (the S_j, taken together as a column vector) we find

$$\frac{d}{dt}\mathbf{S}_H(t) = i[H, \mathbf{S}_H(t)] = i\frac{eg}{2mc}[\mathbf{S}_H(t)\cdot\mathbf{B}, \mathbf{S}_H(t)] \tag{7.1}$$

We know from the discussion above that the solution will be

$$\mathbf{S}_H(t) = U(t)\mathbf{S}_H(0)U(t)^{-1}$$

for

$$U(t) = e^{-it\frac{ge|\mathbf{B}|}{2mc}\mathbf{S}\cdot\frac{\mathbf{B}}{|\mathbf{B}|}}$$

and thus the spin vector observable evolves in the Heisenberg picture by rotating about the magnetic field vector with angular velocity $\frac{ge|\mathbf{B}|}{2mc}$.

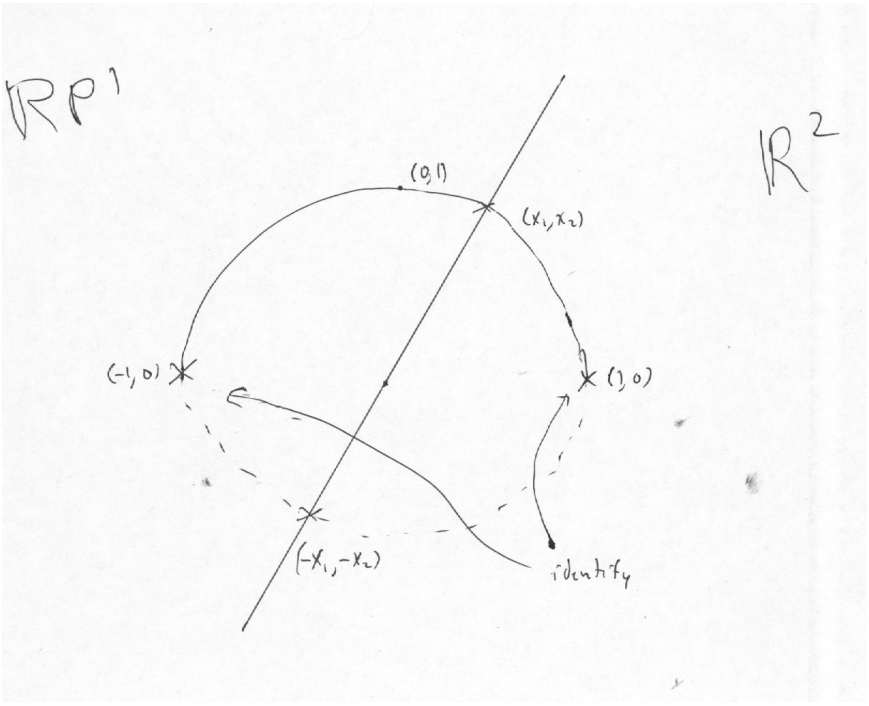
7.4 The Bloch sphere and complex projective space

There is a different approach one can take to characterizing states of a quantum system with $\mathcal{H} = \mathbf{C}^2$. Multiplication of vectors in $\mathcal{H}$ by a non-zero complex number does not change eigenvectors, eigenvalues or expectation values, so arguably has no physical effect. Multiplication by a real scalar just corresponds to a change in normalization of the state, and we will often use this freedom to work with normalized states, those satisfying $\langle\psi|\psi\rangle = 1$. With normalized

states, one still has the freedom to multiply states by a phase $e^{i\theta}$ without changing eigenvectors, eigenvalues or expectation values. In terms of group theory, the overall $U(1)$ in the unitary group $U(2)$ acts on $\mathcal{H}$ by a representation of $U(1)$, which can be characterized by an integer, the corresponding "charge", but this decouples from the rest of the observables and is not of much interest. One is mainly interested in the $SU(2)$ part of the $U(2)$, and the observables that correspond to its Lie algebra.

Working with normalized states in this case corresponds to working with unit-length vectors in $\mathbf{C}^2$, which are given by points on the unit sphere S^3. If we don't care about the overall $U(1)$ action, we can imagine identifying all states that are related by a phase transformation. Using this equivalence relation we can define a new set, whose elements are the "cosets", elements of $S^3 \subset \mathbf{C}^2$, with elements that differ just by multiplication by $e^{i\theta}$ identified. The set of these elements forms a new geometrical space, called the "coset space", often written $S^3/U(1)$. This structure is called a "fibering" of S^3 by circles, and is known as the "Hopf fibration". Try an internet search for various visualizations of the geometrical structure involved, a surprising decomposition of three-dimensional space into non-intersecting curves.

The same space can be represented in a different way, as $\mathbf{C}^2/\mathbf{C}^*$, by taking all elements of $\mathbf{C}^2$ and identifying those related by muliplication by a non-zero complex number. If we were just using real numbers, $\mathbf{R}^2/\mathbf{R}^*$ can be thought of as the space of all lines in the plane going through the origin.



One sees that each such line hits the unit circle in two opposite points, so

this set could be parametrized by a semi-circle, identifying the points at the two ends. This space is given the name $\mathbf{R}P^1$, the "real projective line", and the analog space of lines through the origin in $\mathbf{R}^n$ is called $\mathbf{R}P^{n-1}$. What we are interested in is the complex analog $\mathbf{C}P^1$, which is often called the "complex projective line".

To better understand $\mathbf{C}P^1$, one would like to put coordinates on it. A standard way to choose such a coordinate is to associate to the vector

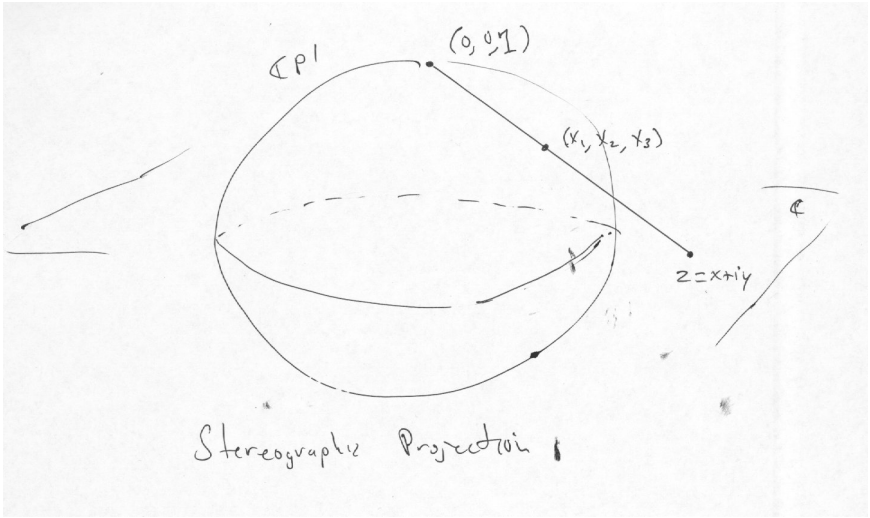
$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \in \mathbf{C}^2$$

the complex number z_1/z_2. Overall multiplication by a complex number will drop out in this ratio, so one gets different values for the coordinate z_1/z_2 for each different coset element, and it appears that elements of $\mathbf{C}P^1$ correspond to points on the complex plane. There is however one problem with this coordinate: the coset of

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

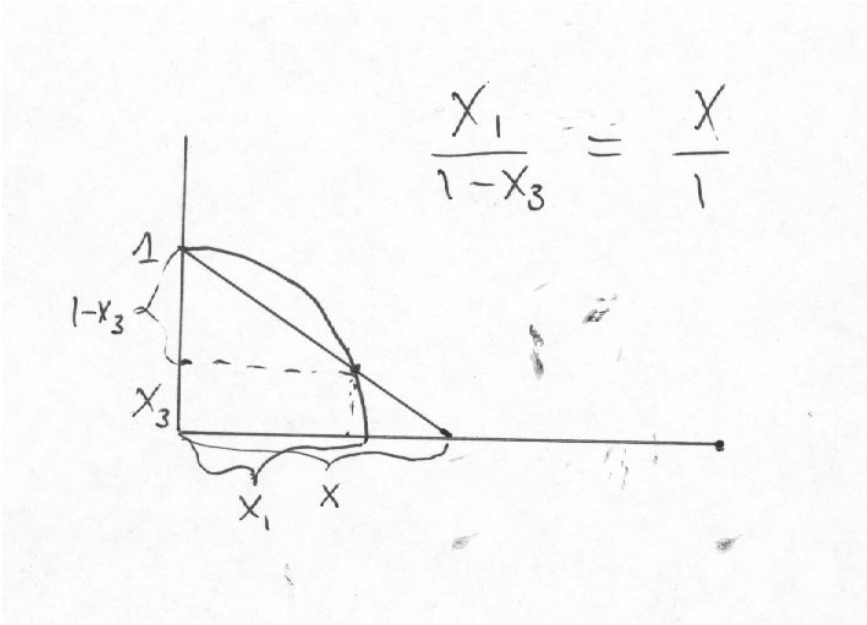
does not have a well-defined value: as one approaches this point one moves off to infinity in the complex plane. In some sense the space $\mathbf{C}P^1$ is the complex plane, but with a "point at infinity" added.

It turns out that $\mathbf{C}P^1$ is best thought of not as a plane together with a point, but as a sphere, with the relation to the plane and the point at infinity given by stereographic projection. Here one creates a one-to-one mapping by considering the lines that go from a point on the sphere to the north pole of the sphere. Such lines will intersect the plane in a point, and give a one-to-one mapping between points on the plane and points on the sphere, except for the north pole. Now, one can identify the north pole with the "point at infinity", and thus the space $\mathbf{C}P^1$ can be identified with the space S^2. The picture looks like this



and the equations relating coordinates (X_1, X_2, X_3) on the sphere and the complex coordinate $z_1/z_2 = z = x + iy$ on the plane are given by

$$x = \frac{X_1}{1 - X_3},\ y = \frac{X_2}{1 - X_3}$$



and

$$X_1 = \frac{2x}{x^2 + y^2 + 1},\ X_2 = \frac{2y}{x^2 + y^2 + 1},\ X_3 = \frac{x^2 + y^2 - 1}{x^2 + y^2 + 1}$$

The action of $SU(2)$ on $\mathcal{H}$ by

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

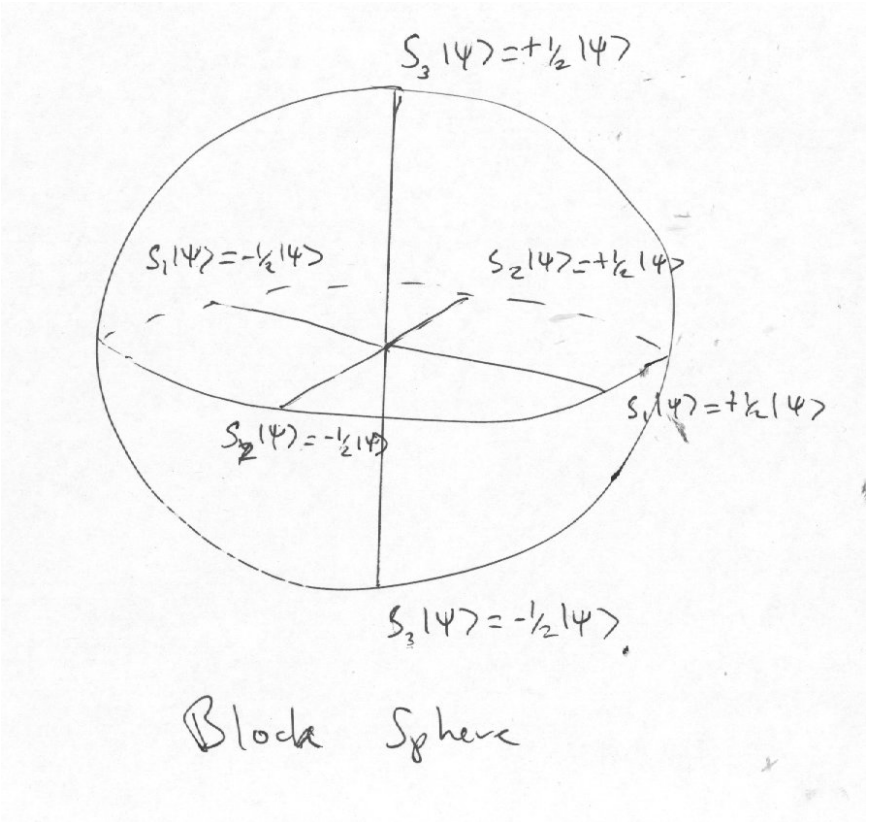
takes

$$z = \frac{z_1}{z_2} \to \frac{\alpha z + \beta}{-\overline{\beta} z + \overline{\alpha}}$$

Such transformations of the complex plane are conformal (angle-preserving) transformations known as "Möbius transformations". One can check that the corresponding transformation on the sphere is the rotation of the sphere in $\mathbf{R}^3$ corresponding to this $SU(2) = Spin(3)$ transformation.

To mathematicians, this sphere identified with $\mathbf{C}P^1$ is known as the "Riemann sphere", whereas physicists often instead use the terminology of "Bloch sphere". It provides a useful parametrization of the states of the qubit system, up to scalar multiplication, which is supposed to be physically irrelevant. The

North pole is the "spin-up" state, the South pole is the "spin-down" state, and along the equator one finds the two states that have definite values for S_1, as well as the two that have definite values for S_2.



Notice that the inner product on vectors in $\mathcal{H}$ does not correspond at all to the inner product of unit vectors in $\mathbf{R}^3$. The North and South poles of the Bloch sphere correspond to orthogonal vectors in $\mathcal{H}$, but they are not at all orthogonal thinking of the corresponding points on the Bloch sphere as vectors in $\mathbf{R}^3$. Similarly, eigenvectors for S_1 and S_2 are orthogonal on the Bloch sphere, but not at all orthogonal in $\mathcal{H}$.

Many of the properties of the Bloch sphere parametrization of states in $\mathcal{H}$ are special to the fact that $\mathcal{H} = \mathbf{C}^2$. In the next class we will study systems of spin $\frac{n}{2}$, where $\mathcal{H} = \mathbf{C}^n$. In these cases there is still a two-dimensional Bloch sphere, but only certain states in $\mathcal{H}$ are parametrized by it. We will see other examples of systems with "coherent states" analogous to the states parametrized by the Bloch sphere, but the case $\mathcal{H}$ has the special property that all states (up to scalar multiplication) are such "coherent states".

7.5 For further reading

Just about every quantum mechanics textbook works out this example of a spin 1/2 particle in a magnetic field. For one example, see chapter 14 of [57]. For an inspirational discussion of spin and quantum mechanics, together with more about the Bloch sphere, see chapter 22 of [45].

Chapter 8

Representations of $SU(2)$ and $SO(3)$

For the case of $G = U(1)$, in chapter 2 we were able to classify all complex irreducible representations by an element of $\mathbf{Z}$ and explicitly construct each irreducible representation. We would like to do the same thing here for representations of $SU(2)$ and $SO(3)$. The end result will be that irreducible representations of $SU(2)$ are classified by a non-negative integer $n = 0, 1, 2, 3, \cdots$, and have dimension $n+1$, so we'll (hoping for no confusion with the irreducible representations $(\pi_n, \mathbf{C})$ of $U(1)$) denote them $(\pi_n, \mathbf{C}^{n+1})$. For even n these will also be irreducible representations of $SO(3)$, but this will not be true for odd n. It is common in physics to label these representations by $s = \frac{n}{2} = 0, \frac{1}{2}, 1, \cdots$ and call the representation labeled by s the "spin s representation". We already know the first three examples:

- Spin 0: $(\pi_0, \mathbf{C})$ is the trivial representation on $\mathbf{V}$, with
$$\pi_0(g) = 1 \ \forall g \in SU(2)$$
This is also a representation of $SO(3)$. In physics, this is sometimes called the "scalar representation". Saying that something transforms under rotations as the "scalar representation" just means that it is invariant under rotations.

- Spin $\frac{1}{2}$: Taking
$$\pi_1(g) = g \in SU(2) \subset U(2)$$
gives the defining representation on $\mathbf{C}^2$. This is the spinor representation discussed in chapter 7. It is not a representation of $SO(3)$.

- Spin 1: Since $SO(3)$ is a group of 3 by 3 matrices, it acts on vectors in $\mathbf{R}^3$. This is just the standard action on vectors by rotation. In other words, the representation is $(\rho, \mathbf{R}^3)$, with ρ the identity homomorphism
$$g \in SO(3) \to \rho(g) = g \in SO(3)$$

One can complexify to get a representation on $\mathbf{C}^3$, which in this case just means acting with $SO(3)$ matrices on column vectors, replacing the real coordinates of vectors by complex coordinates. This is sometimes called the "vector representation", and we saw in chapter 6 that it is isomorphic to the adjoint representation.

One gets a representation $(\pi_2, \mathbf{C}^3)$ of $SU(2)$ by just composing the homomorphisms Φ and ρ:

$$\pi_2 = \rho \circ \Phi : SU(2) \to SO(3)$$

This is the adjoint representation of $SU(2)$.

8.1 Representations of $SU(2)$: classification

8.1.1 Weight decomposition

If we make a choice of a $U(1) \subset SU(2)$, then given any representation (π, V) of $SU(2)$ of dimension m, we get a representation $(\pi_{|U(1)}, V)$ of $U(1)$ by restriction to the $U(1)$ subgroup. Since we know the classification of irreducibles of $U(1)$, we know that

$$(\pi|_{U(1)}, V) = \mathbf{C}_{q_1} \oplus \mathbf{C}_{q_2} \oplus \cdots \oplus \mathbf{C}_{q_m}$$

for $q_1, q_2, \cdots, q_m \in \mathbf{Z}$, where $\mathbf{C}_q$ denotes the one-dimensional representation of $U(1)$ corresponding to the integer q. These are called the "weights" of the representation V. They are exactly the same thing we discussed earlier as "charges", but here we'll favor the mathematician's terminology since the $U(1)$ here occurs in a context far removed from that of electromagnetism and its electric charges.

Since our standard choice of coordinates (the Pauli matrices) picks out the z-direction and diagonalizes the action of the $U(1)$ subgroup corresponding to rotation about this axis, this is the $U(1)$ subgroup we will choose to define the weights of the $SU(2)$ representation V. This is the subgroup of elements of $SU(2)$ of the form

$$\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

Our decomposition of an $SU(2)$ representation (π, V) into irreducible representations of this $U(1)$ subgroup equivalently means that we can choose a basis of V so that

$$\pi \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} = \begin{pmatrix} e^{i\theta q_1} & 0 & \cdots & 0 \\ 0 & e^{i\theta q_2} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & e^{i\theta q_m} \end{pmatrix}$$

An important property of the set of integers q_j is the following:

Theorem. *If q is in the set $\{q_j\}$, so is $-q$.*

Proof. Recall that if we diagonalize a unitary matrix, the diagonal entries are the eigenvalues, but their order is undetermined: acting by permutations on these eigenvalues we get different diagonalizations of the same matrix. In the case of $SU(2)$ the matrix

$$P = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

has the property that conjugation by it permutes the diagonal elements, in particular

$$P \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} P^{-1} = \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

So

$$\pi(P)\pi(\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix})\pi(P)^{-1} = \pi(\begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix})$$

and we see that $\pi(P)$ gives a change of basis of V such that the representation matrices on the $U(1)$ subgroup are as before, with $\theta \to -\theta$. Changing $\theta \to -\theta$ in the representation matrices is equivalent to changing the sign of the weights q_j. The elements of the set $\{q_j\}$ are independent of the basis, so the additional symmetry under sign change implies that for each non-zero element in the set there is another one with the opposite sign. □

Looking at our three examples so far, we see that the scalar or spin 0 representation of course is one-dimensional of weight 0

$$(\pi_0, \mathbf{C}) = \mathbf{C}_0$$

and the spinor or spin $\frac{1}{2}$ representation decomposes into $U(1)$ irreducibles of weights $-1, +1$:

$$(\pi_1, \mathbf{C}^2) = \mathbf{C}_{-1} \oplus \mathbf{C}_{+1}$$

For the spin 1 representation, recall that our double-cover homomorphism Φ takes

$$\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \in SU(2) \to \begin{pmatrix} \cos 2\theta & -\sin 2\theta & 0 \\ \sin 2\theta & \cos 2\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \in SO(3)$$

Acting with the $SO(3)$ matrix on the right on $\mathbf{C}^3$ will give a unitary transformation of $\mathbf{C}^3$, so in the group $U(3)$. One can show that the upper left diagonal 2 by 2 block acts on $\mathbf{C}^2$ with weights $-2, +2$, whereas the bottom right element acts trivially on the remaining part of $\mathbf{C}^3$, which is a one-dimensional representation of weight 0. So, the spin 1 representation decomposes as

$$(\pi_2, \mathbf{C}^3) = \mathbf{C}_{-2} \oplus \mathbf{C}_0 \oplus \mathbf{C}_{+2}$$

Recall that the spin 1 representation of $SU(2)$ is often called the "vector" representation, since it factors in this way through the representation of $SO(3)$ by rotations on three-dimensional vectors.

8.1.2 Lie algebra representations: raising and lowering operators

To proceed further in characterizing a representation (π, V) of $SU(2)$ we need to use not just the action of the chosen $U(1)$ subgroup, but the action of group elements in the other two directions away from the identity. The non-commutativity of the group keeps us from simultaneously diagonalizing those actions and assigning weights to them. We can however work instead with the corresponding Lie algebra representation (π', V) of $\mathfrak{su}(2)$. As in the $U(1)$ case, the group representation is determined by the Lie algebra representation. We will see that for the Lie algebra representation, we can exploit the complexification (recall section 5.4) $\mathfrak{sl}(2, \mathbf{C})$ of $\mathfrak{su}(2)$ to further analyze the possible patterns of weights.

Recall that the Lie algebra $\mathfrak{su}(2)$ can be thought of as the tangent space $\mathbf{R}^3$ to $SU(2)$ at the identity element, with a basis given by the three skew-adjoint 2 by 2 matrices

$$X_j = -i\frac{1}{2}\sigma_j$$

which satisfy the commutation relations

$$[X_1, X_2] = X_3,\ [X_2, X_3] = X_1,\ [X_3, X_1] = X_2$$

We will often use the self-adjoint versions $S_j = iX_j$ that satisfy

$$[S_1, S_2] = iS_3,\ [S_2, S_3] = iS_1,\ [S_3, S_1] = iS_2$$

A unitary representation (π, V) of $SU(2)$ of dimension m is given by a homomorphism

$$\pi : SU(2) \to U(m)$$

and we can take the derivative of this to get a map between the tangent spaces of $SU(2)$ and of $U(m)$, at the identity of both groups, and thus a Lie algebra representation

$$\pi' : \mathfrak{su}(2) \to \mathfrak{u}(m)$$

which takes skew-adjoint 2 by 2 matrices to skew-adjoint m by m matrices, preserving the commutation relations.

We have seen in section 8.1.1 that restricting the representation (π, V) to the diagonal $U(1)$ subgroup of $SU(2)$ and decomposing into irreducibles tells us that we can choose a basis of V so that

$$(\pi, V) = (\pi_{q_1}, \mathbf{C}) \oplus (\pi_{q_2}, \mathbf{C}) \oplus \cdots \oplus (\pi_{q_m}, \mathbf{C})$$

For our choice of $U(1)$ as all matrices of the form

$$e^{i2\theta S_3} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

with $e^{i\theta}$ going around $U(1)$ once as θ goes from 0 to 2π, this means we can choose a basis of V so that

$$\pi(e^{i2\theta S_3}) = \begin{pmatrix} e^{i\theta q_1} & 0 & \cdots & 0 \\ 0 & e^{i\theta q_2} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & e^{i\theta q_m} \end{pmatrix}$$

Taking the derivative of this representation to get a Lie algebra representation, using

$$\pi'(X) = \frac{d}{d\theta}\pi(e^{\theta X})|_{\theta=0}$$

we find for $X = i2S_3$

$$\pi'(i2S_3) = \frac{d}{d\theta}\begin{pmatrix} e^{i\theta q_1} & 0 & \cdots & 0 \\ 0 & e^{i\theta q_2} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & e^{i\theta q_m} \end{pmatrix}_{|\theta=0} = \begin{pmatrix} iq_1 & 0 & \cdots & 0 \\ 0 & iq_2 & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & iq_m \end{pmatrix}$$

Recall that π' is a real-linear map from a real vector space ($\mathfrak{su}(2) = \mathbf{R}^3$) to another real vector space ($\mathfrak{u}(n)$, the skew-Hermitian m by m complex matrices). We can use complex linearity to extend any such map to a complex-linear map from $\mathfrak{su}(2)_{\mathbf{C}}$ (the complexification of $\mathfrak{su}(2)$) to $\mathfrak{u}(m)_{\mathbf{C}}$ (the complexification of $\mathfrak{u}(m)$). $\mathfrak{su}(2)_{\mathbf{C}}$ is all complex linear combinations of the skew-adjoint, trace-free 2 by 2 matrices: the Lie algebra $\mathfrak{sl}(2, \mathbf{C})$ of all complex, trace-free 2 by 2 matrices. $\mathfrak{u}(m)_{\mathbf{C}}$ is $M(m, \mathbf{C}) = \mathfrak{gl}(m, \mathbf{C})$, the Lie algebra of all complex m by m matrices.

As an example, mutiplying $X = i2S_3 \in \mathfrak{su}(2)$ by $\frac{-i}{2}$, we have $S_3 \in \mathfrak{sl}(2, \mathbf{C})$ and the diagonal elements in the matrix $\pi'(i2S_3)$ get also multiplied by $\frac{-i}{2}$ (since π' is a linear map), giving

$$\pi'(S_3) = \begin{pmatrix} \frac{q_1}{2} & 0 & \cdots & 0 \\ 0 & \frac{q_2}{2} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & \frac{q_m}{2} \end{pmatrix}$$

We see that $\pi'(S_3)$ will have half-integral values, and make the following definitions

Definition (Weights and Weight Spaces)**.** *If $\pi'(S_3)$ has an eigenvalue $\frac{k}{2}$, we say that k is a weight of the representation (π, V).*

The subspace $V_k \subset V$ of the representation V satisfying

$$v \in V_k \implies \pi'(S_3)v = \frac{k}{2}v$$

is called the k'th weight space of the representation. All vectors in it are eigenvectors of $\pi'(S_3)$ with eigenvalue $\frac{k}{2}$.

The dimension $\dim V_k$ is called the multiplicity of the weight k in the representation (π, V).

S_1 and S_2 don't commute with S_3, so they may not preserve the subspaces V_k and we can't diagonalize them simultaneously with S_3. We can however exploit the fact that we are in the complexification $\mathfrak{sl}(2,\mathbf{C})$ to construct two complex linear combinations of S_1 and S_2 that do something interesting:

Definition (Raising and lowering operators)**.** *Let*

$$S_+ = S_1 + iS_2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ S_- = S_1 - iS_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We have $S_+, S_- \in \mathfrak{sl}(2,\mathbf{C})$. These are neither self-adjoint nor skew-adjoint, but satisfy

$$(S_\pm)^\dagger = S_\mp$$

and similarly we have

$$\pi'(S_\pm)^\dagger = \pi'(S_\mp)$$

We call $\pi'(S_+)$ a "raising operator" for the representation (π, V), and $\pi'(S_-)$ a "lowering operator".

The reason for this terminology is the following calculation:

$$[S_3, S_+] = [S_3, S_1 + iS_2] = iS_2 + i(-iS_1) = S_1 + iS_2 = S_+$$

which implies (since π' is a Lie algebra homomorphism)

$$\pi'(S_3)\pi'(S_+) - \pi'(S_+)\pi'(S_3) = \pi'([S_3, S_+]) = \pi'(S_+)$$

For any $v \in V_k$, we have

$$\pi'(S_3)\pi'(S_+)v = \pi'(S_+)\pi'(S_3)v + \pi'(S_+)v = (\frac{k}{2} + 1)\pi'(S_+)v$$

so

$$v \in V_k \implies \pi'(S_+)v \in V_{k+2}$$

The linear operator $\pi'(S_+)$ takes vectors with a well-defined weight to vectors with the same weight, plus 2 (thus the terminology "raising operator"). A similar calculation shows that $\pi'(S_-)$ takes V_k to V_{k-2}, lowering the weight by 2.

We're now ready to classify all finite dimensional irreducible unitary representations (π, V) of $SU(2)$. We define

Definition (Highest weights and highest weight vectors)**.** *A non-zero vector $v \in V_n \subset V$ such that*

$$\pi'(S_+)v = 0$$

is called a highest weight vector, with highest weight n.

Irreducible representations will be characterized by a highest weight vector, as follows

Theorem (Highest weight theorem)**.** *Finite dimensional irreducible representations of $SU(2)$ have weights of the form*

$$-n, -n+2, \cdots, n-2, n$$

for n a non-negative integer, each with multiplicity 1, with n a highest weight.

Proof. Finite dimensionality implies there is a highest weight n, and we can choose any highest weight vector $v_n \in V_n$. Repeatedly applying $\pi'(S_-)$ to v_n will give new vectors

$$v_{n-2j} = \pi'(S_-)^j v_n \in V_{n-2j}$$

with weights $n - 2j$.

Consider the span of the $v_{n-2j}, j \geq 0$. To show that this is a representation one needs to show that the $\pi'(S_3)$ and $\pi'(S_+)$ leave it invariant. For $\pi'(S_3)$ this is obvious, for $\pi'(S_+)$ one can show that

$$\pi'(S_+)v_{n-2j} = j(n-j+1)v_{n-2(j-1)} \tag{8.1}$$

by an induction argument. For $j = 0$ this is just the highest weight condition on v_n. Assuming validity for j, one can check validity for $j+1$ by

$$\begin{aligned}
\pi'(S_+)v_{n-2(j+1)} =& \pi'(S_+)\pi'(S_-)v_{n-2j} \\
=& (\pi'([S_+, S_-]) + \pi'(S_-)\pi'(S_+))v_{n-2j} \\
=& (\pi'(2S_3) + \pi'(S_-)\pi'(S_+))v_{n-2j} \\
=& ((n-2j)v_{n-2j} + \pi'(S_-)j(n-j+1)v_{n-2(j-1)} \\
=& ((n-2j) + j(n-j+1))v_{n-2j} \\
=& (j+1)(n-(j+1)+1)v_{n-2((j+1)-1)}
\end{aligned}$$

where we have used the commutation relation

$$[S_+, S_-] = 2S_3$$

The span of the v_{n-2j} is not just a representation, but an irreducible one, since all the non-zero v_{n-2j} arise by repeated application of $\pi'(S_-)$ to v_n and equation 8.1 shows that (up to a constant) $\pi'(S_+)$ is an inverse to $\pi'(S_-)$ for all j up to the value $j = n+1$. In the sequence of v_{n-2j} for increasing j, finite-dimensionality of V^n implies that at some point one one must hit a "lowest weight vector", one annihilated by $\pi'(S_-)$. From that point on, the v_{n-2j} for higher j will be zero. Taking into account the fact that the pattern of weights is invariant under change of sign, one finds that the only possible pattern of weights is

$$-n, -n+2, \cdots, n-2, n$$

This is consistent with equation 8.1, which shows that it is at $j = n$ that $\pi'(S_-)$ will act on v_{n-2j} without having an inverse proportional to $\pi'(S_+)$ (which would act on $v_{n-2(j+1)}$).

□

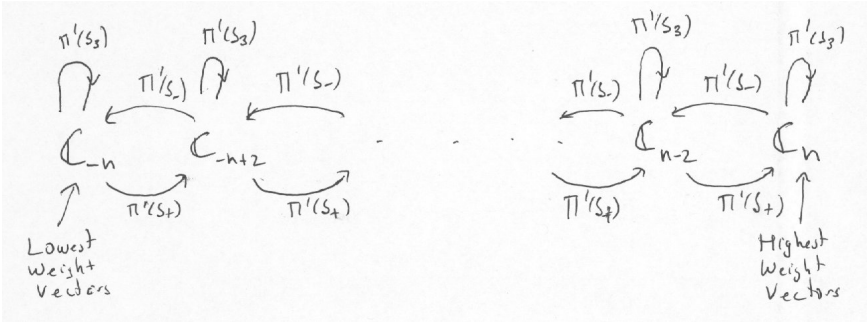
Since we saw in section 8.1.1 that representations can be studied by looking at by the set of their weights under the action of our chosen $U(1) \subset SU(2)$, we can label irreducible representations of $SU(2)$ by a non-negative integer n, the highest weight. Such a representation will be of dimension $n+1$, with weights

$$-n, -n+2, \cdots, n-2, n$$

Each weight occurs with multiplicity one, and we have

$$(\pi, V) = \mathbf{C}_{-n} \oplus \mathbf{C}_{-n+2} \oplus \cdots \mathbf{C}_{n-2} \oplus \mathbf{C}_n$$

Starting with a highest-weight or lowest-weight vector, one can generate a basis for the representation by repeatedly applying raising or lowering operators. The picture to keep in mind is this



where all the vector spaces are copies of $\mathbf{C}$, and all the maps are isomorphisms (multiplications by various numbers).

In summary, we see that all irreducible finite dimensional unitary $SU(2)$ representations can be labeled by a non-negative integer, the highest weight n. These representations have dimension $n+1$ and we will denote them $(\pi_n, V^n = \mathbf{C}^{n+1})$. Note that V_n is the n'th weight space, V^n is the representation with highest weight n. The physicist's terminology for this uses not n, but $\frac{n}{2}$ and calls this number the "spin"of the representation. We have so far seen the lowest three examples $n = 0, 1, 2$, or spin $s = \frac{n}{2} = 0, \frac{1}{2}, 1$, but there is an infinite class of larger irreducibles, with $dim\ V = n + 1 = 2s + 1$.

8.2 Representations of $SU(2)$: construction

The argument of the previous section only tells us what properties possible finite dimensional irreducible representations of $SU(2)$ must have. It shows how to construct such representations given a highest-weight vector, but does not provide any way to construct such highest weight vectors. We would like to find some method to explicitly construct an irreducible (π_n, V^n) for each highest weight n. There are several possible constructions, but perhaps the simplest one is the following, which gives a representation of highest weight n by looking at polynomials in two complex variables, homogeneous of degree n.

Recall from our early discussion of representations that if one has an action of a group on a space M, one can get a representation on functions f on M by taking

$$(\pi(g)f)(x) = f(g^{-1} \cdot x)$$

For $SU(2)$, we have an obvious action of the group on $M = \mathbf{C}^2$ (by matrices acting on column vectors), and we look at a specific class of functions on this space, the polynomials. We can break up the infinite-dimensional space of polynomials on $\mathbf{C}^2$ into finite-dimensional subspaces as follows:

Definition (Homogeneous polynomials)**.** *The complex vector space of homogeneous polynomials of degree m in two complex variables z_1, z_2 is the space of functions on $\mathbf{C}^2$ of the form*

$$f(z_1, z_2) = a_0 z_1^n + a_1 z_1^{n-1} z_2 + \cdots + a_{n-1} z_1 z_2^{n-1} + a_n z_2^n$$

The space of such functions is a complex vector space of dimension $n + 1$.

Using the action of $SU(2)$ on $\mathbf{C}^2$, we will see that this space of functions is exactly the representation space V^n that we need. More explicitly, for

$$g = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}, \; g^{-1} = \begin{pmatrix} \overline{\alpha} & -\beta \\ \overline{\beta} & \alpha \end{pmatrix}$$

we can construct the representation as follows:

$$\begin{aligned}(\pi_n(g)f)(z_1, z_2) =& f(g^{-1} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}) \\ =& f(\overline{\alpha} z_1 - \beta z_2, \overline{\beta} z_1 + \alpha z_2) \\ =& \sum_{k=0}^{n} a_k (\overline{\alpha} z_1 - \beta z_2)^{n-k} (\overline{\beta} z_1 + \alpha z_2)^k\end{aligned}$$

Taking the derivative, the Lie algebra representation is given by

$$\pi_n'(X)f = \frac{d}{dt} \pi_n(e^{tX}) f_{|t=0} = \frac{d}{dt} f(e^{-tX} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix})_{|t=0}$$

By the chain rule this is

$$\begin{aligned}\pi_n'(X)f =& (\frac{\partial f}{\partial z_1}, \frac{\partial f}{\partial z_2})(\frac{d}{dt} e^{-tX} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix})_{|t=0} \\ =& -\frac{\partial f}{\partial z_1}(X_{11} z_1 + X_{12} z_2) - \frac{\partial f}{\partial z_2}(X_{21} z_1 + X_{22} z_2)\end{aligned}$$

where the X_{ij} are the components of the matrix X.

Computing what happens for $X = S_3, S_+, S_-$, we get

$$(\pi_n'(S_3)f)(z_1, z_2) = \frac{1}{2}(-\frac{\partial f}{\partial z_1} z_1 + \frac{\partial f}{\partial z_2} z_2)$$

so

$$\pi'_n(S_3) = \frac{1}{2}(-z_1\frac{\partial}{\partial z_1} + z_2\frac{\partial}{\partial z_2})$$

and similarly

$$\pi'_n(S_+) = -z_2\frac{\partial}{\partial z_1}, \quad \pi'_n(S_-) = -z_1\frac{\partial}{\partial z_2}$$

The $z_1^k z_2^{n-k}$ are eigenvectors for S_3 with eigenvalue $\frac{1}{2}(n-2k)$ since

$$\pi'_n(S_3)z_1^k z_2^{n-k} = \frac{1}{2}(-kz_1^k z_2^{n-k} + (n-k)z_1^k z_2^{n-k}) = \frac{1}{2}(n-2k)z_1^k z_2^{n-k}$$

z_2^n will be an explicit highest weight vector for the representation (π_n, V^n).

An important thing to note here is that the formulas we have found for π' are not in terms of matrices. Instead we have seen that when we construct our representations using functions on $\mathbf{C}^2$, for any $X \in \mathfrak{su}(2)$ (or its complexification $\mathfrak{sl}(2,\mathbf{C})$), $\pi'_n(X)$ is given by a differential operator. Note that these differential operators are independent of n: one gets the same operator $\pi'(X)$ on all the V^n. This is because the original definition of the representation

$$(\pi(g)f)(x) = f(g^{-1}\cdot x)$$

is on the full infinite dimensional space of polynomials on $\mathbf{C}^2$. While this space is infinite-dimensional, issues of analysis don't really come into play here, since polynomial functions are essentially an algebraic construction. Later on in the course we will need to work with function spaces that require much more serious consideration of issues in analysis.

Restricting the differential operators $\pi'(X)$ to a finite dimensional irreducible subspace V^n, the homogeneous polynomials of degree n, if one chooses a basis of V^n, then the linear operator $\pi'(X)$ will be given by a $n+1$ by $n+1$ matrix. Clearly though, the expression as a simple first-order differential operator is much easier to work with. In the examples we will be studying in much of the rest of the course, the representations under consideration will also be on function spaces, with Lie algebra representations appearing as differential operators. Instead of using linear algebra techniques to find eigenvalues and eigenvectors, the eigenvector equation will be a partial differential equation, wtih our focus on using Lie groups and their representation theory to solve such equations.

One issue we haven't addressed yet is that of unitarity of the representation. We need Hermitian inner products on the spaces V^n, inner products that will be preserved by the action of $SU(2)$ that we have defined on these spaces. A standard way to define a Hermitian inner product on functions on a space M is to define them using an integral: for f, g functions on M, take their inner product to be

$$\langle f, g\rangle = \int_M \overline{f}g$$

While for $M = \mathbf{C}^2$ this gives an $SU(2)$ invariant inner product on functions, it is useless for f, g polynomial, since such integrals diverge. What one can do in

this case is define an inner product on polynomial functions on $\mathbf{C}^2$ by

$$\langle f, g\rangle = \frac{1}{\pi^2}\int_{\mathbf{C}^2} \overline{f(z_1, z_2)}g(z_1, z_2)e^{-(|z_1|^2+|z_2|^2)}dx_1dy_1dx_2dy_2 \tag{8.2}$$

Here $z_1 = x_1 + iy_1, z_2 = x_2 + iy_2$. One can do integrals of this kind fairly easily since they factorize into separate integrals over z_1 and z_2, each of which can be treated using polar coordinates and standard calculus methods. One can check by explicit computation that the polynomials

$$\frac{z_1^j z_2^k}{\sqrt{j!k!}}$$

will be an orthornormal basis of the space of polynomial functions with respect to this inner product, and the operators $\pi'(X), X \in \mathfrak{su}(2)$ will be skew-adjoint.

Working out what happens for the first few examples of irreducible $SU(2)$ representations, one finds orthonormal bases for the representation spaces V^n of homogeneous polynomials as follows

- For $n = s = 0$

$$1$$

- For $n = 1, s = \frac{1}{2}$

$$z_1,\ z_2$$

- For $n = 2, s = 1$

$$\frac{1}{\sqrt{2}}z_1^2,\ z_1z_2,\ \frac{1}{\sqrt{2}}z_2^2$$

- For $n = 3, s = \frac{3}{2}$

$$\frac{1}{\sqrt{6}}z_1^3,\ \frac{1}{\sqrt{2}}z_1^2z_2,\ \frac{1}{\sqrt{2}}z_1z_2^2,\ \frac{1}{\sqrt{6}}z_2^3$$

8.3 Representations of $SO(3)$ and spherical harmonics

We would like to now use the classification and construction of representations of $SU(2)$ to study the representations of the closely related group $SO(3)$. For any representation (ρ, V) of $SO(3)$, we can use the double-covering homomorphism $\Phi : SU(2) \to SO(3)$ to get a representation

$$\pi = \rho \circ \Phi$$

of $SU(2)$. It can be shown that if ρ is irreducible, π will be too, so we must have $\pi = \rho \circ \Phi = \pi_n$, one of the irreducible representations of $SU(2)$ found in the last section. Using the fact that $\Phi(-\mathbf{1}) = \mathbf{1}$, we see that

$$\pi_n(-\mathbf{1}) = \rho \circ \Phi(-\mathbf{1}) = \mathbf{1}$$

From knowing that the weights of π_n are $-n, -n+2, \cdots, n-2, n$, we know that

$$\pi_n(-\mathbf{1}) = \pi_n \begin{pmatrix} e^{i\pi} & 0 \\ 0 & e^{-i\pi} \end{pmatrix} = \begin{pmatrix} e^{in\pi} & 0 & \cdots & 0 \\ 0 & e^{i(n-2)\pi} & \cdots & 0 \\ \cdots & & & \cdots \\ 0 & 0 & \cdots & e^{-in\pi} \end{pmatrix} = \mathbf{1}$$

which will only be true for n even, not for n odd. Since the Lie algebra of $SO(3)$ is isomorphic to the Lie algebra of $SU(2)$, the same Lie algebra argument using raising and lowering operators as in the last section also applies. The irreducible representations of $SO(3)$ will be $(\rho_l, V = \mathbf{C}^{2l+1})$ for $l = 0, 1, 2, \cdots$, of dimension $2l+1$ and satisfying

$$\rho_l \circ \Phi = \pi_{2l}$$

Just like in the case of $SU(2)$, we can explicitly construct these representations using functions on a space with an $SO(3)$ action. The obvious space to choose is $\mathbf{R}^3$, with $SO(3)$ matrices acting on $\mathbf{x} \in \mathbf{R}^3$ as column vectors, by the formula we have repeatedly used

$$(\rho(g)f)(x) = f(g^{-1} \cdot \mathbf{x}) = f(g^{-1} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix})$$

Taking the derivative, the Lie algebra representation is given by

$$\rho'(X)f = \frac{d}{dt}\rho(e^{tX})f_{|t=0} = \frac{d}{dt}f(e^{-tX} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix})_{|t=0}$$

where $X \in \mathfrak{so}(3)$. Recall that a basis for $\mathfrak{so}(3)$ is given by

$$l_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad l_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad l_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

which satisfy the commutation relations

$$[l_1, l_2] = l_3, \ [l_2, l_3] = l_1, \ [l_3, l_1] = l_2$$

Digression. *A Note on Conventions*

We're using the notation l_j for the real basis of the Lie algebra $\mathfrak{so}(3) = \mathfrak{su}(2)$. For a unitary representation ρ, the $\rho'(l_j)$ will be skew-adjoint linear operators. For consistency with the physics literature, we'll use the notation $L_j = i\rho'(l_j)$ for the self-adjoint version of the linear operator corresponding to l_j in this representation on functions. The L_j satisfy the commutation relations

$$[L_1, L_2] = iL_3, \ [L_2, L_3] = iL_1, \ [L_3, L_1] = iL_2$$

We'll also use elements $l_\pm = l_1 \pm il_2$ of the complexified Lie algebra to create raising and lowering operators $L_\pm = i\rho'(l_\pm)$.

As with the $SU(2)$ case, we won't include a factor of $\hbar$ as is usual in physics (e.g. the usual convention is $L_j = i\hbar\rho'(l_j)$), since for considerations of the action of the rotation group it would just cancel out (physicists define rotations using $e^{\frac{i}{\hbar}\theta L_j}$). The factor of $\hbar$ is only of significance when L_j is expressed in terms of the momentum operator, a topic discussed in chapter 17.

In the $SU(2)$ case, the $\pi'(S_j)$ had half-integral eigenvalues, with the eigenvalues of $\pi'(2S_3)$ the integral weights of the representation. Here the L_j will have integer eigenvalues, the weights will be the eigenvalues of $2L_3$, which will be even integers.

Computing $\rho'(l_1)$ we find

$$\rho'(l_1)f = \frac{d}{dt}f(e^{-t\begin{pmatrix}0&0&0\\0&0&-1\\0&1&0\end{pmatrix}}\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix})_{|t=0} \tag{8.3}$$

$$= \frac{d}{dt}f(\begin{pmatrix}0&0&0\\0&\cos t&\sin t\\0&-\sin t&\cos t\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix})_{|t=0} \tag{8.4}$$

$$= \frac{d}{dt}f(\begin{pmatrix}0\\x_2\cos t + x_3\sin t\\-x_2\sin t + x_3\cos t\end{pmatrix})_{|t=0} \tag{8.5}$$

$$= (\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \frac{\partial f}{\partial x_3}) \cdot \begin{pmatrix}0\\x_3\\-x_2\end{pmatrix} \tag{8.6}$$

$$= x_3\frac{\partial f}{\partial x_2} - x_2\frac{\partial f}{\partial x_3} \tag{8.7}$$

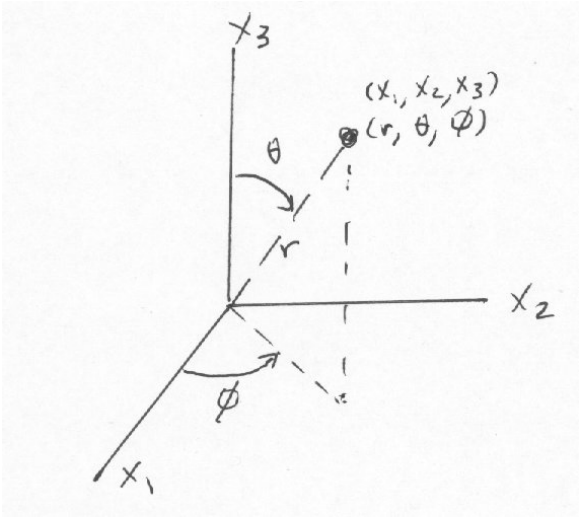
so

$$\rho'(l_1) = x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}$$

and similar calculations give

$$\rho'(l_2) = x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1},\ \rho'(l_3) = x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}$$

The space of all functions on $\mathbf{R}^3$ is much too big: it will give us an infinity of copies of each finite dimensional representation that we want. Notice that when $SO(3)$ acts on $\mathbf{R}^3$, it leaves the distance to the origin invariant. If we work in spherical coordinates (r, θ, ϕ) (see picture)



we will have

$$\begin{aligned} x_1 =& r\sin\theta\cos\phi \\ x_2 =& r\sin\theta\sin\phi \\ x_3 =& r\cos\theta \end{aligned}$$

Acting on $f(r,\phi,\theta)$, $SO(3)$ will leave r invariant, only acting non-trivially on θ,ϕ. It turns out that we can cut down the space of functions to something that will only contain one copy of the representation we want in various ways. One way to do this is to restrict our functions to the unit sphere, i.e. just look at functions $f(\theta,\phi)$. We will see that the representations we are looking for can be found in simple trigonometric functions of these two angular variables.

We can construct our irreducible representations ρ'_l by explicitly constructing a function we will call $Y_l^l(\theta,\phi)$ that will be a highest weight vector of weight l. The weight l condition and the highest weight condition give two differential equations for $Y_l^l(\theta,\phi)$:

$$L_3 Y_l^l = lY_l^l,\ L_+ Y_l^l = 0$$

These will turn out to have a unique solution (up to scalars).

We first need to change coordinates from rectangular to spherical in our expressions for $L_3, L_\pm$. Using the chain rule to compute expressions like

$$\frac{\partial}{\partial r} f(x_1(r,\theta,\phi), x_2(r,\theta,\phi), x_3(r,\theta,\phi))$$

we find

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ r\cos\theta\cos\phi & r\cos\theta\sin\phi & -\sin\theta \\ -r\sin\theta\sin\phi & r\sin\theta\cos\phi & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix}$$

so

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r}\frac{\partial}{\partial \theta} \\ \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix}$$

This is an orthogonal matrix, so one can invert it by taking its transpose, to get

$$\begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r}\frac{\partial}{\partial \theta} \\ \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{pmatrix}$$

So we finally have

$$L_1 = i\rho'(l_1) = i(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}) = i(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi})$$

$$L_2 = i\rho'(l_2) = i(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}) = i(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi})$$

$$L_3 = i\rho'(l_3) = i(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}) = -i\frac{\partial}{\partial\phi}$$

and

$$L_+ = i\rho'(l_+) = e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}), \quad L_- = i\rho'(l_-) = e^{-i\phi}(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})$$

Now that we have expressions for the action of the Lie algebra on functions in spherical coordinates, our two differential equations saying our function $Y_l^l(\theta,\phi)$ is of weight l and in the highest-weight space are

$$L_3Y_l^l(\theta,\phi) = -i\frac{\partial}{\partial\phi}Y_l^l(\theta,\phi) = lY_l^l(\theta,\phi)$$

and

$$L_+Y_l^l(\theta,\phi) = e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})Y_l^l(\theta,\phi) = 0$$

The first of these tells us that

$$Y_l^l(\theta,\phi) = e^{il\phi}F_l(\theta)$$

for some function $F_l(\theta)$, and using the second we get

$$(\frac{\partial}{\partial\theta} - l\cot\theta)F_l(\theta)$$

with solution

$$F_l(\theta) = C_{ll}\sin^l\theta$$

for an arbitrary constant C_{ll}. Finally

$$Y_l^l(\theta,\phi) = C_{ll}e^{il\phi}\sin^l\theta$$

This is a function on the sphere, which is also a highest weight vector in a $2l+1$ dimensional irreducible representation of $SO(3)$. To get functions which give vectors spanning the rest of the weight spaces, one just repeatedly applies the lowering operator L_-, getting functions

$$\begin{aligned} Y_l^m(\theta,\phi) =& C_{lm}(L_-)^{l-m}Y_l^l(\theta,\phi) \\ =& C_{lm}(e^{-i\phi}(-\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}))^{l-m}e^{il\phi}\sin^l\theta \end{aligned}$$

for $m = l, l-1, l-2\cdots, -l+1, -l$

The functions $Y_l^m(\theta,\phi)$ are called "spherical harmonics", and they span the space of complex functions on the sphere in much the same way that the $e^{in\theta}$ span the space of complex valued functions on the circle. Unlike the case of polynomials on $\mathbf{C}^2$, for functions on the sphere, one gets finite numbers by integrating such functions over the sphere. So one can define an inner product on these representations for which they are unitary by simply setting

$$\langle f,g\rangle = \int_{S^2}\overline{f}g\sin\theta d\theta d\phi = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\overline{f(\theta,\phi)}g(\theta,\phi)\sin\theta d\theta d\phi$$

We will not try and show this here, but for the allowable values of l, m the $Y_l^m(\theta,\phi)$ are mutually orthogonal with respect to this inner product.

One can derive various general formulas for the $Y_l^m(\theta,\phi)$ in terms of Legendre polynomials, but here we'll just compute the first few examples, with the proper constants that give them norm 1 with respect to the chosen inner product.

- For the $l=0$ representation

$$Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$$

- For the $l=1$ representation

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi},\quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta,\quad Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}$$

  (one can easily see that these have the correct eigenvalues for $\rho'(L_3) = -i\frac{\partial}{\partial\phi}$).

- For the $l=2$ representation one has

$$Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{i2\phi},\quad Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_2^{-1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{-i\phi},\quad Y_2^{-2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-i2\phi}$$

We will see later that these functions of the angular variables in spherical coordinates are exactly the functions that give the angular dependence of wavefunctions for the physical system of a particle in a spherically symmetric potential. In such a case the $SO(3)$ symmetry of the system implies that the state space (the wavefunctions) will provide a unitary representation π of $SO(3)$, and the action of the Hamiltonian operator H will commute with the action of the operators $L_3, L_\pm$. As a result all of the states in an irreducible representation component of π will have the same energy. States are thus organized into "orbitals", with singlet states called "s" orbitals ($l = 0$), triplet states called "p" orbitals ($l = 1$), multiplicity 5 states called "d" orbitals ($l = 2$), etc.

8.4 The Casimir operator

For both $SU(2)$ and $SO(3)$, we have found that all representations can be constructed out of function spaces, with the Lie algebra acting as first-order differential operators. It turns out that there is also a very interesting second-order differential operator that comes from these Lie algebra representations, known as the Casimir operator. For the case of $SO(3)$

Definition (Casimir operator for $SO(3)$)**.** *The Casimir operator for the representation of $SO(3)$ on functions on S^2 is the second-order differential operator*

$$L^2 \equiv L_1^2 + L_2^2 + L_3^2$$

(the symbol L^2 is not intended to mean that this is the square of an operator L)

A straightforward calculation using the commutation relations satisfied by the L_j shows that

$$[L^2, \rho'(X)] = 0$$

for any $X \in \mathfrak{so}(3)$. Knowing this, a version of Schur's lemma says that L^2 will act on an irreducible representation as a scalar (i.e. all vectors in the representation are eigenvectors of L^2, with the same eigenvalue). This eigenvalue can be used to characterize the irreducible representation.

The easiest way to compute this eigenvalue turns out to be to act with L^2 on a highest weight vector. First one rewrites L^2 in terms of raising and lowering operators.

$$\begin{aligned} L_- L_+ =& (L_1 - iL_2)(L_1 + iL_2) \\ =& L_1^2 + L_2^2 + i[L_1, L_2] \\ =& L_1^2 + L_2^2 - L_3 \end{aligned}$$

so

$$L^2 = L_1^2 + L_2^2 + L_3^2 = L_- L_+ + L_3 + L_3^2$$

For the representation ρ of $SO(3)$ on functions on S^2 constructed above, we know that on a highest weight vector of the irreducible representation ρ_l

(restriction of ρ to the $2l+1$ dimensional irreducible subspace of functions that are linear combinations of the $Y_l^m(\theta,\phi)$), we have the two eigenvalue equations

$$L_+ f = 0, \quad L_3 f = lf$$

with solution the functions proportional to $Y_l^l(\theta,\phi)$. Just from these conditions and our expression for L^2 we can immediately find the scalar eigenvalue of L^2 since

$$L^2 f = L_- L_+ f + (L_3 + L_3^2) f = 0 + l + l^2 = l(l+1)$$

We have thus shown that our irreducible representation ρ_l can be characterized as the representation on which L^2 acts by the scalar $l(l+1)$.

In summary, we have two different sets of partial differential equations whose solutions provide a highest weight vector for and thus determine the irreducible representation ρ_l:

- $$L_+ f = 0, \quad L_3 f = lf$$

  which are first order equations, with the first using complexification and something like a Cauchy-Riemann equation, and

- $$L^2 f = l(l+1) f, \quad L_3 f = lf$$

  where the first equation is a second order equation, something like a Laplace equation.

That a solution of the first set of equations gives a solution of the second set is obvious. Much harder to show is that a solution of the second set gives a solution of the first set. The space of solutions to

$$L^2 f = l(l+1) f$$

for l a non-negative integer includes as we have seen the $2l+1$-dimensional vector space of linear combinations of the $Y_l^m(\theta,\phi)$ (there are no other solutions, although we will not show that). Since the action of $SO(3)$ on functions commutes with the operator L^2, this $2l+1$-dimensional space will provide a representation, the irreducible one of spin l.

One can compute the explicit second order differential operator L^2 in the ρ representation on functions, it is

$$\begin{aligned} L^2 =& L_1^2 + L_2^2 + L_3^2 \\ =& (i(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}))^2 + (i(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}))^2 + (-i\frac{\partial}{\partial\phi})^2 \\ =& -(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}) \end{aligned} \tag{8.8}$$

We will re-encounter this operator later on in the course as the angular part of the Laplace operator on $\mathbf{R}^3$.

For the group $SU(2)$ we can also find irreducible representations as solution spaces of differential equations on functions on $\mathbf{C}^2$. In that case, the differential equation point of view is much less useful, since the solutions we are looking for are just the homogeneous polynomials, which are more easily studied by purely algebraic methods.

8.5 For further reading

The classification of $SU(2)$ representations is a standard topic in all textbooks that deal with Lie group representations. A good example is [28], which covers this material well, and from which the discussion here of the construction of representations as homogeneous polynomials is drawn (see pages 77-79). The calculation of the L_j and the derivation of expressions for spherical harmonics as Lie algebra representations of $\mathfrak{so}(3)$ appears in most quantum mechanics textbooks in one form or another (for example, see Chapter 12 of [57]). Another source used here for the explicit constructions of representations is [13], Chapters 27-30.

Chapter 9

Tensor Products, Entanglement, and Addition of Spin

If one has two independent quantum systems, with state spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, the combined quantum system has a description that exploits the mathematical notion of a "tensor product", with the combined state space the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$. Because of the ability to take linear combinations of states, this combined state space will contain much more than just products of independent states, including states that are described as "entangled", and responsible for some of the most counter-intuitive behavior of quantum physical systems.

This same tensor product construction is a basic one in representation theory, allowing one to construct a new representation $(\pi_{W_1 \otimes W_2}, W_1 \otimes W_2)$ out of representations (π_{W_1}, W_1) and (π_{W_2}, W_2). When we take the tensor product of states corresponding to two irreducible representations of $SU(2)$ of spins s_1, s_2, we will get a new representation $(\pi_{V^{2s_1} \otimes V^{2s_2}}, V^{2s_1} \otimes V^{2s_2})$. It will be reducible, a direct sum of representations of various spins, a situation we will analyze in detail.

Starting with a quantum system with state space $\mathcal{H}$ that describes a single particle, one can describe a system of N particles by taking an N-fold tensor product $\mathcal{H}^{\otimes N} = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}$. A deep fact about the physical world is that for identical particles, we don't get the full tensor product space, but only the subspaces either symmetric or antisymmetric under the action of the permutation group by permutations of the factors, depending on whether our particles are "bosons" or "fermions". An even deeper fact is that elementary particles of half-integral spin s must behave as fermions, those of integral spin, bosons.

Digression. *When physicists refer to "tensors", they generally mean the "tensor fields" used in general relativity or other geometry-based parts of physics,*

not tensor products of state spaces. A tensor field is a function on a manifold, taking values in some tensor product of copies of the tangent space and its dual space. The simplest tensor fields are just vector fields, functions taking values in the tangent space. A more non-trivial example is the metric tensor, which takes values in the dual of the tensor product of two copies of the tangent space.

9.1 Tensor products

Given two vector spaces V and W (over $\mathbf{R}$ or $\mathbf{C}$), one can easily construct the direct sum vector space $V \oplus W$, just by taking pairs of elements (v, w) for $v \in V, w \in W$, and giving them a vector space structure by the obvious addition and multiplication by scalars. This space will have dimension

$$\dim(V \oplus W) = \dim V + \dim W$$

If $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_{\dim V}\}$ is a basis of V, and $\{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_{\dim W}\}$ a basis of W, the

$$\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_{\dim V}, \mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_{\dim W}\}$$

will be a basis of $V \oplus W$.

A less trivial construction is the tensor product of the vector spaces V and W. This will be a new vector space called $V \otimes W$, of dimension

$$\dim(V \otimes W) = (\dim V)(\dim W)$$

One way to motivate the tensor product is to think of vector spaces as vector spaces of functions. Elements

$$v = v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + \cdots + v_{\dim V}\mathbf{e}_{\dim V} \in V$$

can be thought of as functions on the $\dim V$ points $\mathbf{e}_i$, taking values v_i at $\mathbf{e}_i$. If one takes functions on the union of the sets $\{\mathbf{e}_i\}$ and $\{\mathbf{f}_j\}$ one gets elements of $V \oplus W$. The tensor product $V \otimes W$ will be what one gets by taking all functions on not the union, but the product of the sets $\{\mathbf{e}_i\}$ and $\{\mathbf{f}_j\}$. This will be the set with $(\dim V)(\dim W)$ elements, which we will write $\mathbf{e}_i \otimes \mathbf{f}_j$, and elements of $V \otimes W$ will be functions on this set, or equivalently, linear combinations of these basis vectors.

This sort of definition is less than satisfactory, since it is tied to an explicit choice of bases for V and W. We won't however pursue more details of this question or a better definition here. For this, one can consult pretty much any advanced undergraduate text in abstract algebra, but here we will take as given the following properties of the tensor product that we will need:

- Given vectors $v \in V, w \in W$ we get an element $v \otimes w \in V \otimes W$, satisfying bilinearity conditions (for c_1, c_2 constants)

$$v \otimes (c_1 w_1 + c_2 w_2) = c_1(v \otimes w_1) + c_2(v \otimes w_2)$$

$$(c_1 v_1 + c_2 v_2) \otimes w = c_1(v_1 \otimes w) + c_2(v_2 \otimes w)$$

- There are natural isomorphisms

$$\mathbf{C} \otimes V \simeq V, \quad V \otimes W \simeq W \otimes V$$

and

$$U \otimes (V \otimes W) \simeq (U \otimes V) \otimes W$$

for vector spaces U, V, W

- Given a linear operator A on V and another linear operator B on W, we can define a linear operator $A \otimes B$ on $V \otimes W$ by

$$(A \otimes B)(v \otimes w) = Av \otimes Bw$$

for $v \in V, w \in W$.

With respect to the bases $\mathbf{e}_i, \mathbf{f}_j$ of V and W, A will be a $(\dim V)$ by $(\dim V)$ matrix, B will be a $(\dim W)$ by $(\dim W)$ matrix and $A \otimes B$ will be a $(\dim V)(\dim W)$ by $(\dim V)(\dim W)$ matrix (which one can think of as a $(\dim V)$ by $(\dim V)$ matrix of blocks of size $(\dim W)$).

- One often wants to consider tensor products of vector spaces and dual vector spaces. An important fact is that there is an isomorphism between the tensor product $V^* \otimes W$ and linear maps from V to W given by identifying $l \otimes w$ $(l \in V^*)$ with the linear map

$$v \in V \to l(v)w \in W$$

For V a real vector space, its complexification $V_{\mathbf{C}}$ (the vector space one gets by allowing multiplication by both real and imaginary numbers) can be identified with the tensor product

$$V_{\mathbf{C}} = V \otimes_{\mathbf{R}} \mathbf{C}$$

Here the notation $\otimes_{\mathbf{R}}$ indicates a tensor product of two real vector spaces: V of dimension $\dim V$ with basis $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_{\dim V}\}$ and $\mathbf{C} = \mathbf{R}^2$ of dimension 2 with basis $\{1, i\}$.

9.2 Composite quantum systems and tensor products

Consider two quantum systems, one defined by a state space $\mathcal{H}_1$ and a set of operators $\mathcal{O}_1$ on it, the second given by a state space $\mathcal{H}_2$ and set of operators $\mathcal{O}_2$. One can describe the composite quantum system corresponding to considering the two quantum systems as a single one, with no interaction between them, by just taking as a new state space

$$\mathcal{H}_T = \mathcal{H}_1 \otimes \mathcal{H}_2$$

with operators of the form

$$A \otimes \mathbf{Id} + \mathbf{Id} \otimes B$$

with $A \in \mathcal{O}_1, B \in \mathcal{O}_2$. To describe an interacting quantum system, one can use the state space $\mathcal{H}_T$, but with a more general class of operators.

If $\mathcal{H}$ is the state space of a quantum system, one can think of this as describing a single particle, and then to describe a system of N such particles, one uses the multiple tensor product

$$\mathcal{H}^{\otimes N} = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H} \otimes \mathcal{H}}_{\text{N times}}$$

The symmetric group S_N acts on this state space, and one has a representation $(\pi, \mathcal{H}^{\otimes N})$ of S_N as follows. For $\sigma \in S_N$ a permutation of the set $\{1, 2, \ldots, N\}$ of N elements, on a tensor product of vectors one has

$$\pi(\sigma)(v_1 \otimes v_2 \otimes \cdots \otimes v_N) = v_{\sigma(1)} \otimes v_{\sigma(2)} \otimes \cdots \otimes v_{\sigma(N)}$$

The representation of S_N that this gives is in general reducible, containing various components with different irreducible representations of the group S_N.

A fundamental axiom of quantum mechanics is that if $\mathcal{H}^{\otimes N}$ describes N identical particles, then all physical states occur as one-dimensional representations of S_N, which are either symmetric ("bosons") or antisymmetric ("fermions") where

Definition. *A state $v \in \mathcal{H}^{\otimes N}$ is called*

- *symmetric, or bosonic if $\forall \sigma \in S_N$*

  $$\pi(\sigma)v = v$$

  The space of such states is denoted $S^N(\mathcal{H})$.

- *antisymmetric, or fermionic if $\forall \sigma \in S_N$*

  $$\pi(\sigma)v = (-1)^{|\sigma|}v$$

  The space of such states is denoted $\Lambda^N(\mathcal{H})$. Here $|\sigma|$ is the minimal number of transpositions that by composition give σ.

Note that in the fermionic case, for σ a transposition interchanging two particles, the antisymmetric representation π acts on the factor $\mathcal{H} \otimes \mathcal{H}$ by interchanging vectors, taking

$$w \otimes w \in \mathcal{H} \otimes \mathcal{H}$$

to itself. Antisymmetry requires that this state go to its negative, so the state cannot be non-zero. So one cannot have non-zero states in $\mathcal{H}^{\otimes N}$ describing two identical particles in the same state $w \in \mathcal{H}$, a fact that is known as the "Pauli Principle".

While the symmetry or antisymmetry of states of multiple identical particles is a separate axiom when such particles are described in this way as tensor products, we will see later on (chapter 34) that this phenomenon instead finds a natural explanation when particles are described in terms of quantum fields.

9.3 Indecomposable vectors and entanglement

If one is given a function f on a space X and a function g on a space Y, one can form a product function fg on the product space $X \times Y$ by taking (for $x \in X, y \in Y$)

$$(fg)(x, y) = f(x)g(y)$$

However, most functions on $X \times Y$ are not decomposable in this manner. Similarly, for a tensor product of vector spaces, one has:

Definition (Decomposable and indecomposable vectors)**.** *A vector in $V \otimes W$ is called decomposable if it is of the form $v \otimes w$ for some $v \in V, w \in W$. If it cannot be put in this form it is called indecomposable.*

Note that our basis vectors of $V \otimes W$ are all decomposable since they are products of basis vectors of V and W. Linear combinations of these basis vectors however are in general indecomposable. If we think of an element of $V \otimes W$ as a $\dim V$ by $\dim W$ matrix, with entries the coordinates with respect to our basis vectors for $V \otimes W$, then for decomposable vectors we get a special class of matrices, those of rank one.

In the physics context, the language used is:

Definition (Entanglement)**.** *An indecomposable state in the tensor product state space $\mathcal{H}_T = \mathcal{H}_1 \otimes \mathcal{H}_2$ is called an entangled state.*

The phenomenon of entanglement is responsible for some of the most surprising and subtle aspects of quantum mechanical system. The Einstein-Podolsky-Rosen paradox concerns the behavior of an entangled state of two quantum systems, when one moves them far apart. Then performing a measurement on one system can give one information about what will happen if one performs a measurement on the far removed system, introducing a sort of unexpected non-locality.

Measurement theory itself involves crucially an entanglement between the state of a system being measured, thought of as in a state space $\mathcal{H}_{system}$, and the state of the measurement apparatus, thought of as lying in a state space $\mathcal{H}_{apparatus}$. The laws of quantum mechanics presumably apply to the total system $\mathcal{H}_{system} \otimes \mathcal{H}_{apparatus}$, with the counter-intuitive nature of measurements appearing due to this decomposition of the world into two entangled parts: the one under study, and a much larger for which only an approximate description in classical terms is possible. For much more about this, a recommended reading is Chapter 2 of [52].

9.4 Tensor products of representations

Given two representations of a group, one can define a new representation, the tensor product representation, by

Definition (Tensor product representation of a group)**.** *For (π_V, V) and (π_W, W) representations of a group G, one has a tensor product representation $(\pi_{V\otimes W}, V\otimes W)$ defined by*

$$(\pi_{V\otimes W}(g))(v\otimes w) = \pi_V(g)v\otimes \pi_W(g)w$$

One can easily check that $\pi_{V\otimes W}$ is a homomorphism.

To see what happens for the corresponding Lie algebra representation, one computes (for X in the Lie algebra)

$$\begin{aligned}\pi'_{V\otimes W}(X)(v\otimes w) =& \frac{d}{dt}\pi_{V\otimes W}(e^{tX})(v\otimes w)_{t=0}\\ =& \frac{d}{dt}(\pi_V(e^{tX})v\otimes \pi_W(e^{tX})w)_{t=0}\\ =& ((\frac{d}{dt}\pi_V(e^{tX})v)\otimes \pi_W(e^{tX})w)_{t=0} + (\pi_V(e^{tX})v\otimes (\frac{d}{dt}\pi_W(e^{tX})w))_{t=0}\\ =& (\pi'_V(X)v)\otimes w + v\otimes(\pi'_W(X)w)\end{aligned}$$

which could also be written

$$\pi'_{V\otimes W}(X) = (\pi'_V(X)\otimes \mathbf{1}_W) + (\mathbf{1}_V\otimes \pi'_W(X))$$

9.4.1 Tensor products of $SU(2)$ representations

Given two representations (π_V, V) and (π_W, W) of a group G, we can decompose each into irreducibles. To do the same for the tensor product of the two representations, we need to know how to decompose the tensor product of two irreducibles. This is a fundamental non-trivial problem for a group G, with the answer for $G = SU(2)$ as follows:

Theorem 9.1 (Clebsch-Gordan decomposition)**.**
The tensor product $(\pi_{V^{n_1}\otimes V^{n_2}}, V^{n_1}\otimes V^{n_2})$ decomposes into irreducibles as

$$(\pi_{n_1+n_2}, V^{n_1+n_2})\oplus(\pi_{n_1+n_2-2}, V^{n_1+n_2-2})\oplus\cdots\oplus(\pi_{|n_1-n_2|}, V^{|n_1-n_2|})$$

Proof. One way to prove this result is to use highest-weight theory, raising and lowering operators, and the formula for the Casimir operator. We will not try and show the details of how this works out, but in the next section give a simpler argument using characters. However, in outline (for more details, see for instance section 5.2 of [50]), here's how one could proceed:

One starts by noting that if $v_{n_1}\in V_{n_1}, v_{n_2}\in V_{n_2}$ are highest weight vectors for the two representations, $v_{n_1}\otimes v_{n_2}$ will be a highest weight vector in the tensor product representation (i.e. annihilated by $\pi'_{n_1+n_2}(S_+)$), of weight n_1+n_2. So $(\pi_{n_1+n_2}, V^{n_1+n_2})$ will occur in the decomposition. Applying $\pi'_{n_1+n_2}(S_-)$ to $v_{n_1}\otimes v_{n_2}$ one gets a basis of the rest of the vectors in $(\pi_{n_1+n_2}, V^{n_1+n_2})$. However, at weight n_1+n_2-2 one can find another kind of vector, a highest-weight vector orthogonal to the vectors in $(\pi_{n_1+n_2}, V^{n_1+n_2})$. Applying the lowering operator to this gives $(\pi_{n_1+n_2-2}, V^{n_1+n_2-2})$. As before, at weight n_1+n_2-4 one finds another, orthogonal highest weight vector, and gets another representation, with this process only terminating at weight $|n_1-n_2|$. □

9.4.2 Characters of representations

A standard tool for dealing with representations that we have ignored so far is that of associating to a representation an invariant called its character. This will be a conjugation-invariant function on the group that only depends on the equivalence class of the representation. Given two representations constructed in very different ways, one can often check whether they are isomorphic just by seeing if their character functions match. The problem of identifying the possible irreducible representations of a group can be attacked by analyzing the possible character functions of irreducible representations. We will not try and enter into the general theory of characters here, but will just see what the characters of irreducible representations are for the case of $G = SU(2)$. These can be used to give a simple argument for the Clebsch-Gordan decomposition of the tensor product of $SU(2)$ representations. For this we don't need general theorems about the relations of characters and representations, but can directly check that the irreducible representations of $SU(2)$ correspond to distinct character functions which are easily evaluated.

Definition (Character)**.** *The character of a representation (π, V) of a group G is the function on G given by*

$$\chi_V(g) = Tr(\pi(g))$$

Since the trace of a matrix is invariant under conjugation, χ_V in general will be a complex valued, conjugation-invariant function on G. One can easily check that it will satisfy the relations

$$\chi_{V\oplus W} = \chi_V + \chi_W, \quad \chi_{V\otimes W} = \chi_V \chi_W$$

For the case of $G = SU(2)$, any element can be conjugated to be in the subgroup $U(1)$ of diagonal matrices. Knowing the weights of the irreducible representations (π_n, V^n) of $SU(2)$, we know the characters to be the functions

$$\chi_{V^n}(\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}) = e^{in\theta} + e^{i(n-2)\theta} + \cdots + e^{-i(n-2)\theta} + e^{-in\theta} \tag{9.1}$$

As n gets large, this becomes an unwieldy expression, but one has

Theorem (Weyl character formula)**.**

$$\chi_{V^n}(\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}) = \frac{e^{i(n+1)\theta} - e^{-i(n+1)\theta}}{e^{i\theta} - e^{-i\theta}} = \frac{\sin((n+1)\theta)}{\sin(\theta)}$$

Proof. One just needs to use the identity

$$(e^{in\theta} + e^{i(n-2)\theta} + \cdots + e^{-i(n-2)\theta} + e^{-in\theta})(e^{i\theta} - e^{-i\theta}) = e^{i(n+1)\theta} - e^{-i(n+1)\theta}$$

and equation 9.1 for the character. □

To get a proof of 9.1, one can compute the character of the tensor product on the diagonal matrices using the Weyl character formula for the second factor (ordering things so that $n_2 > n_1$)

$$\begin{aligned}\chi_{V^{n_1}\otimes V^{n_2}} =&\chi_{V^{n_1}}\chi_{V^{n_2}}\\ =&(e^{in_1\theta}+e^{i(n_1-2)\theta}+\cdots+e^{-i(n_1-2)\theta}+e^{-in_1\theta})\frac{e^{i(n_2+1)\theta}-e^{-i(n_2+1)\theta}}{e^{i\theta}-e^{-i\theta}}\\ =&\frac{(e^{i(n_1+n_2+1)\theta}-e^{-i(n_1+n_2+1)\theta})+\cdots+(e^{i(n_2-n_1+1)\theta}-e^{-i(n_2-n_1+1)\theta})}{e^{i\theta}-e^{-i\theta}}\\ =&\chi_{V^{n_1+n_2}}+\chi_{V^{n_1+n_2-2}}+\cdots+\chi_{V^{n_2-n_1}}\end{aligned}$$

So, when we decompose the tensor product of irreducibles into a direct sum of irreducibles, the ones that must occur are exactly those of theorem 9.1.

9.4.3 Some examples

Some simple examples of how this works are:

- Tensor product of two spinors:

  $$V^1\otimes V^1 = V^2\oplus V^0$$

  This says that the four complex dimensional tensor product of two spinor representations (which are each two complex dimensional) decomposes into irreducibles as the sum of a three dimensional vector representation and a one dimensional trivial (scalar) representation.

  Using the basis $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$ for V^1, the tensor product $V^1\otimes V^1$ has a basis

  $$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix},\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}$$

  The vector

  $$\frac{1}{\sqrt{2}}(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix})\in V^1\otimes V^1$$

  is clearly antisymmetric under permutation of the two factors of $V^1\otimes V^1$. One can show that this vector is invariant under $SU(2)$, by computing either the action of $SU(2)$ or of its Lie algebra $\mathfrak{su}(2)$. So, this vector is a basis for the component V^0 in the decomposition of $V^1\otimes V^1$ into irreducibles.

  The other component, V^2, is three dimensional, and has a basis

  $$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \frac{1}{\sqrt{2}}(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}),\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}$$

These three vectors span one-dimensional complex subspaces of weights $q = 2, 0, -2$ under the $U(1) \subset SU(2)$ subgroup

$$\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

They are symmetric under permutation of the two factors of $V^1 \otimes V^1$.

We see that if we take two identical quantum systems with $\mathcal{H} = V^1 = \mathbf{C}^2$ and make a composite system out of them, if they were bosons we would get a three dimensional state space $V^2 = S^2(V^1)$, transforming as a vector (spin one) under $SU(2)$. If they were fermions, we would get a one-dimensional state space $V^0 = \Lambda^2(V^1)$ of spin zero (invariant under $SU(2)$). Note that in this second case we automatically get an entangled state, one that cannot be written as a decomposable product.

- Tensor product of three or more spinors:

$$V^1 \otimes V^1 \otimes V^1 = (V^2 \oplus V^0) \otimes V^1 = (V^2 \otimes V^1) \oplus (V^0 \otimes V^1) = V^3 \oplus V^1 \oplus V^1$$

This says that the tensor product of three spinor representations decomposes as a four dimensional ("spin 3/2") representation plus two copies of the spinor representation.

One can clearly generalize this and consider N-fold tensor products $(V^1)^{\otimes N}$ of the spinor representation. Taking N high enough one can get any irreducible representation of $SU(2)$ that one wants this way, giving an alternative to our construction using homogeneous polynomials. Doing this however gives the irreducible as just one component of something larger, and one needs a method to project out the component one wants. One can do this using the action of the symmetric group S_N on $(V^1)^{\otimes N}$ and an understanding of the irreducible representations of S_N. This relationship between irreducible representations of $SU(2)$ and those of S_N coming from looking at how both groups act on $(V^1)^{\otimes N}$ is known as "Schur-Weyl duality", and generalizes to the case of $SU(n)$, where one looks at N-fold tensor products of the defining representation of $SU(n)$ matrices on $\mathbf{C}^n$. For $SU(n)$ this provides perhaps the most straight-forward construction of all irreducible representations of the group.

9.5 Bilinear forms and tensor products

A different sort of application of tensor products that will turn out to be important is to the description of bilinear forms, which generalize the dual space V^* of linear forms on V. We have

Definition (Bilinear forms)**.** *A bilinear form B on a vector space V over a field k (for us, $k = \mathbf{R}$ or $\mathbf{C}$) is a map*

$$B : (u, u') \in V \times V \to B(u, u') \in k$$

that is bilinear in both entries, i.e.

$$B(u+u',u'') = B(u,u'') + B(u',u''), \quad B(cu,u') = cB(u,u')$$

$$B(u,u'+u'') = B(u,u') + B(u,u''), \quad B(u,cu') = cB(u,u')$$

where $c \in k$.

If $B(u',u) = B(u,u')$ *the bilinear form is called symmetric, if* $B(u',u) = -B(u,u')$ *it is antisymmetric.*

The relation to tensor products is

Theorem 9.2. *The space of bilinear forms on* V *is isomorphic to* $V^* \otimes V^*$.

Proof. Given two linear forms $\alpha \in V^*, \beta \in V^*$, one has a map

$$\alpha \otimes \beta \in V^* \otimes V^* \to B : B(u,u') = \alpha(u)\beta(u')$$

Choosing a basis $\mathbf{e}_j$ of V, the coordinate functions $v_j = \mathbf{e}_j^*$ provide a basis of V^*, so the $v_j \otimes v_k$ will be a basis of $V^* \otimes V^*$. The map above takes linear combinations of these to bilinear forms, and is easily seen to be one-to-one and surjective for such linear combinations. □

Given a basis $\mathbf{e}_j$ of V and dual basis v_j of V^* (the coordinates), one can write the element of $V^* \otimes V^*$ corresponding to B as the sum

$$\sum_{j,k} B_{jk} v_j \otimes v_k$$

This expresses the bilinear form B in terms of a matrix $\mathbf{B}$ with entries B_{jk}, which can be computed as

$$B_{jk} = B(\mathbf{e}_j, \mathbf{e}_k)$$

In terms of the matrix $\mathbf{B}$, the bilinear form is computed as

$$B(u,u') = \begin{pmatrix} u_1 & \dots & u_d \end{pmatrix} \begin{pmatrix} B_{11} & \dots & B_{1d} \\ \vdots & \vdots & \vdots \\ B_{d1} & \dots & B_{dd} \end{pmatrix} \begin{pmatrix} u'_1 \\ \vdots \\ u'_d \end{pmatrix} = \mathbf{u} \cdot \mathbf{B}\mathbf{u}'$$

The symmetric bilinear forms lie in $S^2(V^*) \subset V^* \otimes V^*$ and correspond to symmetric matrices. Elements of V^* give linear functions on V, and one can get quadratic functions on V from elements $B \in S^2(V^*)$ by taking

$$u \in V \to B(u,u) = \mathbf{u} \cdot \mathbf{B}\mathbf{u}$$

That one gets quadratic functions by multiplying two linear functions corresponds in terms of tensor products to

$$(\alpha, \beta) \in V^* \times V^* \to \frac{1}{2}(\alpha \otimes \beta + \beta \otimes \alpha) \in S^2(V^*)$$

We will not give the details here, but one can generalize the above from bilinear forms (isomorphic to $V^* \otimes V^*$) to multi-linear forms with N arguments (isomorphic to $(V^*)^{\otimes N}$). Evaluating such a multi-linear form with all arguments set to $u \in V$ gives a homogeneous polynomial of degree N, and one has an isomorphism between symmetric multi-linear forms in $S^N(V^*)$ and such polynomials.

Antisymmetric bilinear forms lie in $\Lambda^2(V^*) \subset V^* \otimes V^*$ and correspond to antisymmetric matrices. One can define a multiplication (called the "wedge product") on V^* that takes values in $\Lambda^2(V^*)$ by

$$(\alpha, \beta) \in V^* \times V^* \to \alpha \wedge \beta = \frac{1}{2}(\alpha \otimes \beta - \beta \otimes \alpha) \in \Lambda^2(V^*)$$

One can use this to get a product on the space of antisymmetric multilinear forms of different degrees, giving something in many ways analogous to the algebra of polynomials. This plays a role in the description of fermions and will be considered in more detail in chapter 27.

9.6 For further reading

For more about the tensor product and tensor product of representations, see section 6 of [67], or appendix B of [59]. Almost every quantum mechanics textbook will contain an extensive discussion of the Clebsch-Gordan decomposition for the tensor product of two irreducible $SU(2)$ representations.

Chapter 10

Energy, Momentum and Translation Groups

We'll now turn to the problem that conventional quantum mechanics courses generally begin with: that of the quantum system describing a free particle moving in physical space $\mathbf{R}^3$. This is something quite different than the classical mechanical decription of a free particle, which will be reviewed in chapter 12. A common way of motivating this is to begin with the 1924 suggestion by de Broglie that, just as photons may behave like particles or waves, the same should be true for matter particles. Photons carry an energy given by $E = \hbar\omega$, where ω is the angular frequency, and de Broglie's proposal was that matter particles behave like a wave with spatial dependence

$$e^{i\mathbf{k}\cdot\mathbf{x}}$$

where $\mathbf{x}$ is the spatial position, and the momentum of the particle is $\mathbf{p} = \hbar\mathbf{k}$.

This proposal was realized in Schrödinger's early 1926 discovery of a version of quantum mechanics, in which the state space $\mathcal{H}$ is a space of complex-valued functions on $\mathbf{R}^3$, called "wavefunctions". The operator

$$\mathbf{P} = -i\hbar\boldsymbol{\nabla}$$

will have eigenvalues $\hbar\mathbf{k}$, the de Broglie momentum, so it can be identified as the momentum operator.

In this chapter our discussion will emphasize the central role of the momentum operator. This operator will have the same relationship to spatial translations as the Hamiltonian operator does to time translations. In both cases, the operators are given by the Lie algebra representation corresponding to a unitary representation on the quantum state space $\mathcal{H}$ of groups of translations (translation in the three space and one time directions respectively).

One way to motivate the quantum theory of a free particle is that, whatever it is, it should have the same sort of behavior as in the classical case under the translational and rotational symmetries of space-time. In chapter 12 we

will see that in the Hamiltonian form of classical mechanics, the components of the momentum vector give a basis of the Lie algebra of the spatial translation group $\mathbf{R}^3$, the energy a basis of the Lie algebra of the time translation group $\mathbf{R}$. Invoking the classical relationship between energy and momentum

$$E = \frac{|\mathbf{p}|^2}{2m}$$

used in non-relativistic mechanics relates the Hamiltonian and momentum operators, giving the conventional Schrödinger differential equation for the wavefunction of a free particle. We will examine the solutions to this equation, beginning with the case of periodic boundary conditions, where spatial translations in each direction are given by the compact group $U(1)$ (whose representations we have already studied in detail).

10.1 Energy, momentum and space-time translations

We have seen that it is a basic axiom of quantum mechanics that the observable operator responsible for infinitesimal time translations is the Hamiltonian operator H, a fact that is expressed as the Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

When H is time-independent, one can understand this equation as reflecting the existence of a unitary representation $(U(t), \mathcal{H})$ of the group $\mathbf{R}$ of time translations on the state space $\mathcal{H}$. For the case of $\mathcal{H}$ infinite-dimensional, this is known as Stone's theorem for one-parameter unitary groups, see for instance chapter 10.2 of [29] for details.

When $\mathcal{H}$ is finite-dimensional, the fact that a differentiable unitary representation $U(t)$ of $\mathbf{R}$ on $\mathcal{H}$ is of the form

$$U(t) = e^{-\frac{i}{\hbar}tH}$$

for H a self-adjoint matrix follows from the same sort of argument as in theorem 2.1. Such a $U(t)$ provides solutions of the Schrödinger equation by

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

The Lie algebra of $\mathbf{R}$ is also $\mathbf{R}$ and we get a Lie algebra representation of $\mathbf{R}$ by taking the time derivative of $U(t)$, which gives us

$$\hbar \frac{d}{dt}U(t)_{|t=0} = -iH$$

Since this Lie algebra representation comes from taking the derivative of a unitary representation, $-iH$ will be skew-adjoint, so H will be self-adjoint. The

minus sign is a convention, for reasons that will be explained in the discussion of momentum to come later.

Note that if one wants to treat the additive group $\mathbf{R}$ as a matrix group, related to its Lie algebra $\mathbf{R}$ by exponentiation of matrices, one can describe the group as the group of matrices of the form

$$\begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}$$

since

$$\begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & a+b \\ 0 & 1 \end{pmatrix}$$

Since

$$e^{\begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix}} = \begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}$$

the Lie algebra is just matrices of the form

$$\begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix}$$

We will mostly though write the group law in additive form. We are interested in the group $\mathbf{R}$ as a group of translations acting on a linear space, and the corresponding infinite dimensional representation induced on functions on the space. The simplest case is when $\mathbf{R}$ acts on itself by translation. Here $a \in \mathbf{R}$ acts on $q \in \mathbf{R}$ (where q is a coordinate on $\mathbf{R}$) by

$$q \to a \cdot q = q + a$$

and the induced representation π on functions uses

$$\pi(g)f(q) = f(g^{-1} \cdot q)$$

to get

$$\pi(a)f(q) = f(q - a)$$

In the Lie algebra version of this representation, we will have

$$\pi'(a) = -a\frac{d}{dq}$$

since

$$\pi(a)f = e^{\pi'(a)}f = e^{-a\frac{d}{dq}}f(q) = f(q) - a\frac{df}{dq} + \frac{a^2}{2!}\frac{d^2f}{dq^2} + \cdots = f(q-a)$$

which for functions with appropriate properties is just Taylor's formula. Note that here the same a labels points of the Lie algebra and of the group. We are not treating the group $\mathbf{R}$ as a matrix group, since we want an additive group

law. So Lie algebra elements are not defined as for matrix groups (things one exponentiates to get group elements). Instead, we think of the Lie algebra as the tangent space to the group at the identity, and then simply identify $\mathbf{R}$ as the tangent space at 0 (the Lie algebra) and $\mathbf{R}$ as the additive group. Note however that the representation obeys a multiplicative law, with the homomorphism property

$$\pi(a+b) = \pi(a)\pi(b)$$

so there is an exponential in the relation between π and π'.

Since we now want to describe quantum systems that depend not just on time, but on space variables $\mathbf{q} = (q_1, q_2, q_3)$, we will have an action by unitary transformations of not just the group $\mathbf{R}$ of time translations, but also the group $\mathbf{R}^3$ of spatial translations. We will define the corresponding Lie algebra representations using self-adjoint operators P_1, P_2, P_3 that play the same role for spatial translations that the Hamiltonian plays for time translations:

Definition (Momentum operators)**.** *For a quantum system with state space $\mathcal{H}$ given by complex valued functions of position variables q_1, q_2, q_3, momentum operators P_1, P_2, P_3 are defined by*

$$P_1 = -i\hbar\frac{\partial}{\partial q_1}, P_2 = -i\hbar\frac{\partial}{\partial q_2}, P_3 = -i\hbar\frac{\partial}{\partial q_3}$$

These are given the name "momentum operators" since we will see that their eigenvalues have an intepretation as the components of the momentum vector for the system, just as the eigenvalues of the Hamiltonian have an interpretation as the energy. Note that while in the case of the Hamiltonian the factor of $\hbar$ kept track of the relative normalization of energy and time units, here it plays the same role for momentum and length units. It can be set to one if appropriate choices of units of momentum and length are made.

The differentiation operator is skew-adjoint since, using integration by parts one has for $\psi \in \mathcal{H}$

$$\int_{-\infty}^{+\infty} \overline{\psi}(\frac{d}{dq}\psi)dq = \int_{-\infty}^{+\infty} (\frac{d}{dq}(\overline{\psi}\psi) - (\frac{d}{dq}\overline{\psi})\psi)dq = -\int_{-\infty}^{+\infty} (\frac{d}{dq}\overline{\psi})\psi dq$$

The P_j are thus self-adjoint operators, with real eigenvalues as expected for an observable operator. Multiplying by $-i$ to get the corresponding skew-adjoint operator of a unitary Lie algebra representation we find

$$-iP_j = -\hbar\frac{\partial}{\partial q_j}$$

Up to the $\hbar$ factor that depends on units, these are exactly the Lie algebra representation operators on basis elements for the action of $\mathbf{R}^3$ on functions on $\mathbf{R}^3$ induced from translation:

$$\pi(a_1, a_2, a_3)f(q_1, q_2, q_3) = f(q_1 - a_1, q_2 - a_2, q_3 - a_3)$$

$$\pi'(a_1, a_2, a_3) = a_1(-iP_1) + a_2(-iP_2) + a_3(-iP_3) = -\hbar(a_1\frac{\partial}{\partial q_1} + a_2\frac{\partial}{\partial q_2} + a_3\frac{\partial}{\partial q_3})$$

Note that the convention for the sign choice here is the opposite from the case of the Hamiltonian ($-iP = -\hbar\frac{d}{dq}$ vs. $-iH = \hbar\frac{d}{dt}$). This means that the conventional sign choice we have been using for the Hamiltonian makes it minus the generator of translations in the time direction. The reason for this comes from considerations of special relativity, where the inner product on space-time has opposite signs for the space and time dimensions . We will review this subject in chapter 37 but for now we just need the relationship special relativity gives between energy and momentum. Space and time are put together in "Minkowski space", which is $\mathbf{R}^4$ with indefinite inner product

$$< (u_0, u_1, u_2, u_3), (v_0, v_1, v_2, v_3) >= -u_0v_0 + u_1v_1 + u_2v_2 + u_3v_3$$

Energy and momentum are the components of a Minkowski space vector ($p_0 = E, p_1, p_2, p_3$) with norm-squared given by minus the mass-squared:

$$< (E, p_1, p_2, p_3), (E, p_1, p_2, p_3) >= -E^2 + |\mathbf{p}|^2 = -m^2$$

This is the formula for a choice of space and time units such that the speed of light is 1. Putting in factors of the speed of light c to get the units right one has

$$E^2 - |\mathbf{p}|^2c^2 = m^2c^4$$

Two special cases of this are:

- For photons, $m = 0$, and one has the energy momentum relation $E = |\mathbf{p}|c$
- For velocities $\mathbf{v}$ small compared to c (and thus momenta $|\mathbf{p}|$ small compared to mc), one has

$$E = \sqrt{|\mathbf{p}|^2c^2 + m^2c^4} = c\sqrt{|\mathbf{p}|^2 + m^2c^2} \approx \frac{c|\mathbf{p}|^2}{2mc} + mc^2 = \frac{|\mathbf{p}|^2}{2m} + mc^2$$

  In the non-relativistic limit, we use this energy-momentum relation to describe particles with velocities small compared to c, typically dropping the momentum-independent constant term mc^2.

In later chapters we will discuss quantum systems that describe photons, as well as other possible ways of constructing quantum systems for relativistic particles. For now though, we will stick to the non-relativistic case. To describe a quantum non-relativistic particle we choose a Hamiltonian operator H such that its eigenvalues (the energies) will be related to the momentum operator eigenvalues (the momenta) by the classical energy-momentum relation $E = \frac{|\mathbf{p}|^2}{2m}$:

$$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2) = \frac{1}{2m}|\mathbf{P}|^2 = \frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} + \frac{\partial^2}{\partial q_3^2})$$

The Schrödinger equation then becomes:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{q},t) = \frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}+\frac{\partial^2}{\partial q_3^2})\psi(\mathbf{q},t) = \frac{-\hbar^2}{2m}\nabla^2\psi(\mathbf{q},t)$$

This is an easily solved simple constant coefficient second-order partial differential equation. One method of solution is to separate out the time-dependence, by first finding solutions ψ_E to the time-independent equation

$$H\psi_E(\mathbf{q}) = \frac{-\hbar^2}{2m}\nabla^2\psi_E(\mathbf{q}) = E\psi_E(\mathbf{q})$$

with eigenvalue E for the Hamiltonian operator and then use the fact that

$$\psi(\mathbf{q},t) = \psi_E(\mathbf{q})e^{-\frac{i}{\hbar}tE}$$

will give solutions to the full-time dependent equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{q},t) = H\psi(\mathbf{q},t)$$

The solutions $\psi_E(\mathbf{q})$ to the time-independent equation are just complex exponentials proportional to

$$e^{i(k_1q_1+k_2q_2+k_3q_3)} = e^{i\mathbf{k}\cdot\mathbf{q}}$$

satisfying

$$\frac{-\hbar^2}{2m}(-i)^2|\mathbf{k}|^2 = \frac{\hbar^2|\mathbf{k}|^2}{2m} = E$$

We have found that solutions to the Schrödinger equation are given by linear combinations of states $|\mathbf{k}\rangle$ labeled by a vector $\mathbf{k}$, which are eigenstates of the momentum and Hamiltonian operators with

$$P_j|\mathbf{k}\rangle = \hbar k_j|\mathbf{k}\rangle, \quad H|\mathbf{k}\rangle = \frac{\hbar^2}{2m}|\mathbf{k}|^2|\mathbf{k}\rangle$$

These are states with well-defined momentum and energy

$$p_j = \hbar k_j, E = \frac{|\mathbf{p}|^2}{2m}$$

so they satisfy exactly the same energy-momentum relations as those for a classical non-relativistic particle.

While the quantum mechanical state space $\mathcal{H}$ contains states with the classical energy-momentum relation, it also contains much, much more since it includes linear combinations of such states. At $t = 0$ one has

$$|\psi\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{q}}$$

where $c_{\mathbf{k}}$ are complex numbers, and the general time-dependent state will be

$$|\psi(t)\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{q}} e^{-it\hbar\frac{|\mathbf{k}|^2}{2m}}$$

or, equivalently in terms of momenta $\mathbf{p} = \hbar\mathbf{k}$

$$|\psi(t)\rangle = \sum_{\mathbf{p}} c_{\mathbf{p}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{q}} e^{-\frac{i}{\hbar}\frac{|\mathbf{p}|^2}{2m}t}$$

10.2 Periodic boundary conditions and the group $U(1)$

We have not yet discussed the inner product on our space of states when they are given as wavefunctions on $\mathbf{R}^3$, and there is a significant problem with doing this. To get unitary representations of translations, we need to use a translation invariant, Hermitian inner product on wavefunctions, and this will have to be of the form

$$\langle \psi_1, \psi_2 \rangle = C \int_{\mathbf{R}^3} \overline{\psi_1(\mathbf{q})}\psi_2(\mathbf{q}) d^3\mathbf{q}$$

for some constant C. But if we try and compute the norm-squared of one of our basis states $|\mathbf{k}\rangle$ we find

$$\langle \mathbf{k}|\mathbf{k}\rangle = C \int_{\mathbf{R}^3} (e^{-i\mathbf{k}\cdot\mathbf{q}})(e^{i\mathbf{k}\cdot\mathbf{q}}) d^3\mathbf{q} = C \int_{\mathbf{R}^3} 1 \; d^3\mathbf{q} = \infty$$

As a result there is no value of C which will give these states a unit norm.

In the finite dimensional case, a linear algebra theorem assures us that given a self-adjoint operator, we can find an orthonormal basis of its eigenvectors. In this infinite dimensional case this is no longer true, and a much more sophisticated formalism (the "spectral theorem for self-adjoint operators") is needed to replace the linear algebra theorem. This is a standard topic in treatments of quantum mechanics aimed at mathematicians emphasizing analysis, but we will not try and enter into this here. One place to find such a discussion is section 2.1 of [64].

One way to deal with the normalization problem is to replace the non-compact space by one of finite volume. We'll consider first the simplified case of a single spatial dimension, since once one sees how this works for one dimension, treating the others the same way is straight-forward. In this one dimensional case, one replaces $\mathbf{R}$ by the circle S^1. This is equivalent to the physicist's method of imposing "periodic boundary conditions", meaning to define the theory on an interval, and then identify the ends of the interval. One can then think of the position variable q as an angle ϕ and define the inner product as

$$\langle \psi_1, \psi_2 \rangle = \frac{1}{2\pi} \int_0^{2\pi} \overline{\psi_1(\phi)}\psi_2(\phi) d\phi$$

The state space is then

$$\mathcal{H} = L^2(S^1)$$

the space of complex-valued square-integrable functions on the circle.

Instead of the translation group $\mathbf{R}$, we have the standard action of the group $SO(2)$ on the circle. Elements $g(\theta)$ of the group are rotations of the circle counterclockwise by an angle θ, or if we parametrize the circle by an angle ϕ, just shifts

$$\phi \to \phi + \theta$$

Recall that in general we can construct a representation on functions from a group action on a space by

$$\pi(g)f(x) = f(g^{-1} \cdot x)$$

so we see that this rotation action on the circle gives a representation on $\mathcal{H}$

$$\pi(g(\theta))\psi(\phi) = \psi(\phi - \theta)$$

If X is a basis of the Lie algebra $\mathfrak{so}(2)$ (for instance taking the circle as the unit circle in $\mathbf{R}^2$, rotations 2 by 2 matrices, $X = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $g(\theta) = e^{\theta X}$) then the Lie algebra representation is given by taking the derivative

$$\pi'(X)f(\phi) = \frac{d}{d\theta} f(\phi - \theta)_{|\theta=0} = -f'(\phi)$$

so we have

$$\pi'(X) = -\frac{d}{d\phi}$$

This operator is defined on a dense subspace of $\mathcal{H} = L^2(S^1)$ and is skew-adjoint, since (using integration by parts)

$$\begin{aligned} \langle \psi_1, \psi_2' \rangle =& \frac{1}{2\pi} \int_0^{2\pi} \overline{\psi_1} \frac{d}{d\phi} \psi_2 d\phi \\ =& \frac{1}{2\pi} \int_0^{2\pi} (\frac{d}{d\phi}(\overline{\psi_1}\psi_2) - (\frac{d}{d\phi}\overline{\psi_1})\psi_2) d\phi \\ =& - \langle \psi_1', \psi_2 \rangle \end{aligned}$$

The eigenfunctions of $\pi'(X)$ are just the $e^{in\phi}$, for $n \in \mathbf{Z}$, which we will also write as state vectors $|n\rangle$. These are orthonormal

$$\langle n|m \rangle = \delta_{nm}$$

and provide a basis for the space $L^2(S^1)$, a basis that corresponds to the decomposition into irreducibles of

$$L^2(S^1)$$

as a representation of $SO(2)$ described above. One has

$$(\pi, L^2(S^1)) = \oplus_{n\in\mathbf{Z}}(\pi_n, \mathbf{C})$$

where π_n are the irreducible one-dimensional representations given by

$$\pi_n(g(\theta)) = e^{in\theta}$$

The theory of Fourier series for functions on S^1 says that one can expand any function $\psi \in L^2(S^1)$ in terms of this basis, i.e.

$$|\psi\rangle = \psi(\phi) = \sum_{n=-\infty}^{+\infty} c_n e^{in\phi} = \sum_{n=-\infty}^{+\infty} c_n |n\rangle$$

where $c_n \in \mathbf{C}$. The condition that $\psi \in L^2(S^1)$ corresponds to the condition

$$\sum_{n=-\infty}^{+\infty} |c_n|^2 < \infty$$

on the coefficients c_n. Using orthonormality of the $|n\rangle$ we find

$$c_n = \langle n|\psi\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-in\phi}\psi(\phi)d\phi$$

The Lie algebra of the group S^1 is the same as that of the group $(\mathbf{R}, +)$, and the $\pi'(X)$ we have found for the S^1 action on functions is related to the momentum operator in the same way as in the $\mathbf{R}$ case. So, we can use the same momentum operator

$$P = -i\hbar\frac{d}{d\phi}$$

which satisfies

$$P|n\rangle = \hbar n|n\rangle$$

By changing space to the compact S^1 we now have momenta that instead of taking on any real value, can only be integral numbers times $\hbar$. Solving the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\phi, t) = \frac{P^2}{2m}\psi(\phi, t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial\phi^2}\psi(\phi, t)$$

as before, we find

$$E\psi_E(\phi) = \frac{-\hbar^2}{2m}\frac{d^2}{d\phi^2}\psi_E(\phi)$$

an eigenvector equation, which has solutions $|n\rangle$, with

$$E = \frac{\hbar^2 n^2}{2m}$$

Writing a solution to the Schrödinger equation as

$$\psi(\phi,t)=\sum_{n=-\infty}^{+\infty}c_n e^{in\phi}e^{-i\frac{\hbar n^2}{2m}t}$$

the c_n will be determined from the initial condition of knowing the wavefunction at time $t=0$, according to the Fourier coefficient formula

$$c_n=\frac{1}{2\pi}\int_0^{2\pi}e^{-in\phi}\psi(\phi,0)d\phi$$

To get something more realistic, we need to take our circle to have an arbitrary circumference L, and we can study our original problem by considering the limit $L\to\infty$. To do this, we just need to change variables from ϕ to ϕ_L, where

$$\phi_L=\frac{L}{2\pi}\phi$$

The momentum operator will now be

$$P=-i\hbar\frac{d}{d\phi_L}$$

and its eigenvalues will be quantized in units of $\frac{2\pi\hbar}{L}$. The energy eigenvalues will be

$$E=\frac{2\pi^2\hbar^2n^2}{mL^2}$$

10.3 The group R and the Fourier transform

In the previous section, we imposed periodic boundary conditions, replacing the group $\mathbf{R}$ of translations by a compact group S^1, and then used the fact that unitary representations of this group are labeled by integers. This made the analysis rather easy, with $\mathcal{H}=L^2(S^1)$ and the self-adjoint operator $P=-i\hbar\frac{\partial}{\partial\phi}$ behaving much the same as in the finite-dimensional case: the eigenvectors of P give a countable orthonormal basis of $\mathcal{H}$. If one wants to, one can think of P as an infinite-dimensional matrix.

Unfortunately, in order to understand many aspects of quantum mechanics, we can't get away with this trick, but need to work with $\mathbf{R}$ itself. One reason for this is that the unitary representations of $\mathbf{R}$ are labeled by the same group, $\mathbf{R}$, and we will find it very important to exploit this and treat positions and momenta on the same footing (see the discussion of the Heisenberg group in chapter 11). What plays the role here of $|n\rangle=e^{in\phi}$, $n\in\mathbf{Z}$ will be the $|k\rangle=e^{ikq}$, $k\in\mathbf{R}$. These are functions on $\mathbf{R}$ that are irreducible representations under the translation action ($\pi(a)$ acts on functions of q by taking $q\to q-a$)

$$\pi(a)e^{ikq}=e^{ik(q-a)}=e^{-ika}e^{ikq}$$

We can try and mimic the Fourier series decomposition, with the coefficients c_n that depend on the labels of the irreducibles replaced by a function $\widetilde{f}(k)$ depending on the label k of the irreducible representation of $\mathbf{R}$.

Definition (Fourier transform)**.** *The Fourier transform of a function ψ is given by*

$$\mathcal{F}\psi = \widetilde{\psi}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikq} \psi(q) dq$$

The definition makes sense for $\psi \in L^1(\mathbf{R})$, Lebesgue integrable functions on $\mathbf{R}$. For the following, it is convenient to instead restrict to the Schwartz space $S(\mathbf{R})$ of functions ψ such that the function and its derivatives fall off faster than any power at infinity (which is a dense subspace of $L^2(\mathbf{R})$). For more details about the analysis and proofs of the theorems quoted here, one can refer to a standard textbook such as [63].

Given the Fourier transform of ψ, one can recover ψ itself:

Theorem (Fourier Inversion)**.** *For $\widetilde{\psi} \in S(\mathbf{R})$ the Fourier transform of a function $\psi \in S(\mathbf{R})$, one has*

$$\psi(q) = \widetilde{\mathcal{F}}\widetilde{\psi} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikq} \widetilde{\psi}(k) dk$$

Note that $\widetilde{\mathcal{F}}$ is the same linear operator as $\mathcal{F}$, with a change in sign of the argument of the function it is applied to. Note also that we are choosing one of various popular ways of normalizing the definition of the Fourier transform. In others, the factor of 2π may appear instead in the exponent of the complex exponential, or just in one of $\mathcal{F}$ or $\widetilde{\mathcal{F}}$ and not the other.

The operators $\mathcal{F}$ and $\widetilde{\mathcal{F}}$ are thus inverses of each other on $S(\mathbf{R})$. One has

Theorem (Plancherel)**.** *$\mathcal{F}$ and $\widetilde{\mathcal{F}}$ extend to unitary isomorphisms of $L^2(\mathbf{R})$ with itself. In other words*

$$\int_{-\infty}^{\infty} |\psi(q)|^2 dq = \int_{-\infty}^{\infty} |\widetilde{\psi}(k)|^2 dk$$

Note that we will be using the same inner product on functions on $\mathbf{R}$

$$\langle \psi_1, \psi_2 \rangle = \int_{-\infty}^{\infty} \overline{\psi_1(q)} \psi_2(q) dq$$

both for functions of q and their Fourier transforms, functions of k.

An important example is the case of Gaussian functions where

$$\begin{aligned}
\mathcal{F} e^{-\alpha \frac{q^2}{2}} =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikq} e^{-\alpha \frac{q^2}{2}} dq \\
=& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{\alpha}{2}((q+i\frac{2k}{\alpha})^2 - (\frac{ik}{\alpha})^2)} dq \\
=& \frac{1}{\sqrt{2\pi}} e^{-\frac{k^2}{2\alpha}} \int_{-\infty}^{+\infty} e^{-\frac{\alpha}{2} q'^2} dq' \\
=& \frac{1}{\sqrt{\alpha}} e^{-\frac{k^2}{2\alpha}}
\end{aligned}$$

A crucial property of the unitary operator $\mathcal{F}$ on $\mathcal{H}$ is that it diagonalizes the differentiation operator and thus the momentum operator P. Under Fourier transform, differential operators become just multiplication by a polynomial, giving a powerful technique for solving differential equations. Computing the Fourier transform of the differentiation operator using integration by parts, we find

$$\begin{aligned}\widetilde{\frac{d\psi}{dq}} =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ikq}\frac{d\psi}{dq}dq \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} (\frac{d}{dq}(e^{-ikq}\psi) - (\frac{d}{dq}e^{-ikq})\psi)dq \\ =& ik\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ikq}\psi dq \\ =& ik\widetilde{\psi}(k)\end{aligned}$$

So under Fourier transform, differentiation by q becomes multiplication by ik. This is the infinitesimal version of the fact that translation becomes multiplication by a phase under Fourier transform. If $\psi_a(q) = \psi(q+a)$, one has

$$\begin{aligned}\widetilde{\psi_a}(k) =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ikq}\psi(q+a)dq \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ik(q'-a)}\psi(q')dq' \\ =& e^{ika}\widetilde{\psi}(k)\end{aligned}$$

Since $p = \hbar k$, we can easily change variables and work with p instead of k, and often will do this from now on. As with the factors of 2π, there's a choice of where to put the factors of $\hbar$ in the normalization of the Fourier transform. We'll make the following choices, to preserve symmetry between the formulas for Fourier transform and inverse Fourier transform:

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{-i\frac{pq}{\hbar}}dq$$

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{i\frac{pq}{\hbar}}dp$$

Note that in this case we have lost an important property that we had for finite dimensional $\mathcal{H}$ and had managed to preserve by using S^1 rather than $\mathbf{R}$ as our space. If we take $\mathcal{H} = L^2(\mathbf{R})$, the eigenvectors for the operator P (the functions e^{ikq}) are not square-integrable, so not in $\mathcal{H}$. The operator P is an unbounded operator and we no longer have a theorem saying that its eigenvectors give an orthornormal basis of $\mathcal{H}$. As mentioned earlier, one way to deal with this uses a general spectral theorem for self-adjoint operators on a Hilbert space, for more details see Chapter 2 of [64].

10.3.1 Delta functions

One would like to think of the eigenvectors of the operator P as in some sense continuing to provide an orthonormal basis for $\mathcal{H}$. One problem is that these eigenvectors are not square-integrable, so one needs to expand one's notion of state space $\mathcal{H}$ beyond a space like $L^2(\mathbf{R})$. Another problem is that Fourier transforms of such eigenvectors (which will be eigenvectors of the position operator) gives something that is not a function but a distribution. The proper general formalism for handling state spaces $\mathcal{H}$ which include eigenvectors of both position and momentum operators seems to be that of "rigged Hilbert spaces" which this author confesses to never have mastered (the standard reference is [21]). As a result we won't here give a rigorous discussion, but will use non-normalizable functions and distributions in the non-rigorous form in which they are used in physics. The physics formalism is set up to work as if $\mathcal{H}$ was finite dimensional and allows easy manipulations which don't obviously make sense. Our interest though is not in the general theory, but in very specific quantum systems, where everything is determined by their properties as unitary group representations. For such systems, the general theory of rigged Hilbert spaces is not needed, since for the statements we are interested in various ways can be found to make them precise (although we will generally not enter into the complexities needed to do so).

Given any function $g(q)$ on $\mathbf{R}$, one can try and define an element of the dual space of the space of functions on $\mathbf{R}$ by integration, i.e by the linear operator

$$f \to \int_{-\infty}^{+\infty} g(q)f(q)dq$$

(we won't try and specify which condition on functions f or g is chosen to make sense of this). There are however some other very obvious linear functionals on such a function space, for instance the one given by evaluating the function at $q = c$:

$$f \to f(c)$$

Such linear functionals correspond to generalized functions, objects which when fed into the formula for integration over $\mathbf{R}$ give the desired linear functional. The most well-known of these is the one that gives this evaluation at $q = c$, it is known as the "delta function" and written as $\delta(q - c)$. It is the object which, if it were a function, would satisfy

$$\int_{-\infty}^{+\infty} \delta(q - c)f(q)dq = f(c)$$

To make sense of such an object, one can take it to be a limit of actual functions. For the δ-function, consider the limit as $\epsilon \to 0$ of

$$g_\epsilon = \frac{1}{\sqrt{2\pi\epsilon}} e^{-\frac{(q-c)^2}{2\epsilon}}$$

which satisfy

$$\int_{-\infty}^{+\infty} g_\epsilon(q)dq = 1$$

for all $\epsilon > 0$ (one way to see this is to use the formula given earlier for the Fourier transform of a Gaussian).

Heuristically (ignoring obvious problems of interchange of integrals that don't make sense), one can write the Fourier inversion formula as follows

$$\begin{aligned}
\psi(x) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikq} \widetilde{\psi}(k)dk \\
=& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikq} (\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikq'} \psi(q')dq')dk \\
=& \frac{1}{2\pi} \int_{-\infty}^{+\infty} (\int_{-\infty}^{+\infty} e^{ik(q-q')} \psi(q')dk)dq' \\
=& \int_{-\infty}^{+\infty} \delta(q'-q)\psi(q')dq'
\end{aligned}$$

Taking the delta function to be an even function (so $\delta(x'-x) = \delta(x-x')$), one can interpret the above calculation as justifying the formula

$$\delta(q-q') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(q-q')} dk$$

One then goes on to consider the eigenvectors

$$|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikq}$$

of the momentum operator as satisfying a replacement for the finite-dimensional orthonormality relation, with the δ-function replacing the δ_{nm}:

$$\langle k'|k\rangle = \int_{-\infty}^{+\infty} \overline{(\frac{1}{\sqrt{2\pi}} e^{ik'q})} (\frac{1}{\sqrt{2\pi}} e^{ikq})dq = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i(k-k')q} dq = \delta(k-k')$$

As mentioned before, we will usually work with the variable $p = \hbar k$, in which case we have

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{pq}{\hbar}}$$

and

$$\delta(p-p') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{i\frac{(p-p')q}{\hbar}} dq$$

For a more mathematically legitimate version of this calculation, one place to look is Lecture 6 in the notes on physics by Dolgachev [12].

10.4 For further reading

Every book about quantum mechanics covers this example of the free quantum particle somewhere very early on, in detail. Our discussion here is unusual just in emphasizing the role of the spatial translation groups and its unitary representations. Discussions of quantum mechanics for mathematicians (such as [64]) typically emphasize the development of the functional analysis needed for a proper description of the Hilbert space $\mathcal{H}$ and of the properties of general self-adjoint operators on this state space. In this class we're restricting attention to a quite limited set of such operators coming from Lie algebra representations, so will avoid the general theory.

Chapter 11

The Heisenberg group and the Schrödinger Representation

In our discussion of the free particle, we used just the actions of the groups $\mathbf{R}^3$ of spatial translations and the group $\mathbf{R}$ of time translations, finding corresponding observables, the self-adjoint momentum (P) and Hamiltonian (H) operators. We've seen though that the Fourier transform involves a perfectly symmetrical treatment of position and momentum variables. This allows us to introduce a position operator Q acting on our state space $\mathcal{H}$. We will analyze in detail in this chapter the implications of extending the algebra of observable operators in this way, most of the time restricting to the case of a single spatial dimension, since the physical case of three dimensions is an easy generalization.

The P and Q operators generate an algebra usually called the Heisenberg algebra, since Werner Heisenberg and collaborators used it in the earliest work on a full quantum-mechanical formalism in 1925. It was quickly recognized by Hermann Weyl that this algebra comes from a Lie algebra representation, with a corresponding group (called the Heisenberg group by mathematicians, the Weyl group by physicists). The state space of a quantum particle, either free or moving in a potential, will be a unitary representation of this group, with the group of spatial translations a subgroup. Note that this particular use of a group and its representation theory in quantum mechanics is both at the core of the standard axioms and much more general than the usual characterization of the significance of groups as "symmetry groups". The Heisenberg group does not in any sense correspond to a group of invariances of the physical situation (there are no states invariant under the group), and its action does not commute with any non-zero Hamiltonian operator. Instead it plays a much deeper role, with its unique unitary representation determining much of the structure of quantum mechanics.

Note: beginning with this chapter, we will always assume units for position

and momentum chosen so that $\hbar = 1$ and no longer keep track of how this dimensional constant appears in equations.

11.1 The position operator and the Heisenberg Lie algebra

In the description of the state space $\mathcal{H}$ as functions of a position variable q, the momentum operator is

$$P = -i\frac{d}{dq}$$

The Fourier transform $\mathcal{F}$ provides a unitary transformation to a description of $\mathcal{H}$ as functions of a momentum variable p in which the momentum operator P is just multiplication by p. Exchanging the role of p and q, one gets a position operator Q that acts as

$$Q = i\frac{d}{dp}$$

when states are functions of p (the sign difference comes from the sign change in $\widetilde{\mathcal{F}}$ vs. $\mathcal{F}$), or as multiplication by q when states are functions of q.

11.1.1 Position space representation

In the position space representation, taking as position variable q', one has normalized eigenfunctions describing a free particle of momentum p

$$|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ipq'}$$

which satisfy

$$P|p\rangle = -i\frac{d}{dq'}(\frac{1}{\sqrt{2\pi}}e^{ipq'}) = p(\frac{1}{\sqrt{2\pi}}e^{ipq'}) = p|p\rangle$$

The operator Q in this representation is just the multiplication operator

$$Q\psi(q') = q'\psi(q')$$

that multiplies a function of the position variable q' by q'. The eigenvectors $|q\rangle$ of this operator will be the δ-functions $\delta(q'-q)$ since

$$Q|q\rangle = q'\delta(q'-q) = q\delta(q'-q)$$

A standard convention in physics is to think of a state written in the notation $|\psi\rangle$ as being representation independent. The wavefunction in the position space representation can then be found by taking the coefficient of $|\psi\rangle$ in the expansion of a state in Q eigenfunctions $|q\rangle$, so

$$\langle q|\psi\rangle = \int_{-\infty}^{+\infty}\delta(q-q')\psi(q')dq' = \psi(q)$$

and in particular

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi}} e^{ipq}$$

11.1.2 Momentum space representation

In the momentum space description of $\mathcal{H}$ as functions of p', the state is the Fourier transform of the state in the position space representation, so the state $|p\rangle$ will be the function (actually, the distribution) on momentum space

$$\mathcal{F}(\frac{1}{\sqrt{2\pi}} e^{ipq'}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ip'q'} e^{ipq'} dq' = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i(p-p')q'} dq' = \delta(p-p')$$

These are eigenfunctions of the operator P, which is a multiplication operator in this representation

$$P|p\rangle = p'\delta(p'-p) = p\delta(p'-p)$$

The position eigenfunctions are also given by Fourier transform

$$|q\rangle = \mathcal{F}(\delta(q-q')) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-ip'q'}\delta(q-q')dq' = \frac{1}{\sqrt{2\pi}} e^{-ip'q}$$

The position operator is

$$Q = i\frac{d}{dp}$$

and $|q\rangle$ is an eigenvector with eigenvalue q

$$Q|q\rangle = i\frac{d}{dp'}(\frac{1}{\sqrt{2\pi\hbar}} e^{-ip'q}) = q(\frac{1}{\sqrt{2\pi}} e^{-ip'q}) = q|q\rangle$$

Another way to see that this is the correct operator is to use the unitary transformation $\mathcal{F}$ and its inverse $\widetilde{\mathcal{F}}$ that relate the position and momentum space representations. Going from position space to momentum space one has

$$Q \to \mathcal{F}Q\widetilde{\mathcal{F}}$$

and one can check that this transformed Q operator will act as $i\frac{d}{dp'}$ on functions of p'.

One can express momentum space wavefunctions as coefficients of the expansion of a state ψ in terms of momentum eigenvectors

$$\langle p|\psi\rangle = \int_{-\infty}^{+\infty}(\frac{1}{\sqrt{2\pi}} e^{-ipq'})\psi(q')dq' = \mathcal{F}(\psi(q)) = \widetilde{\psi}(p)$$

11.1.3 Physical interpretation

With now both momentum and position operators on $\mathcal{H}$, we have the standard set-up for describing a non-relativistic quantum particle that is discussed extensively early on in any quantum mechanics textbook, and one of these should be consulted for more details and for explanations of the physical interpretation of this quantum system. The classically observable quantity corresponding to the operator P is the momentum, and eigenvectors of P are the states that have well-defined values for this (the eigenvalue). The momentum eigenvalues and energy eigenvalues will have the correct non-relativistic energy momentum relationship. Note that for the free particle P commutes with the Hamiltonian $H = \frac{P^2}{2m}$ so there is a conservation law: states with a well-defined momentum at one time always have the same momentum. This corresponds to an obvious physical symmetry, the symmetry under spatial translations.

The operator Q on the other hand does not correspond to a physical symmetry, since it does not commute with the Hamiltonian. We will see that it does generate a group action, and from the momentum space picture we can see that this is a shift in the momentum, but such shifts are not symmetries of the physics and there is no conservation law for Q. The states in which Q has a well-defined numerical value are the ones such that the position wavefunction is a delta-function. If one prepares such a state at a given time, it will not remain a delta-function, but quickly evolve into a wavefunction that spreads out in space.

Since the eigenfunctions of P and Q are non-normalizable, one needs a slightly different formulation of the measurement theory principle used for finite dimensional $\mathcal{H}$. In this case, the probability of observing a position of a particle with wavefunction $\psi(q)$ in the interval $[q_1, q_2]$ will be

$$\frac{\int_{q_1}^{q_2} \overline{\psi}(q)\psi(q)dq}{\int_{-\infty}^{+\infty} \overline{\psi}(q)\psi(q)dq}$$

This will make sense for states $|\psi\rangle \in L^2(\mathbf{R})$, which we will normalize to have norm-squared one when discussing their physical interpretation. Then the statistical expectation value for the measured position variable will be

$$\langle \psi | Q | \psi \rangle$$

which can be computed in either the position or momentum space representation.

Similarly, the probability of observing a momentum of a particle with momentum-space wavefunction $\widetilde{\psi}(q)$ in the interval $[p_1, p_2]$ will be

$$\frac{\int_{p_1}^{p_2} \overline{\widetilde{\psi}}(p)\widetilde{\psi}(p)dp}{\int_{-\infty}^{+\infty} \overline{\widetilde{\psi}}(p)\widetilde{\psi}(p)dp}$$

and for normalized states the statistical expectation value of the measured momentum is

$$\langle \psi | P | \psi \rangle$$

Note that states with a well-defined position (the delta-function states in the position-space representation) are equally likely to have any momentum whatsoever. Physically this is why such states quickly spread out. States with a well-defined momentum are equally likely to have any possible position. The properties of the Fourier transform imply the so-called "Heisenberg uncertainty principle" that gives a lower bound on the product of a measure of uncertainty in position times the same measure of uncertainty in momentum. Examples of this that take on the lower bound are the Gaussian shaped functions whose Fourier transforms were computed earlier.

For much more about these questions, again most quantum mechanics textbooks will contain an extensive discussion.

11.2 The Heisenberg Lie algebra

In either the position or momentum space representation the operators P and Q satisfy the relation

$$[Q, P] = i\mathbf{1}$$

Soon after this commutation relation appeared in early work on quantum mechanics, Weyl realized that it can be interpreted as the relation between operators one would get from a representation of a three-dimensional Lie algebra, now called the Heisenberg Lie algebra.

Definition (Heisenberg Lie algebra, $d = 1$)**.** *The Heisenberg Lie algebra* $\mathfrak{h}_3$ *is the vector space* $\mathbf{R}^3$ *with the Lie bracket defined by its values on a basis* (X, Y, Z) *by*

$$[X, Y] = Z, \quad [X, Z] = [Y, Z] = 0$$

Writing a general element of $\mathfrak{h}_3$ in terms of this basis as $xX + yY + zZ$, and grouping the x, y coordinates together (we will see that it is useful to think of the vector space $\mathfrak{h}_3$ as $\mathbf{R}^2 \oplus \mathbf{R}$), the Lie bracket is given in terms of the coordinates by

$$[(\begin{pmatrix} x \\ y \end{pmatrix}, z), (\begin{pmatrix} x' \\ y' \end{pmatrix}, z')] = (\begin{pmatrix} 0 \\ 0 \end{pmatrix}, xy' - yx')$$

Note that this is a non-trivial Lie algebra, but only minimally so. All Lie brackets of Z with anything else are zero. All Lie brackets of Lie brackets are also zero (as a result, this is an example of what is known as a "nilpotent" Lie algebra).

The Heisenberg Lie algebra is isomorphic to the Lie algebra of 3 by 3 strictly upper triangular real matrices, with Lie bracket the matrix commutator, by the following isomorphism:

$$X \leftrightarrow \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Y \leftrightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad Z \leftrightarrow \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$xX + yY + zZ \leftrightarrow \begin{pmatrix} 0 & x & z \\ 0 & 0 & y \\ 0 & 0 & 0 \end{pmatrix}$$

and one has

$$[\begin{pmatrix} 0 & x & z \\ 0 & 0 & y \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & x' & z' \\ 0 & 0 & y' \\ 0 & 0 & 0 \end{pmatrix}] = \begin{pmatrix} 0 & 0 & xy' - x'y \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The generalization of this to higher dimensions is

Definition (Heisenberg Lie algebra)**.** *The Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$ is the vector space $\mathbf{R}^{2d+1} = \mathbf{R}^{2d} \oplus \mathbf{R}$ with the Lie bracket defined by its values on a basis $X_j, Y_j, Z, (j = 1, \dots d)$ by*

$$[X_j, Y_k] = \delta_{jk} Z, \quad [X_j, Z] = [Y_j, Z] = 0$$

Writing a general element as $\sum_{j=1}^{d} x_j X_j + \sum_{k=1}^{d} y_k Y_k + zZ$, in terms of coordinates the Lie bracket is

$$[(\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}, z), (\begin{pmatrix} \mathbf{x}' \\ \mathbf{y}' \end{pmatrix}, z)] = (\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \mathbf{x} \cdot \mathbf{y}' - \mathbf{y} \cdot \mathbf{x}')$$

One can write this Lie algebra as a Lie algebra of matrices for any d. For instance, in the physical case of $d = 3$, elements of the Heisenberg Lie algebra can be written

$$\begin{pmatrix} 0 & x_1 & x_2 & x_3 & z \\ 0 & 0 & 0 & 0 & y_3 \\ 0 & 0 & 0 & 0 & y_2 \\ 0 & 0 & 0 & 0 & y_1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

11.3 The Heisenberg group

One can easily see that exponentiating matrices in $\mathfrak{h}_3$ gives

$$\exp \begin{pmatrix} 0 & x & z \\ 0 & 0 & y \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & x & z + \frac{1}{2}xy \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}$$

so the group with Lie algebra $\mathfrak{h}_3$ will be the group of upper triangular 3 by 3 real matrices with ones on the diagonal, and this group will be the Heisenberg group H_3. For our purposes though, it is better to work in exponential coordinates (i.e. labeling a group element with the Lie algebra element that exponentiates to it).

Matrix exponentials in general satisfy the Baker-Campbell-Hausdorff formula, which says

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]-\frac{1}{12}[B,[A,B]]+\cdots}$$

where the higher terms can all be expressed as repeated commutators. This provides one way of showing that the Lie group structure is determined (for group elements expressible as exponentials) by knowing the Lie bracket. For the full formula and a detailed proof, see chapter 3 of [27]. One can easily check the first few terms in this formula by expanding the exponentials, but the difficulty of the proof is that it is not at all obvious why all the terms can be organized in terms of commutators.

For the case of the Heisenberg Lie algebra, since all multiple commutators vanish, the Baker-Campbell-Hausdorff formula implies for exponentials of elements of $\mathfrak{h}_3$

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$$

(a proof of this special case of Baker-Campbell-Hausdorff is in section 3.1 of [27]). We can use this to explicitly write the group law in exponential coordinates:

Definition (Heisenberg group, $d = 1$)**.** *The Heisenberg group H_3 is the space $\mathbf{R}^3$ with the group law*

$$(\begin{pmatrix} x \\ y \end{pmatrix}, z)(\begin{pmatrix} x' \\ y' \end{pmatrix} z') = (\begin{pmatrix} x+x' \\ y+y' \end{pmatrix}, z + z' + \frac{1}{2}(xy' - yx')) \tag{11.1}$$

Note that the Lie algebra basis elements X, Y, Z each generate subgroups of H_3 isomorphic to $\mathbf{R}$. Elements of the first two of these subgroups generate the full group, and elements of the third subgroup are "central", meaning they commute with all group elements. Also notice that the non-commutative nature of the Lie algebra or group depends purely on the factor $xy' - yx'$.

The generalization of this to higher dimensions is:

Definition (Heisenberg group)**.** *The Heisenberg group H_{2d+1} is the space $\mathbf{R}^{2d+1}$ with the group law*

$$(\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}, z)(\begin{pmatrix} \mathbf{x}' \\ \mathbf{y}' \end{pmatrix}, z') = (\begin{pmatrix} \mathbf{x}+\mathbf{x}' \\ \mathbf{y}+\mathbf{y}' \end{pmatrix}, z + z' + \frac{1}{2}(\mathbf{x}\cdot\mathbf{y}' - \mathbf{y}\cdot\mathbf{x}'))$$

where the vectors here all live in $\mathbf{R}^d$.

Note that in these exponential coordinates the exponential map relating the Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$ and the Heisenberg Lie group H_{2d+1} is just the identity map.

11.4 The Schrödinger representation

Since it can be defined in terms of 3 by 3 matrices, the Heisenberg group H_3 has an obvious representation on $\mathbf{C}^3$, but this representation is not unitary and not of physical interest. What is of great interest is the infinite dimensional representation on functions of q for which the Lie algebra version is given by the Q, P and unit operators:

Definition (Schrödinger representation, Lie algebra version)**.** *The Schrödinger representation of the Heisenberg Lie algebra $\mathfrak{h}_3$ is the representation $(\Gamma'_S, L^2(\mathbf{R}))$ satisfying*

$$\Gamma'_S(X)\psi(q) = -iQ\psi(q) = -iq\psi(q), \quad \Gamma'_S(Y)\psi(q) = -iP\psi(q) = -\frac{d}{dq}\psi(q)$$

$$\Gamma'_S(Z)\psi(q) = -i\psi(q)$$

Factors of i have been chosen to make these operators skew-adjoint and the representation thus unitary. They can be exponentiated, giving in the exponential coordinates on H_3 of equation 11.1

$$\Gamma_S((\begin{pmatrix} x \\ 0 \end{pmatrix}, 0))\psi(q) = e^{-xiQ}\psi(q) = e^{-ixq}\psi(q)$$

$$\Gamma_S((\begin{pmatrix} 0 \\ y \end{pmatrix},))\psi(q) = e^{-yiP}\psi(q) = e^{-y\frac{d}{dq}}\psi(q) = \psi(q-y)$$

$$\Gamma_S((\begin{pmatrix} 0 \\ 0 \end{pmatrix}, z))\psi(q) = e^{-iz}\psi(q)$$

For general group elements of H_3 one has

Definition (Schrödinger representation, Lie group version)**.** *The Schrödinger representation of the Heisenberg Lie group H_3 is the representation $(\Gamma_S, L^2(\mathbf{R}))$ satisfying*

$$\Gamma_S((\begin{pmatrix} x \\ y \end{pmatrix}, z))\psi(q) = e^{-iz}e^{i\frac{xy}{2}}e^{-ixq}\psi(q-y)$$

To check that this defines a representation, one computes

$$\Gamma_S((\begin{pmatrix} x \\ y \end{pmatrix}, z))\Gamma_S((\begin{pmatrix} x' \\ y' \end{pmatrix}, z'))\psi(q) = \Gamma_S((\begin{pmatrix} x \\ y \end{pmatrix}, z))e^{-iz'}e^{i\frac{x'y'}{2}}e^{-ix'q}\psi(q-y')$$

$$\begin{aligned}
&= e^{-i(z+z')}e^{i\frac{xy+x'y'}{2}}e^{-ixq}e^{-ix'(q-y)}\psi(q-y-y') \\
&= e^{-i(z+z'+\frac{1}{2}(xy'-yx'))}e^{i\frac{(x+x')(y+y')}{2}}e^{-i(x+x')q}\psi(q-(y+y')) \\
&= \Gamma_S((\begin{pmatrix} x+x' \\ y+y' \end{pmatrix}, z+z'+\frac{1}{2}(xy'-yx')))
\end{aligned}$$

The group analog of the Heisenberg commutation relations (often called the "Weyl form" of the commutation relations) is the relation

$$e^{-ixQ}e^{-iyP} = e^{-ixy}e^{-iyP}e^{-ixQ}$$

One can derive this by calculating (using the Baker-Campbell-Hausdorff formula)

$$e^{-ixQ}e^{-iyP} = e^{-i(xQ+yP)+\frac{1}{2}[-ixQ,-iyP])} = e^{-i\frac{xy}{2}}e^{-i(xQ+yP)}$$

as well as the same product in the opposite order, and then comparing the results.

Note that, for the Schrödinger representation, we have

$$\Gamma_S((\begin{pmatrix}0\\0\end{pmatrix}, z + 2\pi)) = \Gamma_S((\begin{pmatrix}0\\0\end{pmatrix}, z))$$

so the representation operators are periodic with period 2π in the z-coordinate. Some authors choose to define the Heisenberg group H_3 as not $\mathbf{R}^2 \oplus \mathbf{R}$, but $\mathbf{R}^2 \oplus S^1$, building this periodicity automatically into the definition of the group, rather than the representation.

We have seen that the Fourier transform $\mathcal{F}$ takes the Schrödinger representation to a unitarily equivalent representation of H_3, in terms of functions of p (the momentum space representation). The operators change as

$$\Gamma_S(g) \to \mathcal{F}\ \Gamma_S(g)\widetilde{\mathcal{F}}$$

when one makes the unitary transformation to the momentum space representation.

In typical physics quantum mechanics textbooks, one often sees calculations made just using the Heisenberg commutation relations, without picking a specific representation of the operators that satisfy these relations. This turns out to be justified by the remarkable fact that, for the Heisenberg group, once one picks the constant with which Z acts, all irreducible representations are unitarily equivalent. By unitarity this constant is $-ic, c \in \mathbf{R}$. We have chosen $c = 1$, but other values of c would correspond to different choices of units. In a sense, the representation theory of the Heisenberg group is very simple: there's just one irreducible representation. This is very different than the theory for even the simplest compact Lie groups ($U(1)$ and $SU(2)$) which have an infinity of inequivalent irreducibles labeled by weight or by spin. Representations of a Heisenberg group will appear in different guises (we've seen two, will see another in the discussion of the harmonic oscillator, and there are yet others that appear in the theory of theta-functions), but they are all unitarily equivalent. This statement is known as the Stone-von Neumann theorem.

So far we've been modestly cavalier about the rigorous analysis needed to make precise statements about the Schrödinger representation. In order to prove a theorem like the Stone-von Neumann theorem, which tries to say something about all possible representations of a group, one needs to invoke a great deal of analysis. Much of this part of analysis was developed precisely to be able to deal with general quantum mechanical systems and prove theorems about them. The Heisenberg group, Lie algebra and its representations are treated in detail in many expositions of quantum mechanics for mathematicians. Some good references for this material are [64], and [29]. In depth discussions devoted to the mathematics of the Heisenberg group and its representations can be found in [35], [19] and [66].

In these references can be found a proof of the (not difficult)

Theorem. *The Schrödinger representation Γ_S described above is irreducible.*

and the much more difficult

Theorem (Stone-von Neumann)**.** *Any irreducible representation π of the group H_3 on a Hilbert space, satisfying*

$$\pi'(Z) = -i\mathbf{1}$$

is unitarily equivalent to the Schrödinger representation $(\Gamma_S, L^2(\mathbf{R}))$

Note that all of this can easily be generalized to the case of d spatial dimensions, for d finite, with the Heisenberg group now H_{2d+1} and the Stone-von Neumann theorem still true. In the case of an infinite number of degrees of freedom, which is the case of interest in quantum field theory, the Stone-von Neumann theorem no longer holds and one has an infinity of inequivalent irreducible representations, leading to quite different phenomena. For more on this topic see chapter 33.

It is also important to note that the Stone-von Neumann theorem is formulated for Heisenberg group representations, not for Heisenberg Lie algebra representations. For infinite-dimensional representations in cases like this, there are representations of the Lie algebra that are "non-integrable": they aren't the derivatives of Lie group representations. For general representations of the Heisenberg Lie algebra, i.e. the Heisenberg commutator relations, there are counter-examples to the analog of the Stone von-Neumann theorem. It is only for integrable representations that the theorem holds and one has a unique sort of irreducible representation.

11.5 For further reading

For a lot more detail about the mathematics of the Heisenberg group, its Lie algebra and the Schrödinger representation, see [7], [35], [19] and [66]. An excellent historical overview of the Stone-von Neumann theorem [51] by Jonathan Rosenberg is well worth reading.

Chapter 12

The Poisson Bracket and Symplectic Geometry

We have seen that the quantum theory of a free particle corresponds to the construction of a representation of the Heisenberg Lie algebra in terms of operators Q and P. One would like to use this to produce quantum systems with a similar relation to more non-trivial classical mechanical systems than the free particle. During the earliest days of quantum mechanics it was recognized by Dirac that the commutation relations of the Q and P operators somehow corresponded to the Poisson bracket relations between the position and momentum coordinates on phase space in the Hamiltonian formalism for classical mechanics. In this chapter we'll give an outline of the topic of Hamiltonian mechanics and the Poisson bracket, including an introduction to the symplectic geometry that characterizes phase space.

The Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$ is usually thought of as quintessentially quantum in nature, but it is already present in classical mechanics, as the Lie algebra of degree zero and one polynomials on phase space, with Lie bracket the Poisson bracket. The full Lie algebra of all functions on phase space (with Lie bracket the Poisson bracket) is infinite dimensional, so not the sort of finite dimensional Lie algebra given by matrices that we have studied so far (although, historically, it is this kind of infinite dimensional Lie algebra that motivated the discovery of the theory of Lie groups and Lie algebras by Sophus Lie during the 1870s). In chapter 14 we will see that degree two polynomials on phase space also provide an important finite-dimensional Lie algebra.

12.1 Classical mechanics and the Poisson bracket

In classical mechanics in the Hamiltonian formalism, the space $M = \mathbf{R}^{2d}$ that one gets by putting together positions and the corresponding momenta is known as "phase space". Points in phase space can be thought of as uniquely parametrizing possible initial conditions for classical trajectories, so another in-

terpretation of phase space is that it is the space that uniquely parametrizes solutions of the equations of motion of a given classical mechanical system. The basic axioms of Hamiltonian mechanics can be stated in a way that parallels the ones for quantum mechanics.

Axiom (States)**.** *The state of a classical mechanical system is given by a point in the phase space $M = \mathbf{R}^{2d}$, with coordinates q_j, p_j, for $j = 1, \ldots, d$.*

Axiom (Observables)**.** *The observables of a classical mechanical system are the functions on phase space.*

Axiom (Dyamics)**.** *There is a distinguished observable, the Hamiltonian function h, and states evolve according to Hamilton's equations*

$$\dot{q_j} = \frac{\partial h}{\partial p_j}$$

$$\dot{p_j} = -\frac{\partial h}{\partial q_j}$$

Specializing to the case $d = 1$, for any observable function f, Hamilton's equations imply

$$\frac{df}{dt} = \frac{\partial f}{\partial q}\frac{dq}{dt} + \frac{\partial f}{\partial p}\frac{dp}{dt} = \frac{\partial f}{\partial q}\frac{\partial h}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial h}{\partial q}$$

We can define

Definition (Poisson bracket)**.** *There is a bilinear operation on functions on the phase space $M = \mathbf{R}^2$ (with coordinates (q, p)) called the Poisson bracket, given by*

$$(f_1, f_2) \to \{f_1, f_2\} = \frac{\partial f_1}{\partial q}\frac{\partial f_2}{\partial p} - \frac{\partial f_1}{\partial p}\frac{\partial f_2}{\partial q}$$

An observable f then evolves in time according to

$$\frac{df}{dt} = \{f, h\}$$

This relation is equivalent to Hamilton's equations since it implies them by taking $f = q$ and $f = p$

$$\dot{q} = \{q, h\} = \frac{\partial h}{\partial p}$$

$$\dot{p} = \{p, h\} = -\frac{\partial h}{\partial q}$$

For a non-relativistic free particle, $h = \frac{p^2}{2m}$ and these equations become

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = 0$$

which just says that the momentum is the mass times the velocity, and is conserved. For a particle subject to a potential $V(q)$ one has

$$h = \frac{p^2}{2m} + V(q)$$

and the trajectories are the solutions to

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial V}{\partial q}$$

which adds Newton's second law

$$F = -\frac{\partial V}{\partial q} = ma = m\ddot{q}$$

to the definition of momentum in terms of velocity.

One can easily check that the Poisson bracket has the properties

- Antisymmetry
$$\{f_1, f_2\} = -\{f_2, f_1\}$$
- Jacobi identity
$$\{\{f_1, f_2\}, f_3\} + \{\{f_3, f_1\}, f_2\} + \{\{f_2, f_3\}, f_1\} = 0$$

These two properties, together with the bilinearity, show that the Poisson bracket fits the definition of a Lie bracket, making the space of functions on phase space into an infinite dimensional Lie algebra. This Lie algebra is responsible for much of the structure of the subject of Hamiltonian mechanics, and it was historically the first sort of Lie algebra to be studied.

The conservation laws of classical mechanics are best understood using this Lie algebra. From the fundamental dynamical equation

$$\frac{df}{dt} = \{f, h\}$$

we see that

$$\{f, h\} = 0 \implies \frac{df}{dt} = 0$$

and in this case the function f is called a "conserved quantity", since it does not change under time evolution. Note that if we have two functions f_1 and f_2 on phase space such that

$$\{f_1, h\} = 0, \quad \{f_2, h\} = 0$$

then using the Jacobi identity we have

$$\{\{f_1, f_2\}, h\} = -\{\{h, f_1\}, f_2\} - \{\{f_2, h\}, f_1\} = 0$$

This shows that if f_1 and f_2 are conserved quantities, so is $\{f_1, f_2\}$, so functions f such that $\{f, h\} = 0$ make up a Lie subalgebra. It is this Lie subalgebra that corresponds to "symmetries" of the physics, commuting with the time translation determined by the dynamical law given by h.

12.2 The Poisson bracket and the Heisenberg Lie algebra

A third fundamental property of the Poisson bracket that can easily be checked is the

- Leibniz rule

$$\{f_1 f_2, f\} = \{f_1, f\} f_2 + f_1 \{f_2, f\}, \quad \{f, f_1 f_2\} = \{f, f_1\} f_2 + f_1 \{f, f_2\}$$

This property says that taking Poisson bracket with a function f acts on a product of functions in a way that satisfies the Leibniz rule for what happens when you take the derivative of a product. Unlike antisymmetry and the Jacobi identity, which reflect the Lie algebra structure on functions, the Leibniz property describes the relation of the Lie algebra structure to multiplication of functions. At least for polynomial functions, it allows one to inductively reduce the calculation of Poisson brackets to the special case of Poisson brackets of the coordinate functions q and p, for instance:

$$\{q^2, qp\} = q\{q^2, p\} + \{q^2, q\}p = q^2\{q, p\} + q\{q, p\}q = 2q^2\{q, p\} = 2q^2$$

The Poisson bracket is thus determined by its values on linear functions. We will define

Definition. $\Omega(\cdot, \cdot)$ *is the restriction of the Poisson bracket to* M^**, the linear functions on* M*. Taking as basis vectors of* M^* *the coordinate functions* q *and* p*,* Ω *is given on basis vectors by*

$$\Omega(q, q) = \Omega(p, p) = 0, \quad \Omega(q, p) = -\Omega(p, q) = 1$$

A general element of M^* will be a linear combination $c_q q + c_p p$ for some constants c_q, c_p. For general pairs of elements in M^*, Ω will be given by

$$\Omega(c_q q + c_p p, c'_q q + c'_p p) = c_q c'_p - c_p c'_q \tag{12.1}$$

We will often write elements of M^* as the column vector of their coefficients c_q, c_p, identifying

$$c_q q + c_p p \leftrightarrow \begin{pmatrix} c_q \\ c_p \end{pmatrix}$$

Then one has

$$\Omega(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, \begin{pmatrix} c'_q \\ c'_p \end{pmatrix}) = c_q c'_p - c_p c'_q$$

Taking together linear functions on M and the constant function, one gets a three dimensional space with basis elements $q, p, 1$, and this space is closed under Poisson bracket. This space is thus a Lie algebra, and is isomorphic to the Heisenberg Lie algebra $\mathfrak{h}_3$ (see section 11.2), with the isomorphism given on basis elements by

$$X \leftrightarrow q, \quad Y \leftrightarrow p, \quad Z \leftrightarrow 1$$

This isomorphism preserves the Lie bracket relations since

$$[X, Y] = Z \leftrightarrow \{q, p\} = 1$$

It is convenient to choose its own notation for the dual phase space, so we will often write $M^* = \mathcal{M}$. The three dimensional space we have identified with the Heisenberg Lie algebra is then

$$\mathcal{M} \oplus \mathbf{R}$$

We will denote elements of this space either by functions $c_q q + c_p p + c$, or as

$$(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c)$$

In this second notation, the Lie bracket is

$$[(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c), (\begin{pmatrix} c'_q \\ c'_p \end{pmatrix}, c)] = (\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Omega(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, \begin{pmatrix} c'_q \\ c'_p \end{pmatrix}))$$

Notice that the non-trivial part of the Lie bracket structure is determined by Ω.

In higher dimensions, coordinate functions $q_1, \cdots, q_d, p_1, \cdots, p_d$ on M provide a basis for the dual space $\mathcal{M}$ consisting of the linear coefficient functions of vectors in M. Taking as an additional basis element the constant function 1, we have a $2d + 1$ dimensional space with basis $q_1, \cdots, q_d, p_1, \cdots, p_d, 1$. The Poisson bracket relations

$$\{q_j, q_k\} = \{p_j, p_k\} = 0, \quad \{q_j, p_k\} = \delta_{jk}$$

turn this space into a Lie algebra, isomorphic to the Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$. On general functions, the Poisson bracket will be given by the obvious generalization of the $d = 1$ case

$$\{f_1, f_2\} = \sum_{j=1}^{d} (\frac{\partial f_1}{\partial q_j}\frac{\partial f_2}{\partial p_j} - \frac{\partial f_1}{\partial p_j}\frac{\partial f_2}{\partial q_j}) \tag{12.2}$$

Elements of $\mathfrak{h}_{2d+1}$ are functions on $M = \mathbf{R}^{2d}$ of the form

$$c_{q_1} q_1 + \cdots + c_{q_d} q_d + c_{p_1} p_1 + \cdots + c_{p_d} p_d + c = \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p} + c$$

(using the notation $\mathbf{c}_q = (c_{q_1}, \ldots, c_{q_d})$, $\mathbf{c}_p = (c_{p_1}, \ldots, c_{p_d})$). We will often denote these by

$$(\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c)$$

This Lie bracket on $\mathfrak{h}_{2d+1}$ is given by

$$[(\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c), (\begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix}, c)] = (\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \Omega(\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, \begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix}))$$

which depends just on the antisymmetric bilinear form

$$\Omega(\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, \begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix}) = \mathbf{c}_q \cdot \mathbf{c}'_p - \mathbf{c}_p \cdot \mathbf{c}'_q \tag{12.3}$$

Digression. *We have been careful here to keep track of the difference between phase space $M = \mathbf{R}^{2d}$ and its dual $\mathcal{M} = M^*$, since it is $\mathcal{M} \oplus \mathbf{R}$ that is given the structure of a Lie algebra (in this case $\mathfrak{h}_{2d+1}$) by the Poisson bracket, and it is this Lie algebra we want to use in chapter 15 when we define a quantization of the classical system. Taking duals, we find an isomorphism*

$$M \oplus \mathbf{R} \leftrightarrow \mathfrak{h}_{2d+1}^*$$

It is a general phenomenon that one can define a version of the Poisson bracket on functions on $\mathfrak{g}^*$, the dual of any Lie algebra $\mathfrak{g}$. This is because the Leibniz property ensures that the Poisson bracket only depends on Ω, its restriction to linear functions, and linear functions on $\mathfrak{g}^*$ are just elements of $\mathfrak{g}$. So one can define a Poisson bracket on functions on $\mathfrak{g}^*$ by first defining

$$\Omega(X, X') = [X, X'] \tag{12.4}$$

for $X, X' \in \mathfrak{g} = (\mathfrak{g}^*)^*$, and then extending this to all functions on $\mathfrak{g}^*$ by the Leibniz property.

12.3 Symplectic geometry

We saw in chapter 4 that given a basis $\mathbf{e}_j$ of a vector space V, a dual basis $\mathbf{e}_j^*$ of V^* is given by taking $\mathbf{e}_j^* = v_j$, where v_j are the coordinate functions. If one instead is initially given the coordinate functions v_j, one can construct a dual basis of $V = (V^*)^*$ by taking as basis vectors the first order linear differential operators given by differentiation with respect to the v_j, in other words by taking

$$\mathbf{e}_j = \frac{\partial}{\partial v_j}$$

Elements of V are then identified with linear combinations of these operators. In effect, one is identifying vectors $\mathbf{v}$ with the directional derivative along the vector

$$\mathbf{v} \leftrightarrow \mathbf{v} \cdot \boldsymbol{\nabla}$$

We also saw in chapter 4 that an inner product $\langle \cdot, \cdot \rangle$ on V provides an isomorphism of V and V^* by

$$v \in V \leftrightarrow l_v(\cdot) = \langle v, \cdot \rangle \in V^* \tag{12.5}$$

Such an inner product is the fundamental structure in Euclidean geometry, giving a notion of length of a vector and angle between two vectors, as well a group, the orthogonal group of linear transformations preserving the inner product. It is a symmetric, non-degenerate bilinear form on V.

A phase space M does not usually come with a choice of inner product. We have seen that the Poisson bracket gives us not a symmetric bilinear form, but an antisymmetric bilinear form Ω, defined on the dual space $\mathcal{M}$. We will define an analog of an inner product, with symmetry replaced by antisymmetry:

Definition (Symplectic form)**.** *A symplectic form ω on a vector space V is a bilinear map*

$$\omega : V \times V \to \mathbf{R}$$

such that

- *ω is antisymmetric: $\omega(v, v') = -\omega(v, v')$*
- *ω is nondegenerate: if $v \neq 0$, then $\omega(v, \cdot) \in V^*$ is non-zero.*

A vector space V with a symplectic form ω is called a symplectic vector space. The analog of Euclidean geometry, replacing the inner product by a symplectic form, is called symplectic geometry. In this sort of geometry, there is no notion of length (since antisymmetry implies $\omega(v, v) = 0$). There is an analog of the orthogonal group, called the symplectic group, which consists of linear transformations preserving ω, a group we will study in detail in chapter 14.

Just as an inner product gives an identification of V and V^*, a symplectic form can be used in a similar way, giving an identification of M and $\mathcal{M}$. Using the symplectic form Ω on $\mathcal{M}$, we can define an isomorphism by identifying basis vectors by

$$q_j \in \mathcal{M} \leftrightarrow \Omega(\cdot, q_j) = -\Omega(q_j, \cdot) = -\frac{\partial}{\partial p_j} \in M$$
$$p_j \in \mathcal{M} \leftrightarrow \Omega(\cdot, p_j) = -\Omega(p_j, \cdot) = \frac{\partial}{\partial q_j} \in M$$

and in general

$$u \in \mathcal{M} \leftrightarrow \Omega(\cdot, u) \tag{12.6}$$

Note that unlike the inner product case, a choice of convention of minus sign must be made and is done here.

Recalling the discussion of bilinear forms from section 9.5, a bilinear form on a vector space V can be identified with an element of $V^* \otimes V^*$. Taking $V = M^*$ we have $V^* = (M^*)^* = M$, and the bilinear form Ω on M^* is an element of $M \otimes M$ given by

$$\Omega = \sum_{j=1}^{d} \left(\frac{\partial}{\partial q_j} \otimes \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_j} \otimes \frac{\partial}{\partial q_j}\right)$$

Under the identification 12.6 of M and M^*, $\Omega \in M \otimes M$ corresponds to

$$\omega = \sum_{j=1}^{d} (q_j \otimes p_j - p_j \otimes q_j) \in M^* \otimes M^* \tag{12.7}$$

Another version of the identification of M and $\mathcal{M}$ is then given by

$$v \in M \to \omega(v, \cdot) \in \mathcal{M}$$

In the case of Euclidean geometry, one can show by Gram-Schmidt orthogonalization that a basis $\mathbf{e}_j$ can always be found that puts the inner product (which is a symmetric element of $V^* \otimes V^*$) in the standard form

$$\sum_{j=1}^{n} v_j \otimes v_j$$

in terms of basis elements of V^*, the coordinate functions v_j. There is an analogous theorem in symplectic geometry (for a proof, see for instance Proposition 1.1 of [7]), which says that a basis of a symplectic vector space V can always be found so that the dual basis coordinate functions come in pairs q_j, p_j, with the symplectic form ω the same one we have found based on the Poisson bracket, that given by equation 12.7. Note that one difference between Euclidean and symplectic geometry is that a symplectic vector space will always be even-dimensional.

Digression. *For those familiar with differential manifolds, vector fields and differential forms, the notion of a symplectic vector space can be extended to:*

Definition (Symplectic manifold)**.** *A symplectic manifold M is a manifold with a differential two-form $\omega(\cdot, \cdot)$ (called a symplectic two-form) satisfying the conditions*

- *ω is non-degenerate, i.e. for a nowhere zero vector field X, $\omega(X, \cdot)$ is a nowhere zero one-form.*
- *$d\omega = 0$, in which case ω is said to be closed.*

The cotangent bundle T^*N of a manifold N (i.e. the space of pairs of a point on N together with a linear function on the tangent space at that point) provides one class of symplectic manifolds, generalizing the linear case $N = \mathbf{R}^d$, and corresponding physically to a particle moving on N. A simple example that is neither linear nor a cotangent bundle is the sphere $M = S^2$, with ω the area two-form. The Darboux theorem says that, by an appropriate choice of local coordinates, symplectic two-forms ω can always be put in the form

$$\omega = \sum_{j=1}^{d} dq_j \wedge dp_j$$

Unlike the linear case though, there will in general be no global choice of coordinates for which this true. Later on, our discussion of quantization will rely crucially on having a linear structure on phase space, so will not apply to general symplectic manifolds.

Note that there is no assumption here that M has a metric (i.e. it may not be a Riemannian manifold). A symplectic two-form ω is a structure on a manifold analogous to a metric but with opposite symmetry properties. Whereas a metric is a symmetric non-degenerate bilinear form on the tangent space at

each point, a symplectic form is an antisymmetric non-degenerate bilinear form on the tangent space.

Returning to vector spaces V, one can generalize the notion of a symplectic structure by dropping the non-degeneracy condition on ω. The Leibniz property can still be used to extend this to a Poisson bracket on functions on V, which is then called a Poisson structure on V. In particular, one can do this for $V = \mathfrak{g}^*$ for any Lie algebra $\mathfrak{g}$, using the choice of ω discussed at the end of section 12.2. So $\mathfrak{g}^*$ always has a Poisson structure, and on subspaces where ω is non-degenerate, a symplectic structure.

For instance, for

$$V = \mathfrak{h}_{2d+1}^* = M \oplus \mathbf{R}$$

one has a Poisson bracket on functions on V, but only on the subspace M is this Poisson bracket non-degenerate on linear functions, making M a symplectic vector space. For another example one can take $\mathfrak{g} = \mathfrak{so}(3)$, which is just $\mathbf{R}^3$, with antisymmetric bilinear form ω given by the vector cross-product. In this case it turns out that if one considers spheres of fixed radius in $\mathbf{R}^3$, ω provides a non-degenerate symplectic form on their tangent spaces and such spheres are symplectic manifolds with symplectic two-form their area two-form.

12.4 For further reading

Some good sources for discussions of symplectic geometry and the geometrical formulation of Hamiltonian mechanics are [2], [7] and [9].

Chapter 13

Hamiltonian Vector Fields and the Moment Map

A basic feature of Hamiltonian mechanics is that, for any function f on phase space M, one gets trajectories in phase space that solve Hamilton's equations, and the velocity vectors of these trajectories provide a vector field on phase space. Such vector fields are called Hamiltonian vector fields. When a Lie group G acts on phase space, the infinitesimal action of the group also associates to each element of $\mathfrak{g}$ a vector field on phase space. When these are Hamiltonian vector fields, we get (up to a constant) for each $L \in \mathfrak{g}$ a function μ_L that corresponds to that vector field. This map from $\mathfrak{g}$ to functions on M is called the moment map, and it characterizes the action of G on phase space. Quantization of such functions will give us the quantum observables corresponding to the group action. For the case of the action of $G = \mathbf{R}^3$ on $M = \mathbf{R}^6$ by translations, the moment map gives the momentum, for the action of $G = SO(3)$ by rotations, the angular momentum.

13.1 Vector fields and the exponential map

One can think of a vector field on $M = \mathbf{R}^2$ as a choice of a two-dimensional vector at each point in $\mathbf{R}^2$, so given by a vector-valued function

$$\mathbf{F}(q,p) = \begin{pmatrix} F_q(q,p) \\ F_p(q,p) \end{pmatrix}$$

Such a vector field determines a system of differential equations

$$\frac{dq}{dt} = F_q, \quad \frac{dp}{dt} = F_p$$

Once we specify initial conditions

$$q(0) = q_0, \quad p(0) = p_0$$

if F_q and F_p are differentiable functions these differential equations have a unique solution $q(t), p(t)$, at least for some neighborhood of $t = 0$ (from the existence and uniqueness theorem that can be found for instance in [34]). These solutions $q(t), p(t)$ describe trajectories in $\mathbf{R}^2$ with velocity vector $\mathbf{F}(q(t), p(t))$ and such trajectories can be used to define the "flow" of the vector field: for each t this is the map that takes the initial point $(q(0), p(0)) \in \mathbf{R}^2$ to the point $(q(t), p(t)) \in \mathbf{R}^2$.

Another equivalent way to define vector fields on $\mathbf{R}^2$ is to use instead the directional derivative along the vector field, identifying

$$\mathbf{F}(q,p) \leftrightarrow \mathbf{F}(q,p) \cdot \boldsymbol{\nabla} = F_q(q,p)\frac{\partial}{\partial q} + F_p(q,p)\frac{\partial}{\partial p}$$

The case of $\mathbf{F}$ a constant vector is just our previous identification of the vector space M with linear combinations of $\frac{\partial}{\partial q}$ and $\frac{\partial}{\partial p}$.

An advantage of defining vector fields in this way as first order linear differential operators is that it shows that vector fields form a Lie algebra, where one takes as Lie bracket the commutator of the differential operators. The commutator of two first-order differential operators is another first-order differential operator since higher order derivatives will cancel, using equality of mixed partial derivatives. In addition, such a commutator will satisfy the Jacobi identity. Not only do we get a Lie algebra, but also a representation of the Lie algebra, on functions on $\mathbf{R}^2$.

Given this Lie algebra of vector fields, one can ask what the corresponding group might be. This is not a finite dimensional matrix Lie algebra, so exponentiation of matrices will not give the group. One can however use the flow of the vector field X to define an analog of the exponential of a parameter t times X:

Definition (Exponential map of a vector field)**.** *An exponential map for the vector field X on M is a map*

$$exp(tX) : M \to M$$

that depends on a parameter $t \in \mathbf{R}$, is the identity map at $t = 0$, and satisfies

$$\frac{d}{dt}exp(tX)(m) = X(exp(tX)(m))$$

for $m \in M$.

The flow of the vector field X is the map

$$\Phi_X : (t, m) \in \mathbf{R} \times M \to \Phi_X(t, m) = exp(tX)(m)$$

If the vector field X is differentiable, $exp(tX)$ will be a well-defined map for some neighborhood of $t = 0$, and satisfy

$$exp(t_1X)exp(t_2X) = exp((t_1 + t_2)X)$$

thus providing a one-parameter group with derivative X at the identity.

Digression. *For any manifold M, one has a Lie algebra of differentiable vector fields with an associated Lie bracket. One also has an infinite dimensional Lie group, the group of invertible maps from M to itself, such that the maps and their inverses are both differentiable. This group is called the diffeomorphism group of M and written $Diff(M)$. Its Lie algebra is the Lie algebra of vector fields.*

The representation of the Lie algebra of vector fields on functions is the differential of the representation of $Diff(M)$ on functions induced in the usual way from the action of $Diff(M)$ on the space M.

13.2 Hamiltonian vector fields and canonical transformations

Our interest is not in general vector fields, but in vector fields corresponding to Hamilton's equations for some Hamiltonian function f, i.e. the case

$$F_q = \frac{\partial f}{\partial p}, \quad F_p = -\frac{\partial f}{\partial q}$$

We call such vector fields Hamiltonian vector fields, defining:

Definition (Hamiltonian Vector Field)**.** *A vector field on $M = \mathbf{R}^2$ given by*

$$\frac{\partial f}{\partial p}\frac{\partial}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial}{\partial p} = -\{f, \cdot\}$$

for some function f on $M = \mathbf{R}^2$ is called a Hamiltonian vector field and will be denoted by X_f. In higher dimensions, Hamiltonian vector fields will be those of the form

$$X_f = \sum_{j=1}^{d} \left(\frac{\partial f}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial f}{\partial q_j}\frac{\partial}{\partial p_j}\right) = -\{f, \cdot\} \tag{13.1}$$

for some function f on $M = \mathbf{R}^{2d}$.

The simplest non-zero Hamiltonian vector fields are those for f a linear function. For c_q, c_p constants, if

$$f = c_q q + c_p p$$

then

$$X_f = c_p \frac{\partial}{\partial q} - c_q \frac{\partial}{\partial p}$$

and the map

$$f \to X_f$$

is just the isomorphism of $\mathcal{M}$ and M of equation 12.6.

For example, taking $f = p$, we have $X_p = \frac{\partial}{\partial q}$. The exponential map for this vector field is

$$exp(tX_p)(q_0, p_0) = (q_0 + t, p_0) \tag{13.2}$$

Similarly, for $f = q$ one has $X_q = -\frac{\partial}{\partial p}$ and

$$exp(tX_q)(q_0, p_0) = (q_0, p_0 - t) \tag{13.3}$$

For quadratic functions f one gets vector fields X_f with components linear in the coordinates. An important example, which describes a harmonic oscillator and will be treated in much more detail in chapter 20, is the case

$$f = \frac{1}{2}(q^2 + p^2)$$

for which

$$X_f = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}$$

The trajectories satisfy

$$\frac{dq}{dt} = p, \quad \frac{dp}{dt} = -q$$

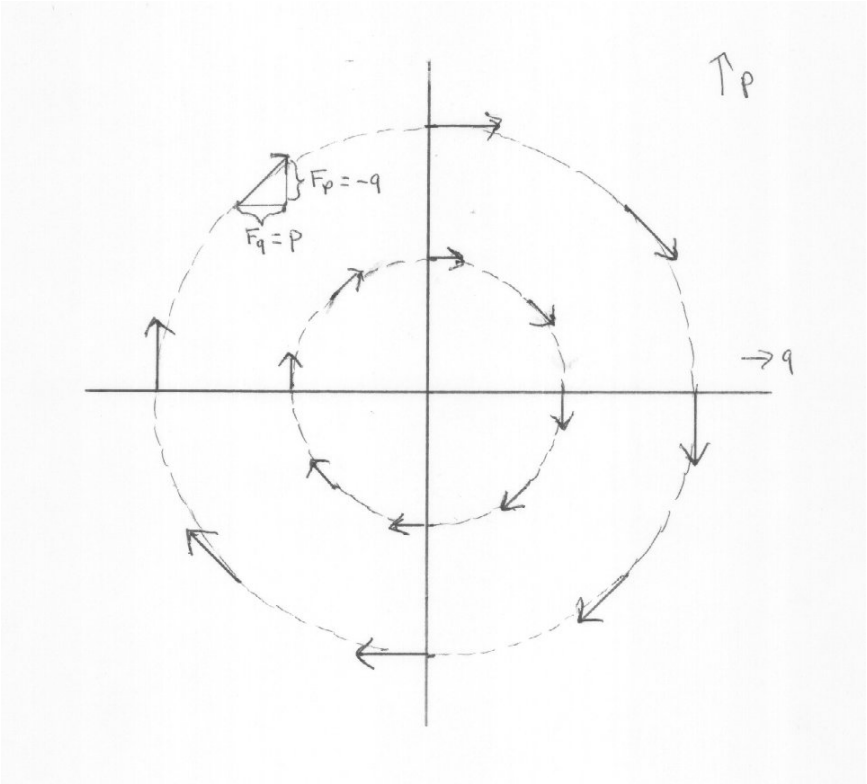
and are given by

$$q(t) = q(0)\cos t + p(0)\sin t, \quad p(t) = p(0)\cos t - q(0)\sin t$$

The exponential map is given by clockwise rotation through an angle t

$$exp(tX_f)(q_0, p_0) = (q_0 \cos t + p_0 \sin t, p_0 \cos t - q_0 \sin t)$$

The vector field X_f and the trajectories in the $q - p$ plane look like this



The relation of vector fields to the Poisson bracket is given by

$$\{f_1, f_2\} = X_{f_2}(f_1) = -X_{f_1}(f_2)$$

so one has in particular

$$\{q, f\} = \frac{\partial f}{\partial p}, \quad \{p, f\} = -\frac{\partial f}{\partial q}$$

The definition we have given here of X_f (equation 13.1) carries with it a choice of how to deal with a confusing sign issue. Recall that vector fields on M form a Lie algebra with Lie bracket the commutator of differential operators. A natural question is that of how this Lie algebra is related to the Lie algebra of functions on M (with Lie bracket the Poisson bracket).

The Jacobi identity implies

$$\{f, \{f_1, f_2\}\} = \{\{f, f_1\}, f_2\} + \{\{f_2, f\}, f_1\} = \{\{f, f_1\}, f_2\} - \{\{f, f_2\}, f_1\}$$

so

$$X_{\{f_1, f_2\}} = X_{f_2} X_{f_1} - X_{f_1} X_{f_2} = -[X_{f_1}, X_{f_2}] \tag{13.4}$$

This shows that the map $f \to X_f$ of equation 13.1 that we defined between these Lie algebras is not quite a Lie algebra homomorphism because of the -

sign in equation 13.4 (it is called a Lie algebra "antihomomorphism"). The map that is a Lie algebra homomorphism is

$$f \to -X_f$$

To keep track of the minus sign here, one needs to keep straight the difference between

- The functions on phase space M are a Lie algebra, with adjoint action

$$ad(f)(\cdot) = \{f, \cdot\}$$

  and

- The functions f provide vector fields X_f acting on functions on M, where

$$X_f(\cdot) = \{\cdot, f\} = -\{f, \cdot\}$$

The first of these is what will be most relevant to us later when we quantize functions on M to get operators, preserving the Lie algebra structure. The second is what one naturally gets from the geometrical action of a Lie group G on the phase space M (see section 13.3). As a simple example, the function p satisfies

$$\{p, F(q)\} = -\frac{\partial F}{\partial q}$$

so

$$\{p, \cdot\} = -\frac{\partial(\cdot)}{\partial q}$$

is the infinitesimal action of translation in q on functions, whereas $\frac{\partial}{\partial q}$ is the vector field on M corresponding to infinitesimal translation in the position coordinate.

It is important to note that the Lie algebra homomorphism

$$f \to X_f$$

is not an isomorphism, for two reasons:

- It is not injective (one-to-one), since functions f and $f+C$ for any constant C correspond to the same X_f.

- It is not surjective since not all vector fields are Hamiltonian vector fields (i.e. of the form X_f for some f). One property that a vector field must satisfy in order to possibly be a Hamiltonian vector field (this condition is sufficient but we will not show this) is

$$X\{g_1, g_2\} = \{Xg_1, g_2\} + \{g_1, Xg_2\} \tag{13.5}$$

  for g_1 and g_2 on M. This is just the Jacobi identity for f, g_1, g_2, when $X = X_f$.

Digression. *For a general symplectic manifold M, the symplectic two-form ω gives one an analog of Hamilton's equations. This is the following equality of one-forms, relating a Hamiltonian function h and a vector field X_h determining time evolution of trajectories in M*

$$i_{X_h}\omega = \omega(X_h, \cdot) = dh$$

(here i_X is interior product with the vector field X). The Poisson bracket in this context can be defined as

$$\{f_1, f_2\} = \omega(X_{f_1}, X_{f_2})$$

Recall that a symplectic two-form is defined to be closed, satisfying the equation $d\omega = 0$, which is then a condition on a three-form $d\omega$. Standard differential form computations allow one to express $d\omega(X_{f_1}, X_{f_2}, X_{f_3})$ in terms of Poisson brackets of functions f_1, f_2, f_3, and one finds that $d\omega = 0$ is the Jacobi identity for the Poisson bracket.

The theory of "prequantization" (see [36], [29]) enlarges the phase space M to a $U(1)$ bundle with connection, where the curvature of the connection is the symplectic form ω. Then the problem of lack of injectivity of the Lie algebra homomorphism

$$f \to -X_f$$

is resolved by instead using the map

$$f \to -\nabla_{X_f} + if \tag{13.6}$$

where ∇_X is the covariant derivative with respect to the connection. For details of this, see [36] or [29].

In our treatment of functions on phase space M, we have always been taking such functions to be time-independent. One can abstractly interpret M as the space of trajectories of a classical mechanical system, with coordinates q, p having the interpretation of initial conditions $q(0), p(0)$ of the trajectories. The exponential maps $exp(tX_h)$ give an action on the space of trajectories for Hamiltonian function h, taking the trajectory with initial conditions given by $m \in M$ to the time-translated one with initial conditions given by $exp(tX_h)(m)$. One should really interpret the formula for Hamilton's equations

$$\frac{df}{dt} = \{f, h\}$$

as meaning

$$\frac{d}{dt} f(exp(tX_f)(m))|_{t=0} = \{f(m), h(m)\}$$

for each $m \in M$.

Given a Hamiltonian vector field X_f, the maps

$$exp(tX_f) : M \to M$$

are known to physicists as "canonical transformations", and to mathematicians as "symplectomorphisms". We will not try and work out in any more detail how the exponential map behaves in general. In chapter 14 we will see what happens for f an order-two homogeneous polynomial in the q_j, p_k. In that case the vector field X_f will take linear functions on M to linear functions, thus acting on $\mathcal{M}$, in which case its behavior can be studied using the matrix for the linear transformation with respect to the basis elements q_j, p_k.

Digression. *The exponential map $exp(tX)$ can be defined as above on a general manifold. For a symplectic manifold M, Hamiltonian vector fields X_f will have the property that*

$$exp(tX_f)^*\omega = \omega$$

This is because

$$\mathcal{L}_{X_f}\omega = (di_{X_f} + i_{X_f}d)\omega = di_{X_f}\omega = d\omega(X_f, \cdot) = ddf = 0$$

13.3 Group actions on M and the moment map

Whenever one has an action of a Lie group G on a space M, an infinitesimal version of this action is the map

$$L \in \mathfrak{g} \to X_L$$

from $\mathfrak{g}$ to vector fields on M that takes L to the vector field X_L which acts on functions on M by

$$X_L F(m) = \frac{d}{dt} F(e^{tL} \cdot m)_{|t=0}$$

This map however is not a homomorphism (for the Lie bracket on vector fields the commutator of derivatives), but an anti-homomorphism. To see why this is, recall that when a group G acts on a space, we get a representation π on functions F on the space by

$$\pi(g)F(m) = F(g^{-1} \cdot m)$$

The derivative of this representation will be the Lie algebra representation

$$\pi'(L)F(m) = \frac{d}{dt} F(e^{-tL} \cdot m)_{|t=0} = -X_L F(m)$$

so we see that it is the map

$$L \to \pi'(L) = -X_L$$

that will be a homomorphism.

Given an action of a group G on M, if for $L \in \mathfrak{g}$ the vector field X_L is a Hamiltonian vector field, we would like to find the function f such that $X_L = X_f$. This will allow us to study infinitesimal group actions on M by using functions

on M and the Poisson bracket. Quantization will turn functions on M into operators, turning the function f into an operator which will be the observable corresponding to the infinitesimal group action by a Lie algebra element L.

Only for certain actions of G on M will the X_L be Hamiltonian vector fields. A necessary condition is that X_L satisfy equation 13.5

$$X_L\{g_1, g_2\} = \{X_L g_1, g_2\} + \{g_1, X_L g_2\}$$

which is a property of Hamiltonian vector fields. Even when a function f exists such that $X_f = X_L$, it is only unique up to a constant, since f and $f + C$ will give the same vector field. We would like to choose these constants in such a way that the map

$$L \to f$$

is a Lie algebra homomorphism from $\mathfrak{g}$ to the Lie algebra of functions on M. When this is possible, the G-action is said to be a Hamiltonian G-action. When it is not possible, the G-symmetry of the classical phase space is said to have an "anomaly".

We can define

Definition (Moment map)**.** *Given a Hamiltonian action of a Lie group G on M, a Lie algebra homomorphism*

$$L \to \mu_L$$

from $\mathfrak{g}$ to functions on M is said to be a moment map if

$$X_L = X_{\mu_L}$$

Equivalently, for functions F on M, μ_L satisfies

$$X_{\mu_L} F = -\{\mu_L, F\} = X_L F$$

Note what we are calling a moment map is sometimes called a "co-moment map", with the term "moment map" referring to a repackaged form of the same information, the map

$$\mu : M \to \mathfrak{g}^*$$

where

$$(\mu(m))(L) = \mu_L(m)$$

For $G = H_3$, the moment map is just our identification of the Heisenberg Lie algebra with functions on phase space:

$$\mu_L = L = c_q q + c_p p + c \in \mathfrak{h}_3$$

Here

$$X_{\mu_L} = -c_q \frac{\partial}{\partial p} + c_p \frac{\partial}{\partial q}$$

The action of H_3 on M for which this is the moment map will have $X_L = X_{\mu_L}$ and one can check that this action is

$$(\begin{pmatrix} x \\ y \end{pmatrix}, z) \cdot (q_0, p_0) = (q_0 + y, p_0 - x) \tag{13.7}$$

See equations 13.2 and 13.3, which show that this action corresponds to the exponential map for vector fields associated to Lie algebra basis elements q and p. For central elements of the Lie algebra (the constant functions), the vector field is zero, and the exponential map takes these to the identity map on M.

For $d = 3$ the translation group $G = \mathbf{R}^3$ is a subgroup of H_7 of elements of the form

$$(\begin{pmatrix} \mathbf{0} \\ \mathbf{a} \end{pmatrix}, 0)$$

since it acts on the phase space by translation in the position coordinates

$$(\mathbf{q}_0, \mathbf{p}_0) \to (\mathbf{q}_0 + \mathbf{a}, \mathbf{p}_0)$$

Taking $\mathbf{a}$ to be the corresponding element in the Lie algebra of $G = \mathbf{R}^3$, the vector field on M is

$$X_{\mathbf{a}} = \mathbf{a} \cdot \boldsymbol{\nabla}$$

and the moment map is given by

$$\mu_{\mathbf{a}}(\mathbf{q}_0, \mathbf{p}_0) = \mathbf{a} \cdot \mathbf{p}_0$$

(a function on M for each element $\mathbf{a}$ of the Lie algebra) or

$$\mu(\mathbf{q}_0, \mathbf{p}_0)(\mathbf{a}) = \mathbf{a} \cdot \mathbf{p}_0$$

(an element of the dual of the Lie algebra for each point $m = (\mathbf{q}_0, \mathbf{p}_0)$ in phase space).

For another example, consider the action of the group $G = SO(3)$ of rotations on phase space $M = \mathbf{R}^6$, which gives a map from $\mathfrak{so}(3)$ to vector fields on $\mathbf{R}^6$, taking for example

$$l_1 \in \mathfrak{so}(3) \to X_{l_1} = -q_3 \frac{\partial}{\partial q_2} + q_2 \frac{\partial}{\partial q_3} - p_3 \frac{\partial}{\partial p_2} + p_2 \frac{\partial}{\partial p_3}$$

(this is the vector field for an infinitesimal clockwise rotation in the $q_2 - q_3$ and $p_2 - p_3$ planes, in the opposite direction to the case of the vector field $X_{\frac{1}{2}(q^2+p^2)}$ in the $q - p$ plane of section 13.2). The moment map here gives the usual expression for the 1-component of the angular momentum

$$\mu_{l_1} = q_2 p_3 - q_3 p_2$$

since one can check from equation 13.1 that $X_{l_1} = X_{\mu_{l_1}}$. On basis elements of $\mathfrak{so}(3)$ one has

$$\mu_{l_j}(\mathbf{q}_0, \mathbf{p}_0) = (\mathbf{q}_0 \times \mathbf{p}_0)_j$$

Formulated as a map from M to $\mathfrak{so}(3)^*$, the moment map is

$$\mu(\mathbf{q}_0, \mathbf{p}_0)(\mathbf{l}) = (\mathbf{q}_0 \times \mathbf{p}_0) \cdot \mathbf{l}$$

where $\mathbf{l} \in \mathfrak{so}(3)$.

Digression. *For the case of M a general symplectic manifold, one can still define the moment map, whenever one has a Lie group G acting on M, preserving the symplectic form ω. The infinitesimal condition for such a G action is that*

$$\mathcal{L}_X \omega = 0$$

where $\mathcal{L}_X$ is the Lie derivative along the vector field X. Using the formula

$$\mathcal{L}_X = (d + i_X)^2 = di_X + i_X d$$

for the Lie derivative acting on differential forms (i_X is contraction with the vector field X), one has

$$(di_X + i_X d)\omega = 0$$

and since $d\omega = 0$ we have

$$di_X \omega = 0$$

When M is simply-connected, one-forms $i_X\omega$ whose differential is 0 (called "closed") will be the differentials of a function (and called "exact"). So there will be a function μ such that

$$i_X\omega(\cdot, \cdot) = \omega(X, \cdot) = d\mu(\cdot)$$

although such a μ is only unique up to a constant.

Given an element $L \in \mathfrak{g}$, the G action on M gives a vector field X_L. When we can choose the constants appropriately and find functions μ_L satisfying

$$i_{X_L}\omega(\cdot, \cdot) = d\mu_L(\cdot)$$

such that the map

$$L \to \mu_L$$

taking Lie algebra elements to functions on M (with Lie bracket the Poisson bracket) is a Lie algebra homomorphism, then this is called the moment map. One can equivalently work with

$$\mu : M \to \mathfrak{g}^*$$

by defining

$$(\mu(m))(L) = \mu_L(m)$$

An important class of symplectic manifolds M with an action of a Lie group G, preserving the symplectic form, are the co-adjoint orbits $\mathcal{O}_l$. These are the

manifolds one gets by acting on a chosen $l \in \mathfrak{g}^*$ by the co-adjoint action Ad^*, meaning the action of g on $\mathfrak{g}^*$ satisfying

$$(Ad^*(g) \cdot l)(X) = l(Ad(g)X)$$

where $X \in \mathfrak{g}$, and $Ad(g)$ is the usual adjoint action on $\mathfrak{g}$. For these cases, the moment map

$$\mu : \mathcal{O}_l \to \mathfrak{g}^*$$

is just the inclusion map. Two simple examples are

- *For $\mathfrak{g} = \mathfrak{h}_3$, fixing a choice of c elements of $\mathfrak{g}$ are linear functions on $M = \mathbf{R}^2$, so $l \in \mathfrak{g}^*$ is a point in M (evaluation of the function at that point). The co-adjoint action is the action of H_3 on M of equation 13.7.*
- *For $\mathfrak{g} = \mathfrak{so}(3)$ the non-zero co-adjoint orbits are spheres, with radius the length of l.*

13.4 For further reading

For a general discussion of vector fields on $\mathbf{R}^n$, see [34]. See [2], [7] and [9] for more on Hamiltonian vector fields and the moment map. For more on the duals of Lie algebras and co-adjoint orbits, see [8] and [35].

Chapter 14

Quadratic Polynomials and the Symplectic Group

The Poisson bracket on functions on phase space $M = \mathbf{R}^{2d}$ is determined by an antisymmetric bilinear form Ω on the dual phase space $\mathcal{M} = M^*$. Just as there is a group of linear transformations (the orthogonal group) leaving invariant an inner product, which is a symmetric bilinear form, here there is a group leaving invariant Ω, the symplectic group $Sp(2d, \mathbf{R})$. The Lie algebra $\mathfrak{sp}(2d, \mathbf{R})$ of this group can be identified with the Lie algebra of order-two polynomials on M, with Lie bracket the Poisson bracket. Elements of $Sp(2d, \mathbf{R})$ act on $\mathcal{M}$, preserving Ω, and so provide a map of the Heisenberg Lie algebra $\mathfrak{h}_{2d+1} = \mathcal{M} \oplus \mathbf{R}$ to itself, preserving the Lie bracket (which is defined using Ω). The symplectic group thus acts by automorphisms on $\mathfrak{h}_{2d+1}$. This action has an infinitesimal version, reflected in the non-trivial Poisson brackets between order two and order one polynomials on M.

The identification of elements L of the Lie algebra $\mathfrak{sp}(2d, \mathbf{R})$ with order-two polynomials μ_L on M is just the moment map for the action of the symplectic group $Sp(2d, \mathbf{R})$ on phase space. The corresponding vector fields will have linear coefficient functions. Quantization of these polynomial functions will provide quantum observables corresponding to any Lie subgroup $G \subset Sp(2d, \mathbf{R})$ (any Lie group G that acts on M preserving the symplectic form). Such group actions will give rise to quantum observables, but they may or may not be "symmetries", with the term "symmetry" usually meaning that one has $\{\mu_L, h\} = 0$ for h the Hamiltonian function.

14.1 The symplectic group

Recall that the orthogonal group can be defined as the group of linear transformations preserving an inner product, which is a symmetric bilinear form. We now want to study the analog of the orthogonal group one gets by replacing

the inner product by the antisymmetric bilinear form Ω that determines the symplectic geometry of phase space. We will define

Definition (Symplectic Group)**.** *The symplectic group $Sp(2d, \mathbf{R})$ is the subgroup of linear transformations g of $M^* = \mathbf{R}^{2d}$ that satisfy*

$$\Omega(gv_1, gv_2) = \Omega(v_1, v_2)$$

for $v_1, v_2 \in M^*$

While this definition uses the dual phase space M^* and Ω, it would have been equivalent to have made the definition using M and ω, since these transformations preserve the isomorphism between M and M^* given by Ω (see equation 12.6). For an action on M^*

$$u \in M^* \to gu \in M^*$$

the action on elements of M, which correspond to linear functions $\Omega(u, \cdot)$ on M^* is given by

$$\Omega(u, \cdot) \in M \to g \cdot \Omega(u, \cdot) = \Omega(u, g^{-1}(\cdot)) = \Omega(gu, \cdot) \in M$$

Here the first equality uses the definition of the dual representation (see 4.2) and the second uses the invariance of Ω.

14.1.1 The symplectic group for $d = 1$

In order to study symplectic groups as groups of matrices, we'll begin with the case $d = 1$ and the group $Sp(2, \mathbf{R})$. We can write Ω as

$$\Omega(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, \begin{pmatrix} c'_q \\ c'_p \end{pmatrix}) = c_q c'_p - c_p c'_q = \begin{pmatrix} c_q & c_p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} c'_q \\ c'_p \end{pmatrix} \tag{14.1}$$

Note that for the analogous case of the inner product, the same formula holds with the elementary antisymmetric matrix replaced by the identity matrix.

A linear transformation g of M^* will be given by

$$\begin{pmatrix} c_q \\ c_p \end{pmatrix} \to \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} c_q \\ c_p \end{pmatrix}$$

The condition for Ω to be invariant under such a transformation is

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{14.2}$$

or

$$\begin{pmatrix} 0 & \alpha\delta - \beta\gamma \\ -\alpha\delta + \beta\gamma & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

so

$$det \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \alpha\delta - \beta\gamma = 1$$

This says that we can have any linear transformation with unit determinant. In other words, we find that $Sp(2,\mathbf{R}) = SL(2,\mathbf{R})$. We will see later that this isomorphism with a special linear group only happens for $d = 1$.

For the analog of equation 14.2 in the inner product case, replace the elementary antisymmetric matrices by unit matrices, giving the condition that defines orthogonal matrices, $g^T g = 1$.

Now turning to the Lie algebra, for group elements $g \in GL(2,\mathbf{R})$ near the identity, one can write g in the form $g = e^{tL}$ where L is in the Lie algebra $\mathfrak{gl}(2,\mathbf{R})$. The condition that g acts on $\mathcal{M}$ preserving Ω implies that (differentiating 14.2)

$$\frac{d}{dt}((e^{tL})^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} e^{tL}) = (e^{tL})^T (L^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} L) e^{tL} = 0$$

Setting $t = 0$, the condtion on L is

$$L^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} L = 0 \tag{14.3}$$

This requires that L must be of the form

$$L = \begin{pmatrix} a & b \\ c & -a \end{pmatrix}$$

which is what one expects: L is in the Lie algebra $\mathfrak{sl}(2,\mathbf{R})$ of 2 by 2 real matrices with zero trace. The analog in the inner product case is just the condition defining elements of the Lie algebra of the orthogonal group, $L^T + L = 0$.

The homogeneous degree two polynomials in p and q form a three-dimensional sub-Lie algebra of the Lie algebra of functions on phase space, since the non-zero Poisson bracket relations between them on a basis $\frac{q^2}{2}, \frac{p^2}{2}, qp$ are

$$\{\frac{q^2}{2}, \frac{p^2}{2}\} = qp \quad \{qp, p^2\} = 2p^2 \quad \{qp, q^2\} = -2q^2$$

This Lie algebra is isomorphic to $\mathfrak{sl}(2,\mathbf{R})$, with an explicit isomorphism given by identifying basis elements as follows:

$$\frac{q^2}{2} \leftrightarrow E = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad -\frac{p^2}{2} \leftrightarrow F = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad -qp \leftrightarrow G = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{14.4}$$

The commutation relations amongst these matrices are

$$[E, F] = G \quad [G, E] = 2E \quad [G, F] = -2F$$

which are the same as the Poisson bracket relations between the corresponding quadratic polynomials.

We thus see that we have an isomorphism between the Lie algebra of degree two homogeneous polynomials with the Poisson bracket and the Lie algebra

of 2 by 2 trace-zero real matrices with the commutator as Lie bracket. The isomorphism on general elements of these Lie algebras is

$$\mu_L = -aqp + \frac{bq^2}{2} - \frac{cp^2}{2} = \frac{1}{2}\begin{pmatrix} q & p \end{pmatrix}\begin{pmatrix} b & -a \\ -a & -c \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} \leftrightarrow L = \begin{pmatrix} a & b \\ c & -a \end{pmatrix} \quad (14.5)$$

We have seen that this is a Lie algebra isomorphism on basis elements, but one can explicitly check that.

$$\{\mu_L, \mu_{L'}\} = \mu_{[L,L']}$$

The use of the notation μ_L for these quadratic functions reflects the fact that

$$L \in \mathfrak{sl}(2, \mathbf{R}) \to \mu_L$$

is a moment map. This is for the $SL(2, \mathbf{R})$ action on phase space $M = \mathbf{R}^2$ corresponding to the above $SL(2, \mathbf{R})$ action on $\mathcal{M}$ (under the identification between M and $\mathcal{M}$ given by Ω). One can check the condition $X_L = X_{\mu_L}$ on vector fields on M, but we will not do this here, since for our purposes it is the action on $\mathcal{M}$ that is important.

Two important subgroups of $SL(2, \mathbf{R})$ are

- The subgroup of elements one gets by exponentiating G, which is isomorphic to the multiplicative group of positive real numbers

$$e^{tG} = \begin{pmatrix} e^t & 0 \\ 0 & e^{-t} \end{pmatrix}$$

  Here one can explicitly see that this group has elements going off to infinity.

- Exponentiating the Lie algebra element $E - F$ gives rotations of the plane

$$e^{\theta(E-F)} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

  Note that the Lie algebra element being exponentiated here is

$$E - F \leftrightarrow \frac{1}{2}(p^2 + q^2)$$

  which we will later re-encounter as the Hamiltonian function for the harmonic oscillator.

The group $SL(2, \mathbf{R})$ is non-compact and thus its representation theory is quite unlike the case of $SU(2)$. In particular, all of its non-trivial irreducible unitary representations are infinite-dimensional, forming an important topic in mathematics, but one that is beyond our scope. We will be studying just one such irreducible representation, and it is a representation only of a double-cover of $SL(2, \mathbf{R})$, not $SL(2, \mathbf{R})$ itself.

14.1.2 The symplectic group for arbitary d

For general d, the symplectic group $Sp(2d, \mathbf{R})$ is the group of linear transformations g of $\mathcal{M}$ that leave Ω (see 12.3) invariant, i.e. satisfy

$$\Omega(g\begin{pmatrix}\mathbf{c}_q\\ \mathbf{c}_p\end{pmatrix}, g\begin{pmatrix}\mathbf{c}'_q\\ \mathbf{c}'_p\end{pmatrix}) = \Omega(\begin{pmatrix}\mathbf{c}_q\\ \mathbf{c}_p\end{pmatrix}, \begin{pmatrix}\mathbf{c}'_q\\ \mathbf{c}'_p\end{pmatrix})$$

where $\mathbf{c}_q, \mathbf{c}_p$ are d-dimensional vectors. By essentially the same calculation as in the $d = 1$ case, we find the d-dimensional generalization of equation 14.2. This says that $Sp(2d, \mathbf{R})$ is the group of real $2d$ by $2d$ matrices g satisfying

$$g^T \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix} g = \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix}$$

where $\mathbf{0}$ is the d by d zero matrix, $\mathbf{1}$ the d by d unit matrix.

Again by a similar argument to the $d = 1$ case where the Lie algebra $\mathfrak{sp}(2, \mathbf{R})$ was determined by the condition 14.3, $\mathfrak{sp}(2d, \mathbf{R})$ is the Lie algebra of $2d$ by $2d$ matrices L satisfying

$$L^T \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix} + \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix} L = 0$$

Such matrices will be those with the block-diagonal form

$$L = \begin{pmatrix}A & B\\ C & -A^T\end{pmatrix} \tag{14.6}$$

where A, B, C are d by d real matrices, with B and C symmetric, i.e.

$$B = B^T, \quad C = C^T$$

The generalization of 14.5 is

Theorem 14.1. *The Lie algebra $\mathfrak{sp}(2d, \mathbf{R})$ is isomorphic to the Lie algebra of order two homogeneous polynomials on $M = \mathbf{R}^{2d}$ by the isomorphism (using a vector notation for the coefficient functions $q_1, \cdots, q_d, p_1, \cdots, p_d$)*

$$L \leftrightarrow \mu_L$$

where

$$\begin{aligned}\mu_L =& \frac{1}{2}\begin{pmatrix}\mathbf{q} & \mathbf{p}\end{pmatrix} L \begin{pmatrix}\mathbf{0} & -\mathbf{1}\\ \mathbf{1} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix}\\ =& \frac{1}{2}\begin{pmatrix}\mathbf{q} & \mathbf{p}\end{pmatrix}\begin{pmatrix}B & -A\\ -A^T & -C\end{pmatrix}\begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix}\\ =& \frac{1}{2}(\mathbf{q}\cdot B\mathbf{q} - 2\mathbf{q}\cdot A\mathbf{p} - \mathbf{p}\cdot C\mathbf{p})\end{aligned} \tag{14.7}$$

We will postpone the proof of this theorem until section 14.2, since it is easier to first study Poisson brackets between order two and order one polynomials, then use this to prove the theorem about Poisson brackets between order two polynomials.

The Lie algebra $\mathfrak{sp}(2d, \mathbf{R})$ has a subalgebra $\mathfrak{gl}(d, \mathbf{R})$ consisting of matrices of the form

$$L = \begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & -A^T \end{pmatrix}$$

or, in terms of polynomials, polynomials

$$-\mathbf{q} \cdot A\mathbf{p} = -(A^T\mathbf{p}) \cdot \mathbf{q}$$

Here A is any real d by d matrix. This shows that one way to get symplectic transformations is to take any linear transformation of the position coordinates, together with the dual linear transformation on momentum coordinates. In this way, any linear group of symmetries of the position space becomes a group of symmetries of phase-space. An example of this is the group $SO(d)$ of spatial rotations, with Lie algebra $\mathfrak{so}(d) \subset \mathfrak{gl}(d, \mathbf{R})$, the antisymmetric d by d matrices. In the case $d = 3$, μ_L gives the standard expression for the angular momentum as a function of the q_j, p_k coordinates on phase space. For example, taking $L = l_1$, one has

$$\mu_{l_1} = q_2p_3 - q_3p_2$$

the standard expression for angular momentum about the 1-axis.

Another important subgroup comes from taking $A = 0, B = \mathbf{1}, C = -\mathbf{1}$, which gives

$$\mu_L = \frac{1}{2}(|\mathbf{q}|^2 + |\mathbf{p}|^2)$$

which will be the Hamiltonian function for a d-dimensional harmonic oscillator. Exponentiating, one gets an $SO(2)$ subgroup, one that acts on phase space in a way that mixes position and momentum coordinates, so cannot be understood just in terms of configuration space.

14.2 The symplectic group and automorphisms of the Heisenberg group

Returning to the $d = 1$ case, we have found two three-dimensional Lie algebras ($\mathfrak{h}_3$ and $\mathfrak{sl}(2, \mathbf{R})$) as subalgebras of the infinite dimensional Lie algebra of functions on phase space:

- $\mathfrak{h}_3$, the Lie algebra of linear polynomials on M, with basis $1, q, p$.
- $\mathfrak{sl}(2, \mathbf{R})$, the Lie algebra of order two homogeneous polynomials on M, with basis q^2, p^2, qp.

Taking all quadratic polynomials, we get a six-dimensional Lie algebra with basis elements $1, q, p, qp, q^2, p^2$. This is not the direct product of $\mathfrak{h}_3$ and $\mathfrak{sl}(2,\mathbf{R})$ since there are nonzero Poisson brackets

$$\begin{aligned} \{qp, q\} &= -q, \quad \{qp, p\} = \quad p \\ \{\frac{p^2}{2}, q\} &= -p, \quad \{\frac{q^2}{2}, p\} = \quad q \end{aligned} \tag{14.8}$$

These relations show that operating on a basis of linear functions on M by taking the Poisson bracket with something in $\mathfrak{sl}(2,\mathbf{R})$ (a quadratic function) provides a linear transformation on M^*. In this section we will see that this is a reflection of the fact that $SL(2,\mathbf{R})$ acts on the Heisenberg group H_3 by automorphisms.

Recall the definition 11.1 of the Heisenberg group H_3 as elements

$$(\begin{pmatrix} x \\ y \end{pmatrix}, z) \in \mathcal{M} \oplus \mathbf{R}$$

with the group law

$$(\begin{pmatrix} x \\ y \end{pmatrix}, z)(\begin{pmatrix} x' \\ y' \end{pmatrix}, z') = (\begin{pmatrix} x+x' \\ y+y' \end{pmatrix}, z + z' + \frac{1}{2}\Omega(\begin{pmatrix} x \\ y \end{pmatrix}, \begin{pmatrix} x' \\ y' \end{pmatrix}))$$

Elements $g \in SL(2,\mathbf{R})$ act on H_3 by

$$(\begin{pmatrix} x \\ y \end{pmatrix}, z) \to \phi_g((\begin{pmatrix} x \\ y \end{pmatrix}, z)) = (g \begin{pmatrix} x \\ y \end{pmatrix}, z) \tag{14.9}$$

This is an example of

Definition (Group automorphisms)**.** *If an action of elements g of a group G on a group H*

$$h \in H \to \phi_g(h) \in H$$

satisfies

$$\phi_g(h_1)\phi_g(h_2) = \phi_g(h_1 h_2)$$

for all $g \in G$ and $h_1, h_2 \in H$, the group G is said to act on H by automorphisms. Each map ϕ_g is an automorphism of H. Note that since ϕ_g is an action of G, we have $\phi_{g_1 g_2} = \phi_{g_1}\phi_{g_2}$.

Here $G = SL(2,\mathbf{R})$, $H = H_3$ and ϕ_g given above is an action by automorphisms since

$$\begin{aligned} \phi_g(\begin{pmatrix} x \\ y \end{pmatrix}, z)\phi_g(\begin{pmatrix} x' \\ y' \end{pmatrix}, z') =& (g \begin{pmatrix} x \\ y \end{pmatrix}, z)(g \begin{pmatrix} x' \\ y' \end{pmatrix}, z') \\ =& (g \begin{pmatrix} x+x' \\ y+y' \end{pmatrix}, z + z' + \frac{1}{2}\Omega(g \begin{pmatrix} x \\ y \end{pmatrix}, g \begin{pmatrix} x' \\ y' \end{pmatrix})) \\ =& (g \begin{pmatrix} x+x' \\ y+y' \end{pmatrix}, z + z' + \frac{1}{2}\Omega(\begin{pmatrix} x \\ y \end{pmatrix}, \begin{pmatrix} x' \\ y' \end{pmatrix})) \\ =& \phi_g((\begin{pmatrix} x \\ y \end{pmatrix}, z)(\begin{pmatrix} x' \\ y' \end{pmatrix}, z')) \end{aligned} \tag{14.10}$$

One can consider the Lie algebra $\mathfrak{h}_3$ instead of the group H_3, and there will again be an action of $SL(2,\mathbf{R})$ by automorphisms. Denoting elements $c_q q + c_p p + c$ of the Lie algebra $\mathfrak{h}_3 = \mathcal{M} \oplus \mathbf{R}$ (see section 12.2) by

$$(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c)$$

the Lie bracket is

$$[(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c), (\begin{pmatrix} c'_q \\ c'_p \end{pmatrix}, c')] = (\begin{pmatrix} 0 \\ 0 \end{pmatrix}, c_q c'_p - c_p c'_q) = (\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Omega(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, \begin{pmatrix} c'_q \\ c'_p \end{pmatrix}))$$

This Lie bracket just depends on Ω, so acting on $\mathcal{M}$ by $g \in SL(2,\mathbf{R})$ will give a map of $\mathfrak{h}_3$ to itself preserving the Lie bracket. More explicitly, an $SL(2,\mathbf{R})$ group element acts on the Lie algebra $\mathfrak{h}_3$ by

$$X = (\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c) \in \mathfrak{h}_3 \to \phi_g(X) = (g \begin{pmatrix} c_q \\ c_p \end{pmatrix}, c)$$

These ϕ_g are just the same maps ϕ_g that give automorphisms of the group structure of H_3 since the exponential map relating $\mathfrak{h}_3$ and H_3 in these coordinates is just the identification

$$(\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c) \leftrightarrow (\begin{pmatrix} x \\ y \end{pmatrix}, z)$$

The ϕ_g provide an example of

Definition (Lie algebra automorphisms)**.** *If an action of elements g of a group G on a Lie algebra $\mathfrak{h}$*

$$X \in \mathfrak{h} \to \phi_g(X) \in \mathfrak{h}$$

satisfies

$$[\phi_g(X), \phi_g(Y)] = \phi_g([X,Y])$$

for all $g \in G$ and $X, Y \in \mathfrak{h}$, the group is said to act on $\mathfrak{h}$ by automorphisms. The action of ϕ_g on $\mathfrak{h}$ is an automorphism of $\mathfrak{h}$ and we have the relation $\phi_{g_1 g_2} = \phi_{g_1}\phi_{g_2}$.

Two examples are

- In the case discussed above, $SL(2,\mathbf{R})$ acts on $\mathfrak{h}_3$ by automorphisms. With respect to the decomposition

  $$\mathfrak{h}_3 = \mathcal{M} \oplus \mathbf{R}$$

  $SL(2,\mathbf{R})$ acts just on $\mathcal{M}$, by linear transformations preserving Ω.

- If $\mathfrak{h}$ is the Lie algebra of a Lie group H, the adjoint representation $(Ad, \mathfrak{h})$ gives an action

  $$X \in \mathfrak{h} \to Ad(h)(X) = hXh^{-1}$$

of H on $\mathfrak{h}$ by automorphisms $\phi_h = Ad(h)$. For the case of the Heisenberg group, one can check that the adjoint representation of H_3 on $\mathfrak{h}_3$ leaves invariant the $\mathcal{M}$ component, only acting on the $\mathbf{R}$ component. Note that this is opposite behavior to the co-adjoint action of H_3 on $\mathfrak{h}_3^*$, which acts on M by translations (as in equation 13.7).

The $SL(2,\mathbf{R})$ action on $\mathfrak{h}_3$ by Lie algebra automorphisms has an infinitesimal version (i.e. for group elements infinitesimally close to the identity), an action of the Lie algebra of $SL(2,\mathbf{R})$ on $\mathfrak{h}_3$. This is defined for $L \in \mathfrak{sl}(2,\mathbf{R})$ and $X \in \mathfrak{h}_3$ by

$$L \cdot X = \frac{d}{dt}(e^{tL} \cdot X)_{|t=0} \tag{14.11}$$

Computing this, one finds

$$L \cdot (\begin{pmatrix} c_q \\ c_p \end{pmatrix}, c) = (L \begin{pmatrix} c_q \\ c_p \end{pmatrix}, 0) \tag{14.12}$$

so L acts on $\mathfrak{h}_3 = \mathcal{M} \oplus \mathbf{R}$ just by matrix multiplication on vectors in $\mathcal{M}$.

More generally, one has

Definition 14.1 (Lie algebra derivations)**.** *If an action of a Lie algebra $\mathfrak{g}$ on a Lie algebra $\mathfrak{h}$*

$$X \in \mathfrak{h} \to Z \cdot X \in \mathfrak{h}$$

satisfies

$$[Z \cdot X, Y] + [X, Z \cdot Y] = Z \cdot [X, Y]$$

for all $Z \in \mathfrak{g}$ and $X, Y \in \mathfrak{h}$, the Lie algebra $\mathfrak{g}$ is said to act on $\mathfrak{h}$ by derivations. The action of an element Z on $\mathfrak{h}$ is a derivation of $\mathfrak{h}$.

Given an action of a Lie group G on a Lie algebra $\mathfrak{h}$ by automorphisms, taking the derivative as in 14.11 gives an action of $\mathfrak{g}$ on $\mathfrak{h}$ by derivations since

$$Z \cdot [X, Y] = \frac{d}{dt}(\phi_{e^{tL}}([X, Y]))_{|t=0} = \frac{d}{dt}([\phi_{e^{tL}} X, \phi_{e^{tL}} Y])_{|t=0} = [Z \cdot X, Y] + [X, Z \cdot Y]$$

We will often refer to this action of $\mathfrak{g}$ on $\mathfrak{h}$ as the infinitesimal version of the action of G on $\mathfrak{h}$.

Two examples are

- The case above, where $\mathfrak{sl}(2,\mathbf{R})$ acts on $\mathfrak{h}_3$ by derivations.
- The adjoint representation of a Lie algebra $\mathfrak{h}$ on itself gives an action of $\mathfrak{h}$ on itself by derivations, with

$$X \in \mathfrak{h} \to Z \cdot X = ad(Z)(X) = [Z, X]$$

The Poisson brackets between degree two and degree one polynomials discussed at the beginning of this section give explicitly the action of $\mathfrak{sl}(2,\mathbf{R})$ on $\mathfrak{h}_3$ by derivations. For a general $L \in \mathfrak{sl}(2,\mathbf{R})$ and $c_q q + c_p p + c \in \mathfrak{h}_3$ we have

$$\{\mu_L, c_q q + c_p p + c\} = c'_q q + c'_p p, \quad \begin{pmatrix} c'_q \\ c'_p \end{pmatrix} = \begin{pmatrix} a c_q + b c_p \\ c c_q - a c_p \end{pmatrix} = L \begin{pmatrix} c_q \\ c_p \end{pmatrix} \tag{14.13}$$

(here μ_L is given by 14.5). We see that this is just the action of $\mathfrak{sl}(2,\mathbf{R})$ by derivations on $\mathfrak{h}_3$ of equation 14.12, the infinitesimal version of the action of $SL(2,\mathbf{R})$ on $\mathfrak{h}_3$ by automorphisms.

Note that in the larger Lie algebra of all polynomials on M of order two or less, the action of $\mathfrak{sl}(2,\mathbf{R})$ on $\mathfrak{h}_3$ by derivations is part of the adjoint action of the Lie algebra on itself, since it is given by the Poisson bracket (which is the Lie bracket), between order two and order one polynomials.

The generalization to the case of arbitrary d is

Theorem. *The $\mathfrak{sp}(2d,\mathbf{R})$ action on $\mathfrak{h}_{2d+1} = \mathcal{M} \oplus \mathbf{R}$ by derivations is*

$$L \cdot (\mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p} + c) = \{\mu_L, \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p} + c\} = \mathbf{c}'_q \cdot \mathbf{q} + \mathbf{c}'_p \cdot \mathbf{p} \qquad (14.14)$$

where

$$\begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix} = L \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}$$

or, equivalently (see section 4.1), on coordinate function basis vectors of $\mathcal{M}$ one has

$$\{\mu_L, \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}\} = L^T \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}$$

Proof. One can first prove 14.14 for the cases when only one of A, B, C is non-zero, then the general case follows by linearity. For instance, taking the special case

$$L = \begin{pmatrix} \mathbf{0} & B \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mu_L = \frac{1}{2}\mathbf{q} \cdot B\mathbf{q}$$

one can show that the action on coordinate functions (the basis vectors of $\mathcal{M}$) is

$$\{\frac{1}{2}\mathbf{q} \cdot B\mathbf{q}, \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}\} = L^T \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ B\mathbf{q} \end{pmatrix}$$

by computing

$$\begin{aligned} \{\frac{1}{2}\sum_{j,k} q_j B_{jk} q_k, p_l\} =& \frac{1}{2}\sum_{j,k} (q_j \{B_{jk} q_k, p_l\} + \{q_j B_{jk}, p_l\} q_k) \\ =& \frac{1}{2}(\sum_j q_j B_{jl} + \sum_k B_{lk} q_k) \\ =& \sum_j B_{lj} q_j \quad (\text{since } B = B^T) \end{aligned}$$

Repeating for A and C one finds that for general L one has

$$\{\mu_L, \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}\} = L^T \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}$$

Since an element in $\mathcal{M}$ can be written as

$$\begin{pmatrix} \mathbf{c}_q & \mathbf{c}_p \end{pmatrix} L^T \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = (L \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix})^T \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}$$

we have

$$\begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix} = L \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}$$

□

We can now prove theorem 14.1 as follows:

Proof.

$$L \to \mu_L$$

is clearly a vector space isomorphism of a space of matrices and one of quadratic polynomials. To show that it is a Lie algebra isomorphism, one can use the Jacobi identity for the Poisson bracket to show

$$\{\mu_L, \{\mu_{L'}, \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p}\}\} - \{\mu_{L'}, \{\mu_L, \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p}\}\} = \{\{\mu_L, \mu_{L'}\}, \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p}\}$$

The left-hand side of this equation is $\mathbf{c}''_q \cdot \mathbf{q} + \mathbf{c}''_p \cdot \mathbf{p}$, where

$$\begin{pmatrix} c''_{\mathbf{q}} \\ c''_{\mathbf{p}} \end{pmatrix} = (LL' - L'L) \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}$$

As a result, the right-hand side is the linear map given by

$$\{\mu_L, \mu_{L'}\} = \mu_{[L,L']}$$

□

14.3 For further reading

For more on symplectic groups and the isomorphism between $\mathfrak{sp}(2d, \mathbf{R})$ and homogeneous degree two polynomials, see chapter 14 of [25] or chapter 4 of [19]. Chapter 15 of [25] and chapter 1 of [19] discuss the action of the symplectic group on the Heisenberg group and Lie algebra by automorphisms.

Chapter 15

Quantization

Given any Hamiltonian classical mechanical system with phase space $\mathbf{R}^{2d}$, physics textbooks have a standard recipe for producing a quantum system, by a method known as "canonical quantization". We will see that for linear functions on phase space, this is just the construction we have already seen of a unitary representation Γ'_S of the Heisenberg Lie algebra, the Schrödinger representation, and the Stone-von Neumann theorem assures us that this is the unique such construction, up to unitary equivalence. We will also see that this recipe can only ever be partially successful, with the Schrödinger representation extending to give us a representation of a sub-algebra of the algebra of all functions on phase space (the polynomials of degree two and below), and a no-go theorem showing that this cannot be extended to a representation of the full infinite dimensional Lie algebra. Recipes for quantizing higher-order polynomials will always suffer from a lack of uniqueness, a phenomenon known to physicists as the existence of "operator ordering ambiguities".

In later chapters we will see that this quantization prescription does give unique quantum systems corresponding to some Hamiltonian systems (in particular the harmonic oscillator and the hydrogen atom), and does so in a manner that allows a description of the quantum system purely in terms of representation theory.

15.1 Canonical quantization

Very early on in the history of quantum mechanics, when Dirac first saw the Heisenberg commutation relations, he noticed an analogy with the Poisson bracket. One has

$$\{q, p\} = 1 \quad \text{and} \quad -\frac{i}{\hbar}[Q, P] = \mathbf{1}$$

as well as

$$\frac{df}{dt} = \{f, h\} \quad \text{and} \quad \frac{d}{dt}\mathcal{O}(t) = -\frac{i}{\hbar}[\mathcal{O}, H]$$

where the last of these equations is the equation for the time dependence of a Heisenberg picture observable $\mathcal{O}(t)$ in quantum mechanics. Dirac's suggestion was that given any classical Hamiltonian system, one could "quantize" it by finding a rule that associates to a function f on phase space a self-adjoint operator O_f (in particular $O_h = H$) acting on a state space $\mathcal{H}$ such that

$$O_{\{f,g\}} = -\frac{i}{\hbar}[O_f, O_g]$$

This is completely equivalent to asking for a unitary representation $(\pi', \mathcal{H})$ of the infinite dimensional Lie algebra of functions on phase space (with the Poisson bracket as Lie bracket). To see this, note that one can choose units for momentum p and position q such that $\hbar = 1$. Then, as usual getting a skew-adjoint Lie algebra representation operator by multiplying a self-adjoint operator by $-i$, setting

$$\pi'(f) = -iO_f$$

the Lie algebra homomorphism property

$$\pi'(\{f, g\}) = [\pi'(f), \pi'(g)]$$

corresponds to

$$-iO_{\{f,g\}} = [-iO_f, -iO_g] = -[O_f, O_g]$$

so one has Dirac's suggested relation.

Recall that the Heisenberg Lie algebra is isomorphic to the three-dimensional sub-algebra of functions on phase space given by linear combinations of the constant function, the function q and the function p. The Schrödinger representation Γ_S provides a unitary representation not of the Lie algebra of all functions on phase space, but of these polynomials of degree at most one, as follows

$$O_1 = \mathbf{1}, \quad O_q = Q, \quad O_p = P$$

so

$$\Gamma'_S(1) = -i\mathbf{1}, \quad \Gamma'_S(q) = -iQ = -iq, \quad \Gamma'_S(p) = -iP = -\frac{d}{dq}$$

Moving on to quadratic polynomials, these can also be quantized, as follows

$$O_{\frac{p^2}{2}} = \frac{P^2}{2}, \quad O_{\frac{q^2}{2}} = \frac{Q^2}{2}$$

For the function pq one can no longer just replace p by P and q by Q since the operators P and Q don't commute, and PQ or QP is not self-adjoint. What does work, satisfying all the conditions to give a Lie algebra homomorphism is

$$O_{pq} = \frac{1}{2}(PQ + QP)$$

This shows that the Schrödinger representation Γ'_S that was defined as a representation of the Heisenberg Lie algebra $\mathfrak{h}_3$ extends to a unitary Lie algebra

representation of a larger Lie algebra, that of all quadratic polynomials on phase space, a representation that we will continue to denote by Γ'_S and refer to as the Schrödinger representation. On a basis of homogeneous order two polynomials we have

$$\Gamma'_S(\frac{p^2}{2}) = -i\frac{P^2}{2} = \frac{i}{2}\frac{d^2}{dq^2}$$

$$\Gamma'_S(\frac{q^2}{2}) = -i\frac{Q^2}{2} = -\frac{i}{2}q^2$$

$$\Gamma'_S(pq) = \frac{-i}{2}(PQ + QP)$$

Restricting Γ'_S to just linear combinations of these homogeneous order two polynomials (which give the Lie algebra $\mathfrak{sl}(2,\mathbf{R})$, recall equation 14.4) we get a Lie algebra representation of $\mathfrak{sl}(2,\mathbf{R})$ called the metaplectic representation.

Restricted to the Heisenberg Lie algebra, the Schrödinger representation Γ'_S exponentiates to give a representation Γ_S of the corresponding Heisenberg Lie group (see 11.4). As an $\mathfrak{sl}(2,\mathbf{R})$ representation however, one can show that Γ'_S has the same sort of problem as the spinor representation of $\mathfrak{su}(2) = \mathfrak{so}(3)$, which was not a representation of $SO(3)$, but only of its double cover $SU(2) = Spin(3)$. To get a group representation, one must go to a double cover of the group $SL(2,\mathbf{R})$, which will be called the metaplectic group and denoted $Mp(2,\mathbf{R})$.

The source of the problem is the subgroup of $SL(2,\mathbf{R})$ generated by exponentiating the Lie algebra element

$$\frac{1}{2}(p^2 + q^2) \leftrightarrow E - F = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

When we study the Schrödinger representation using its action on the quantum harmonic oscillator state space $\mathcal{H}$ in chapter 20 we will see that the Hamiltonian is the operator

$$\frac{1}{2}(P^2 + Q^2)$$

and this has half-integer eigenvalues. As a result, trying to exponentiate Γ'_S gives a representation of $SL(2,\mathbf{R})$ only up to a sign, and one needs to go to the double cover $Mp(2,\mathbf{R})$ to get a true representation.

One should keep in mind though that, since $SL(2,\mathbf{R})$ acts non-trivially by automorphisms on H_3, elements of these two groups do not commute. The Schrödinger representation is a representation not of the product group, but of something called a "semi-direct product" which will be discussed in more detail in chapter 16.

15.2 The Groenewold-van Hove no-go theorem

If one wants to quantize polynomial functions on phase space of degree greater than two, it quickly becomes clear that the problem of "operator ordering ambiguities" is a significant one. Different prescriptions involving different ways

of ordering the P and Q operators lead to different O_f for the same function f, with physically different observables (although the differences involve the commutator of P and Q, so higher-order terms in $\hbar$).

When physicists first tried to find a consistent prescription for producing an operator O_f corresponding to a polynomial function on phase space of degree greater than two, they found that there was no possible way to do this consistent with the relation

$$O_{\{f,g\}} = -\frac{i}{\hbar}[O_f, O_g]$$

for polynomials of degree greater than two. Whatever method one devises for quantizing higher degree polynomials, it can only satisfy that relation to lowest order in $\hbar$, and there will be higher order corrections, which depend upon one's choice of quantization scheme. Equivalently, it is only for the six-dimensional Lie algebra of polynomials of degree up to two that the Schrödinger representation gives one a Lie algebra representation, and this cannot be consistently extended to a representation of a larger subalgebra of the functions on phase space. This problem is made precise by the following no-go theorem

Theorem (Groenewold-van Hove)**.** *There is no map $f \to O_f$ from polynomials on $\mathbf{R}^2$ to self-adjoint operators on $L^2(\mathbf{R})$ satisfying*

$$O_{\{f,g\}} = -\frac{i}{\hbar}[O_f, O_g]$$

and

$$O_p = P, \quad O_q = Q$$

for any Lie subalgebra of the functions on $\mathbf{R}^2$ larger than the subalgebra of polynomials of degree less than or equal to two.

Proof. For a detailed proof, see section 5.4 of [7], section 4.4 of [19], or chapter 16 of [25]. In outline, the proof begins by showing that taking Poisson brackets of polynomials of degree three leads to higher order polynomials, and that furthermore for degree three and above there will be no finite-dimensional subalgebras of polynomials of bounded degree. The assumptions of the theorem force certain specific operator ordering choices in degree three. These are then used to get a contradiction in degree four, using the fact that the same degree four polynomial has two different expressions as a Poisson bracket:

$$q^2p^2 = \frac{1}{3}\{q^2p, p^2q\} = \frac{1}{9}\{q^3, p^3\}$$

□

15.3 Canonical quantization in d dimensions

One can easily generalize the above to the case of d dimensions, with the Schrödinger representation Γ_S now giving a unitary representation of the Heisenberg group H_{2d+1}, with the corresponding Lie algebra representation given by

$$\Gamma'_S(q_j) = -iQ_j, \quad \Gamma'_S(p_j) = -iP_j$$

which satisfy the Heisenberg relations

$$[Q_j, P_k] = i\delta_{jk}$$

Generalizing to quadratic polynomials in the phase space coordinate functions, we have

$$\Gamma'_S(q_j q_k) = -iQ_j Q_k, \quad \Gamma'_S(p_j p_k) = -iP_j P_k, \quad \Gamma'_S(q_j p_k) = -\frac{i}{2}(Q_j P_k + P_k Q_j) \tag{15.1}$$

One can exponentiate these operators to get a representation on the same $\mathcal{H}$ of $Mp(2d, \mathbf{R})$, a double cover of the symplectic group $Sp(2d, \mathbf{R})$. This phenomenon will be examined carefully in later chapters, starting with chapter 18 and the calculation in section 18.2.1, followed by discussion in later chapters using a different (but unitarily equivalent) representation that appears in the quantization of the harmonic oscillator. The Groenewold-van Hove theorem implies that we cannot find a unitary representation of a larger group of canonical transformations extending this one on the Heisenberg and metaplectic groups.

15.4 Quantization and symmetries

The Schrödinger representation is thus a representation of the groups H_{2d+1} and $Mp(2d, \mathbf{R})$, with the Lie algebra representation providing observables corresponding to elements of the Lie algebras $\mathfrak{h}_{2d+1}$ (linear combinations of Q_j and P_k) and $\mathfrak{sp}(2d, \mathbf{R})$ (linear combinations of order-two combinations of Q_j and P_k). The observables that commute with the Hamiltonian operator H will make up a Lie algebra of symmetries of the quantum system, and will take energy eigenstates to energy eigenstates of the same energy. Some examples for the physical case of $d = 3$ are:

- The group $\mathbf{R}^3$ of translations in coordinate space is a subgroup of the Heisenberg group and has a Lie algebra representation as linear combinations of the operators $-iP_j$. If the Hamiltonian is position-independent, for instance the free particle case of

  $$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2)$$

  then the momentum operators correspond to symmetries. Note that the position operators Q_j do not commute with this Hamiltonian, and so do not correspond to a symmetry of the dynamics.

- The group $SO(3)$ of spatial rotations is a subgroup of $Sp(6, \mathbf{R})$ and the operators

  $$-i(Q_2 P_3 - Q_3 P_2), \quad -i(Q_3 P_1 - Q_1 P_3, \quad -i(Q_1 P_2 - Q_2 P_1)$$

  are a basis for a Lie algebra representation of $\mathfrak{so}(3)$. These are the same operators that were studied in chapter 8 under the name $\rho'(l_j)$. They will

be symmetries of rotationally invariant Hamiltonians, for instance the free particle as above, or the particle in a potential

$$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2) + V(Q_1, Q_2, Q_3)$$

when the potential only depends on the combination $Q_1^2 + Q_2^2 + Q_3^2$.

15.5 More general notions of quantization

The definition given here of quantization using the Schrödinger representation of $\mathfrak{h}_{2d+1}$ only allows the construction of a quantum system based on a classical phase space for the linear case of $M = \mathbf{R}^{2d}$. For other sorts of classical systems one needs other methods to get a corresponding quantum system. One possible approach is the path integral method, which starts with a choice of configuration space and Lagrangian, and will be discussed in chapter 32.

Digression. *The name "geometric quantization" refers to attempt to generalize quantization to the case of any symplectic manifold M, starting with the idea of prequantization (see equation 13.6). This gives a representation of the Lie algebra of functions on M on a space of sections of a line bundle with connection ∇, with ∇ a connection with curvature ω, where ω is the symplectic form on M. One then has to deal with two problems*

- *The space of all functions on M is far too big, allowing states localized in both position and coordinate variables in the case $M = \mathbf{R}^{2d}$. One needs some way to cut down this space to something like a space of functions depending on only half the variables (e.g. just the positions, or just the momenta). This requires finding an appropriate choice of a so-called "polarization" that will accomplish this.*

- *To get an inner product on the space of states, one needs to introduce a twist by a "square root" of a certain line bundle, something called the "metaplectic correction".*

For more details, see for instance [29] or [75].

Geometric quantization focuses on finding an appropriate state space. Another general method, the method of "deformation quantization" focuses instead on the algebra of operators, with a quantization given by finding an appropriate non-commutative algebra that is in some sense a deformation of a commutative algebra of functions. To first order the deformation in the product law is determined by the Poisson bracket.

Starting with any Lie algebra $\mathfrak{g}$, one can in principle use 12.4 to get a Poisson bracket on functions on the dual space $\mathfrak{g}^*$, and then take the quantization of this to be the algebra of operators known as the universal enveloping algebra $U(\mathfrak{g})$. This will in general have many different irreducible representations and corresponding possible quantum state spaces. The co-adjoint orbit philosophy posits an approximate matching between orbits in $\mathfrak{g}^*$ under the dual of the

adjoint representation (which are symplectic manifolds) and irreducible representations. Geometric quantization provides one possible method for trying to associate representations to orbits. For more details, see [35].

None of the general methods of quantization is fully satisfactory, with each running into problems in certain cases, or not providing a construction with all the properties that one would want.

15.6 For further reading

Just about all quantum mechanics textbooks contain some version of the discussion here of canonical quantization starting with classical mechanical systems in Hamiltonian form. For discussions of quantization from the point of view of representation theory, see [7] and chapters 14-16 of [25]. For a detailed discussion of the Heisenberg group and Lie algebra, together with their representation theory, also see chapter 2 of [35].

Chapter 16

Semi-direct Products

The theory of a free particle depends crucially on the group of symmetries of three-dimensional space, a group which includes a subgroup $\mathbf{R}^3$ of spatial translations, and a subgroup $SO(3)$ of rotations. The second subgroup acts non-trivially on the first, since the direction of a translation is rotated by an element of $SO(3)$. In later chapters dealing with special relativity, these symmetry groups get enlarged to include a fourth dimension, time, and the theory of a free particle will again be determined by these symmetry groups. In chapters 13 and 14 we saw that there are two groups acting on phase space: the Heisenberg group H_{2d+1} and the symplectic group $Sp(2d, \mathbf{R})$. In this situation also, the second group acts non-trivially on the first by automorphisms (see 14.10).

This situation of two groups, with one acting on the other by automorphisms, allows one to construct a new sort of product of the two groups, called the semi-direct product, and this will be the topic for this chapter. We'll also begin the study of representations of such groups, outlining what happens when the first group is commutative. Chapter 18 will describe how the Schrödinger representation of H_{2d+1} extends to become a representation (up to a sign ambiguity) of the semi-direct product of H_{2d+1} and $Sp(2d, \mathbf{R})$. In chapter 17 we'll consider the cases of the semi-direct product of translations and rotations in two and three dimensions, and there see how the irreducible representations are provided by the quantum state space of a free particle.

16.1 An example: the Euclidean group

Given two groups G' and G'', one can form the product group by taking pairs of elements $(g', g'') \in G' \times G''$. However, when the two groups act on the same space, but elements of G' and G'' don't commute, a different sort of product group is needed. As an example, consider the case of pairs $(\mathbf{a}_2, R_2)$ of elements $\mathbf{a}_2 \in \mathbf{R}^3$ and $R_2 \in SO(3)$, acting on $\mathbf{R}^3$ by translation and rotation

$$\mathbf{v} \to (\mathbf{a}_2, R_2) \cdot \mathbf{v} = \mathbf{a}_2 + R_2 \mathbf{v}$$

If we then act on the result with $(\mathbf{a}_1, R_1)$ we get

$$(\mathbf{a}_1, R_1) \cdot ((\mathbf{a}_2, R_2) \cdot \mathbf{v}) = (\mathbf{a}_1, R_1) \cdot (\mathbf{a}_2 + R_2\mathbf{v}) = \mathbf{a}_1 + R_1\mathbf{a}_2 + R_1R_2\mathbf{v}$$

Note that this is not what we would get if we took the product group law on $\mathbf{R}^3 \times SO(3)$, since then the action of $(\mathbf{a}_1, R_1)(\mathbf{a}_2, R_2)$ on $\mathbf{R}^3$ would be

$$\mathbf{v} \to \mathbf{a}_1 + \mathbf{a}_2 + R_1R_2\mathbf{v}$$

To get the correct group action on $\mathbf{R}^3$, we need to take $\mathbf{R}^3 \times SO(3)$ not with the product group law, but instead with the group law

$$(\mathbf{a}_1, R_1)(\mathbf{a}_2, R_2) = (\mathbf{a}_1 + R_1\mathbf{a}_2, R_1R_2)$$

This group law differs from the standard product law, by a term $R_1\mathbf{a}_2$, which is the result of $R_1 \in SO(3)$ acting non-trivially on $\mathbf{a}_2 \in \mathbf{R}^3$. We will denote the set $\mathbf{R}^3 \times SO(3)$ with this group law by

$$\mathbf{R}^3 \rtimes SO(3)$$

This is the group of transformations of $\mathbf{R}^3$ preserving the standard inner product.

The same construction works in arbitrary dimensions, where one has

Definition (Euclidean group)**.** *The Euclidean group $E(d)$ (sometimes written $ISO(d)$ for "inhomogeneous" rotation group) in dimension d is the product of the translation and rotation groups of $\mathbf{R}^d$ as a set, with multiplication law*

$$(\mathbf{a}_1, R_1)(\mathbf{a}_2, R_2) = (\mathbf{a}_1 + R_1\mathbf{a}_2, R_1R_2)$$

(where $\mathbf{a}_j \in \mathbf{R}^d, R_j \in SO(d)$) and can be denoted by

$$\mathbf{R}^d \rtimes SO(d)$$

$E(d)$ can also be written as a matrix group, taking it to be the subgroup of $GL(d+1, \mathbf{R})$ of matrices of the form (R is a d by d orthogonal matrix, $\mathbf{a}$ a d-dimensional column vector)

$$\begin{pmatrix} R & \mathbf{a} \\ \mathbf{0} & 1 \end{pmatrix}$$

One gets the multiplication law for $E(d)$ from matrix multiplication since

$$\begin{pmatrix} R_1 & \mathbf{a}_1 \\ \mathbf{0} & 1 \end{pmatrix} \begin{pmatrix} R_2 & \mathbf{a}_2 \\ \mathbf{0} & 1 \end{pmatrix} = \begin{pmatrix} R_1R_2 & \mathbf{a}_1 + R_1\mathbf{a}_2 \\ \mathbf{0} & 1 \end{pmatrix}$$

16.2 Semi-direct product groups

The Euclidean group example of the previous section can be generalized to the following

Definition (Semi-direct product group)**.** *Given a group K, a group N, and an action ϕ of K on N by automorphisms*

$$\phi_k : n \in N \to \phi_k(n) \in N$$

the semi-direct product $N \rtimes K$ is the set of pairs $(n, k) \in N \times K$ with group law

$$(n_1, k_1)(n_2, k_2) = (n_1 \phi_{k_1}(n_2), k_1 k_2)$$

One can easily check that this satisfies the group axioms. The inverse is

$$(n, k)^{-1} = (\phi_{k^{-1}}(n^{-1}), k^{-1})$$

Checking associativity, one finds

$$\begin{aligned}((n_1, k_1)(n_2, k_2))(n_3, k_3) =& (n_1 \phi_{k_1}(n_2), k_1 k_2)(n_3, k_3) \\ =& (n_1 \phi_{k_1}(n_2) \phi_{k_1 k_2}(n_3), k_1 k_2 k_3) \\ =& (n_1 \phi_{k_1}(n_2) \phi_{k_1}(\phi_{k_2}(n_3)), k_1 k_2 k_3) \\ =& (n_1 \phi_{k_1}(n_2 \phi_{k_2}(n_3)), k_1 k_2, k_3) \\ =& (n_1, k_1)(n_2 \phi_{k_2}(n_3), k_2 k_3) \\ =& (n_1, k_1)((n_2, k_2)(n_3, k_3))\end{aligned}$$

The notation $N \rtimes K$ for this construction has the weakness of not explicitly indicating the automorphism ϕ which it depends on. There may be multiple possible choices for ϕ, and these will always include the trivial choice $\phi_k = 1$ for all $k \in K$, which will give the standard product of groups.

Digression. *For those familiar with the notion of a normal subgroup, N is a normal subgroup of $N \rtimes K$. A standard notation for "N is a normal subgroup of G" is $N \lhd G$. The symbol $N \rtimes K$ is supposed to be a mixture of the $\times$ and $\lhd$ symbols (note that some authors define it to point in the other direction).*

The Euclidean group $E(d)$ is an example with $N = \mathbf{R}^d, K = SO(d)$. For $\mathbf{a} \in \mathbf{R}^d, R \in SO(d)$ one has

$$\phi_R(\mathbf{a}) = R\mathbf{a}$$

In chapter 39 we will see another important example, the Poincaré group which generalizes $E(3)$ to include a time dimension, treating space and time according to the principles of special relativity.

The most important example for quantum theory is

Definition (Jacobi group)**.** *The Jacobi group in d dimensions is the semi-direct product group*

$$G^J(d) = H_{2d+1} \rtimes Sp(2d, \mathbf{R})$$

If we write elements of the group as

$$((\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c), k)$$

where $k \in Sp(2d, \mathbf{R})$, then the automorphism ϕ_k that defines the Jacobi group is given by

$$\phi_k((\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c)) = (k \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c) \tag{16.1}$$

Note that the Euclidean group $E(d)$ is a subgroup of the Jacobi group $G^J(d)$, the subgroup of elements of the form

$$((\begin{pmatrix} \mathbf{0} \\ \mathbf{c}_p \end{pmatrix}, 0), \begin{pmatrix} R & \mathbf{0} \\ \mathbf{0} & R \end{pmatrix})$$

where $R \in SO(d)$. The

$$(\begin{pmatrix} \mathbf{0} \\ \mathbf{c}_p \end{pmatrix}, 0) \subset H_{2d+1}$$

make up the group $\mathbf{R}^d$ of translations in the q_j coordinates, and the

$$k = \begin{pmatrix} R & \mathbf{0} \\ \mathbf{0} & R \end{pmatrix} \subset Sp(2d, \mathbf{R})$$

are symplectic transformations since

$$\begin{aligned} \Omega(k \begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, k \begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix}) =& R\mathbf{c}_q \cdot R\mathbf{c}'_p - R\mathbf{c}_p \cdot R\mathbf{c}'_q \\ =& \mathbf{c}_q \cdot \mathbf{c}'_p - \mathbf{c}_p \cdot \mathbf{c}'_q \\ =& \Omega(\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, \begin{pmatrix} \mathbf{c}'_q \\ \mathbf{c}'_p \end{pmatrix}) \end{aligned}$$

(R is orthogonal so preserves dot products).

16.3 Semi-direct product Lie algebras

We have seen that semi-direct product Lie groups can be constructed by taking a product $N \times K$ of Lie groups as a set, and imposing a group multiplication law that uses an action of K on N by automorphisms. In a similar manner, one can construct semi-direct product Lie algebras $\mathfrak{n} \rtimes \mathfrak{k}$ by taking the direct sum of $\mathfrak{n}$ and $\mathfrak{k}$ as vector spaces, and defining a Lie bracket that uses an action of $\mathfrak{n}$ on $\mathfrak{k}$ by derivations (the infinitesimal version of automorphisms, see definition 14.1).

Considering first the example $E(d) = \mathbf{R}^d \rtimes SO(d)$, recall that elements $E(d)$ can be written in the form

$$\begin{pmatrix} R & \mathbf{a} \\ \mathbf{0} & 1 \end{pmatrix}$$

for $R \in SO(d)$ and $\mathbf{a} \in \mathbf{R}^d$. The tangent space to this group at the identity will be given by matrices of the form

$$\begin{pmatrix} X & \mathbf{a} \\ \mathbf{0} & 0 \end{pmatrix}$$

where X is an antisymmetric d by d matrix and $\mathbf{a} \in \mathbf{R}^d$. Exponentiating such matrices will give elements of $E(d)$.

The Lie bracket is then given by the matrix commutator, so

$$[\begin{pmatrix} X_1 & \mathbf{a}_1 \\ \mathbf{0} & 0 \end{pmatrix}, \begin{pmatrix} X_2 & \mathbf{a}_2 \\ \mathbf{0} & 0 \end{pmatrix}] = \begin{pmatrix} [X_1, X_2] & X_1\mathbf{a}_2 - X_2\mathbf{a}_1 \\ \mathbf{0} & 0 \end{pmatrix} \tag{16.2}$$

So the Lie algebra of $E(d)$ will be given by taking the sum of $\mathbf{R}^d$ (the Lie algebra of $\mathbf{R}^d$) and $\mathfrak{so}(d)$, with elements pairs $(\mathbf{a}, X)$ with $\mathbf{a} \in \mathbf{R}^d$ and X an antisymmetric d by d matrix. The infinitesimal version of the rotation action of $SO(d)$ on $\mathbf{R}^d$ by automorphisms

$$\phi_R(a) = Ra$$

is

$$\frac{d}{dt}\phi_{e^{tX}}(\mathbf{a})_{|t=0} = \frac{d}{dt}(e^{tX}\mathbf{a})_{|t=0} = X\mathbf{a}$$

Just in terms of such pairs, the Lie bracket can be written

$$[(\mathbf{a}_1, X_1), (\mathbf{a}_2, X_2)] = (X_1\mathbf{a}_2 - X_2\mathbf{a}_1, [X_1, X_2])$$

We can define in general

Definition (Semi-direct product Lie algebra)**.** *Given Lie algebras $\mathfrak{k}$ and $\mathfrak{n}$, and an action of elements $Y \in \mathfrak{k}$ on $\mathfrak{n}$ by derivations*

$$X \in \mathfrak{n} \to Y \cdot X \in \mathfrak{n}$$

the semi-direct product $\mathfrak{n} \rtimes \mathfrak{k}$ is the set of pairs $(X, Y) \in \mathfrak{n} \oplus \mathfrak{k}$ with the Lie bracket

$$[(X_1, Y_1), (X_2, Y_2)] = ([X_1, X_2] + Y_1 \cdot X_2 - Y_2 \cdot X_1, [Y_1, Y_2])$$

One can easily see that in the special case of the Lie algebra of $E(d)$ this agrees with the construction above.

In section 14.1.2 we studied the Lie algebra of all polynomials of degree at most two in d-dimensional phase space coordinates q_j, p_j, with the Poisson bracket as Lie bracket. There we found two Lie subalgebras, the degree zero and one polynomials (isomorphic to $\mathfrak{h}_{2d+1}$), and the homogeneous degree two polynomials (isomorphic to $\mathfrak{sp}(2d, \mathbf{R})$) with the second subalgebra acting on the first by derivations as in equation 14.14.

Recall from chapter 14 that elements of this Lie algebra can also be written as pairs

$$((\begin{pmatrix} \mathbf{c}_q \\ \mathbf{c}_p \end{pmatrix}, c), L)$$

of elements in $\mathfrak{h}_{2d+1}$ and $\mathfrak{sp}(2d, \mathbf{R})$, with this pair corresponding to the polynomial

$$\mu_L + \mathbf{c}_q \cdot \mathbf{q} + \mathbf{c}_p \cdot \mathbf{p} + c$$

In terms of such pairs, the Lie bracket is given by

$$[(\begin{pmatrix}\mathbf{c}_q\\ \mathbf{c}_p\end{pmatrix}, c), L), (\begin{pmatrix}\mathbf{c}'_q\\ \mathbf{c}'_p\end{pmatrix}, c), L')] = ((L\begin{pmatrix}\mathbf{c}'_q\\ \mathbf{c}'_p\end{pmatrix} - L'\begin{pmatrix}\mathbf{c}_q\\ \mathbf{c}_p\end{pmatrix}, \Omega(\begin{pmatrix}\mathbf{c}_q\\ \mathbf{c}_p\end{pmatrix}, \begin{pmatrix}\mathbf{c}'_q\\ \mathbf{c}'_p\end{pmatrix})), [L, L'])$$

which satisfies the definition above.

So one example of a semi-direct product Lie algebra is

$$\mathfrak{h}_{2d+1} \rtimes \mathfrak{sp}(2d, \mathbf{R})$$

and from the discussion in chapter 14.2 one can see that this is the Lie algebra of the semi-direct product group

$$G^J(d) = H_{2d+1} \rtimes Sp(2d, \mathbf{R})$$

.

The Lie algebra of $E(d)$ will be a sub-Lie algebra of this, consisting of elements of the form

$$((\begin{pmatrix}\mathbf{0}\\ \mathbf{c}_p\end{pmatrix}, 0), \begin{pmatrix}X & \mathbf{0}\\ \mathbf{0} & X\end{pmatrix})$$

where X is an antisymmetric d by d matrix.

Digression. *Just as $E(d)$ can be identified with a group of $d+1$ by $d+1$ matrices, the Jacobi group $G_J(d)$ is also a matrix group and one can in principle work with it and its Lie algebra using usual matrix methods. The construction is slightly complicated and represents elements of $G_J(d)$ as matrices in $Sp(2d+1, \mathbf{R})$. See section 8.5 of [8] for details of the $d = 1$ case.*

16.4 For further reading

Semi-direct products are not commonly covered in detail in either physics or mathematics textbooks, with the exception of the case of the Poincaré group of special relativity, which will be discussed in chapter 39. Some textbooks that do cover the subject include section 3.8 of [59], chapter 6 of [26] and [8].

Chapter 17

The Quantum Free Particle as a Representation of the Euclidean Group

In this chapter we will explicitly construct unitary representations of the Euclidean groups $E(2)$ and $E(3)$ of spatial symmetries in two and three dimensions. These groups commute with the Hamiltonian of the free particle, and their irreducible representations will be given just by the quantum state space of a free particle (of fixed energy) in either two ot three spatial dimensions. The momentum operators P_j will provide the infinitesimal action of translations on the state space, while angular momentum operators L_k will provide the infinitesimal rotation action (there will be only one of these in two dimensions, three in three dimensions).

The Hamiltonian of the free particle is proportional to the operator $|\mathbf{P}|^2$. This is a quadratic operator that commutes with the action of all the elements of the Lie algebra of the Euclidean group, and so is a Casimir operator playing an analogous role to that of the $SO(3)$ Casimir operator $|\mathbf{L}|^2$ of section 8.4. Irreducible representations will be labeled by the eigenvalue of this operator, which in this case will be proportional to the energy. In the Schrödinger representation where the P_j are differentiation operators, this will be a second-order differential operator, and the eigenvalue equation will be a second-order differential equation (the time-independent Schrödinger equation).

Using the Fourier transform, the space of solutions of the Schrödinger equation of fixed energy becomes something much easier to analyze, the space of functions on momentum space supported only on the subspace of momenta of a fixed length. In the case of $E(2)$ this is just a circle, whereas for $E(3)$ it is a sphere. In both cases, for each radius one gets an irreducible representation.

In the case of $E(3)$ other classes of irreducible representations can be constructed. This can be done by introducing multi-component wavefunctions, with a new action of the rotation group $SO(3)$. A second Casimir operator is

available in this case, and irreducible representations are eigenfunctions of this operator in the space of wavefunctions of fixed energy. The eigenvalue of the second Casimir operator turns out to be an integer, known to physicists as the "helicity".

17.1 The quantum free particle and representations of $E(2)$

We'll begin with the case of two spatial dimensions, partly for simplicity, partly because physical systems that are translationally invariant in one direction can often be treated as effectively two dimensional. A basis for the Lie algebra of $E(2)$ is given by the functions

$$l = q_1 p_2 - q_2 p_1, \quad p_1, \quad p_2$$

on the $d = 2$ phase space $M = \mathbf{R}^4$. The non-zero Lie bracket relations are given by the Poisson brackets

$$\{l, p_1\} = p_2, \quad \{l, p_2\} = -p_1$$

and there is an isomorphism of this Lie algebra with a matrix Lie algebra of 3 by 3 matrices given by

$$l \leftrightarrow \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad p_1 \leftrightarrow \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad p_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

Writing this Lie algebra in terms of linear and quadratic functions on the phase space shows that it can be realized as a sub-Lie algebra of the Jacobi Lie algebra $\mathfrak{g}^J(2)$. Quantization via the Schrödinger representation Γ'_S then provides a unitary representation of the Lie algebra of $E(2)$ on the state space $\mathcal{H}$ of functions of the position variables q_1, q_2, in terms of operators

$$\Gamma'_S(p_1) = -iP_1 = -\frac{\partial}{\partial q_1}, \quad \Gamma'_S(p_2) = -iP_1 = -\frac{\partial}{\partial q_2} \tag{17.1}$$

and

$$\Gamma'_S(l) = -iL = -i(Q_1 P_2 - Q_2 P_1) = -(q_1 \frac{\partial}{\partial q_2} - q_2 \frac{\partial}{\partial q_1}) \tag{17.2}$$

The Hamiltonian operator for the free particle is

$$H = \frac{1}{2m}(P_1^2 + P_2^2) = -\frac{1}{2m}(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2})$$

and solutions to the Schrödinger equation can be found by solving the eigenvalue equation

$$H\psi(q_1, q_2) = -\frac{1}{2m}(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2})\psi(q_1, q_2) = E\psi(q_1, q_2)$$

The operators L, P_1, P_2 commute with H and so provide a representation of the Lie algebra of $E(2)$ on the space of wavefunctions of energy E.

This construction of irreducible representations of $E(2)$ is similar in spirit to the construction of irreducible representations of $SO(3)$ in section 8.4. There the Casimir operator L^2 commuted with the $SO(3)$ action, and gave a differential operator on functions on the sphere whose eigenfunctions were spaces of dimension $2l+1$ with eigenvalue $l(l+1)$, for l non-negative and integral. For $E(2)$ the quadratic function $p_1^2 + p_2^2$ Poisson commutes with l, p_1, p_2. After quantization,

$$|\mathbf{P}|^2 = P_1^2 + P_2^2$$

is a second-order differential operator which commutes with L, P_1, P_2. This operator has infinite-dimensional eigenspaces that each carry an irreducible representation of $E(2)$. They are characterized by a non-negative eigenvalue that has physical interpretation as $2mE$ where m, E are the mass and energy of a free quantum particle moving in two spatial dimensions.

Recall from our discussion of the free particle in chapter 10 that

$$\psi_{\mathbf{p}}(\mathbf{q}) = e^{i\mathbf{p}\cdot\mathbf{q}} = |\mathbf{p}\rangle$$

is a solution of the time-independent Schrödinger equation with energy

$$E = \frac{|\mathbf{p}|^2}{2m} > 0$$

and such $|\mathbf{p}\rangle$ give a sort of continuous basis of $\mathcal{H}$, even though these are not square-integrable functions. The formalism for working with them uses distributions and the orthonormality relation

$$\langle \mathbf{p}|\mathbf{p}'\rangle = \delta(\mathbf{p}-\mathbf{p}')$$

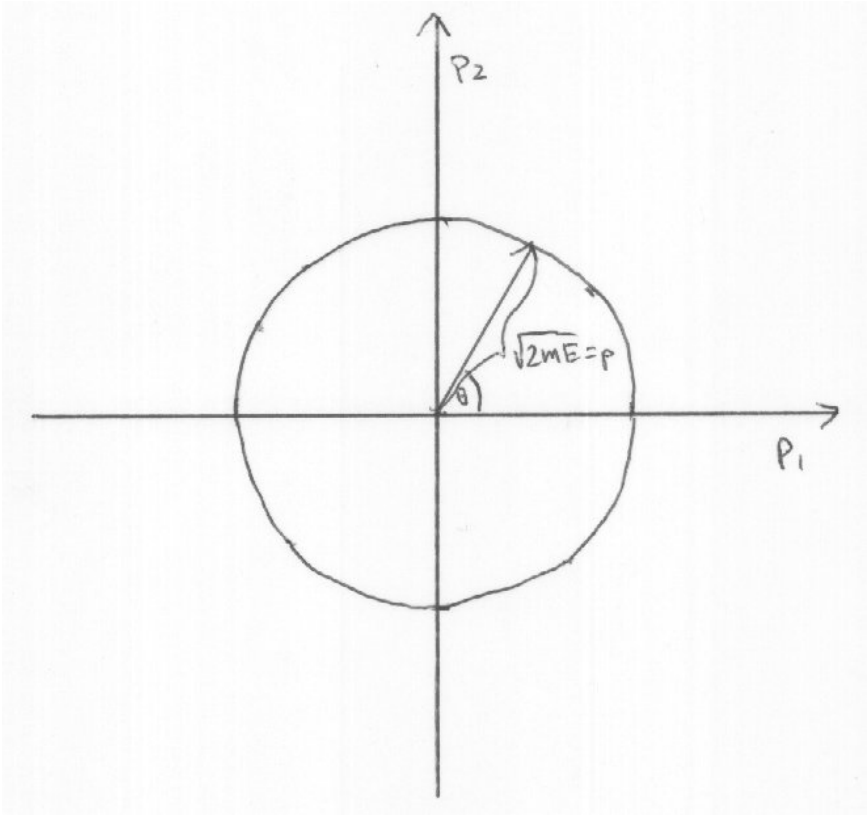
An arbitrary $\psi(\mathbf{q}) \in \mathcal{H}$ can be written as a continuous linear combination of the $|\mathbf{p}\rangle$, i.e. as an inverse Fourier transform of a function $\widetilde{\psi}(\mathbf{p})$ on momentum space as

$$\psi(\mathbf{q}) = \frac{1}{2\pi}\iint e^{i\mathbf{p}\cdot\mathbf{q}}\widetilde{\psi}(\mathbf{p})d^2\mathbf{p}$$

In momentum space the time-independent Schrödinger equation becomes

$$(\frac{|\mathbf{p}|^2}{2m} - E)\widetilde{\psi}(\mathbf{p}) = 0$$

so we get a solution for any choice of $\widetilde{\psi}(\mathbf{p})$ that is non-zero only on the circle $|\mathbf{p}|^2 = 2mE$ (we won't try to characterize which class of such functions to consider, which would determine which class of functions solving the Schrödinger equation we end up with after Fourier transform).



Going to polar coordinates $\mathbf{p} = (p\cos\theta, p\sin\theta)$, the space of solutions to the time-independent Schrödinger equation at energy E is given by $\widetilde{\psi}(\mathbf{p})$ of the form

$$\widetilde{\psi}(\mathbf{p}) = \widetilde{\psi}_E(\theta)\delta(p^2 - 2mE)$$

To put this delta-function in a more useful form, note that for $p \approx \sqrt{2mE}$ one has the linear approximation

$$p^2 - 2mE \approx \frac{1}{2\sqrt{2mE}}(p - \sqrt{2mE})$$

so one has the equality of distributions

$$\delta(p^2 - 2mE) = \frac{1}{2\sqrt{2mE}}\delta(p - \sqrt{2mE})$$

It is this space of functions $\widetilde{\psi}_E(\theta)$ of functions on the circle of radius $\sqrt{2mE}$ that will provide an infinite-dimensional representation of the group $E(2)$, one that turns out to be irreducible, although we will not show that here. The

position space wavefunction corresponding to $\widetilde{\psi}_E(\theta)$ will be

$$\begin{aligned}\psi(\mathbf{q}) =& \frac{1}{2\pi}\iint e^{i\mathbf{p}\cdot\mathbf{q}}\widetilde{\psi}_E(\theta)\delta(p^2-2mE)pdpd\theta \\ =& \frac{1}{2\pi}\iint e^{i\mathbf{p}\cdot\mathbf{q}}\widetilde{\psi}_E(\theta)\frac{1}{2\sqrt{2mE}}\delta(p-\sqrt{2mE})pdpd\theta \\ =& \frac{1}{4\pi}\int_0^{2\pi} e^{i\sqrt{2mE}(q_1\cos\theta+q_2\sin\theta)}\widetilde{\psi}_E(\theta)d\theta\end{aligned}$$

Functions $\widetilde{\psi}_E(\theta)$ with simple behavior in θ will correspond to wavefunctions with more complicated behavior in position space. For instance, taking $\widetilde{\psi}_E(\theta) = e^{-in\theta}$ one finds that the wavefunction along the q_2 direction is given by

$$\begin{aligned}\psi(0,q) =& \frac{1}{4\pi}\int_0^{2\pi} e^{i\sqrt{2mE}(q\sin\theta)}e^{-in\theta}d\theta \\ =& \frac{1}{2}J_n(\sqrt{2mE}q)\end{aligned}$$

where J_n is the n'th Bessel function.

Equations 17.1 and 17.2 give the representation of the Lie algebra of $E(2)$ on wavefunctions $\psi(\mathbf{q})$. The representation of this Lie algebra on the $\widetilde{\psi}_E(\theta)$ is just given by the Fourier transform, and we'll denote this $\widetilde{\Gamma}'_S$. Using the formula for the Fourier transform we find that

$$\widetilde{\Gamma}'_S(p_1) = -\widetilde{\frac{\partial}{\partial q_1}} = -ip_1 = -i\sqrt{2mE}\cos\theta$$

$$\widetilde{\Gamma}'_S(p_2) = -\widetilde{\frac{\partial}{\partial q_2}} = -ip_2 = -i\sqrt{2mE}\sin\theta$$

are multiplication operators and, taking the Fourier transform of 17.2 gives the differentiation operator

$$\begin{aligned}\widetilde{\Gamma}'_S(l) =& -(p_1\frac{\partial}{\partial p_2} - p_2\frac{\partial}{\partial p_1}) \\ =& -\frac{\partial}{\partial\theta}\end{aligned}$$

(use integration by parts to show $q_j = i\frac{\partial}{\partial p_j}$ and thus the first equality, then the chain rule for functions $f(p_1(\theta), p_2(\theta))$ for the second).

This construction of a representation of $E(2)$ starting with the Schrödinger representation gives the same result as starting with the action of $E(2)$ on configuration space, and taking the induced action on functions on $\mathbf{R}^2$ (the wavefunctions). To see this, note that $E(2)$ has elements $(\mathbf{a}, R(\phi))$ which can be written as a product $(\mathbf{a}, R(\phi)) = (\mathbf{a}, \mathbf{1})(\mathbf{0}, R(\phi))$ or, in terms of matrices

$$\begin{pmatrix}\cos\phi & -\sin\phi & a_1 \\ \sin\phi & \cos\phi & a_2 \\ 0 & 0 & 1\end{pmatrix} = \begin{pmatrix}1 & 0 & a_1 \\ 0 & 1 & a_2 \\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1\end{pmatrix}$$

The group has a unitary representation

$$(\mathbf{a}, R(\phi)) \to u(\mathbf{a}, R(\phi))$$

on the position space wavefunctions $\psi(\mathbf{q})$, given by the induced action on functions from the action of $E(2)$ on position space $\mathbf{R}^2$

$$\begin{aligned} u(\mathbf{a}, R(\phi))\psi(\mathbf{q}) =& \psi((\mathbf{a}, R(\phi))^{-1} \cdot \mathbf{q}) \\ =& = \psi((-R(-\phi)\mathbf{a}, R(-\phi)) \cdot \mathbf{q}) \\ =& \psi(R(-\phi)(\mathbf{q} - \mathbf{a})) \end{aligned}$$

This is just the Schrödinger representation Γ_S of the Jacobi group $G^J(2)$, restricted to the subgroup $E(2)$ of transformations of phase space that are translations in $\mathbf{q}$ and rotations in both $\mathbf{q}$ and $\mathbf{p}$ vectors, preserving their inner product (and thus the symplectic form). One can see this by considering the action of translations as the exponential of the Lie algebra representation operators $\Gamma'_S(p_j) = -iP_j$

$$u(\mathbf{a}, \mathbf{1})\psi(\mathbf{q}) = e^{-i(a_1 P_1 + a_2 P_2)}\psi(\mathbf{q}) = \psi(\mathbf{q} - \mathbf{a})$$

and the action of rotations as the exponential of the $\Gamma'_S(l) = -iL$

$$u(0, R(\phi))\psi(\mathbf{q}) = e^{-i\phi L}\psi(\mathbf{q}) = \psi(R(-\phi)\mathbf{q})$$

One also has a Fourier-transformed version $\widetilde{u}$ of this representation, with translations now acting by multiplication operators on the $\widetilde{\psi}_E$

$$\widetilde{u}(\mathbf{a}, \mathbf{1})\widetilde{\psi}_E(\theta) = e^{-i(\mathbf{a}\cdot\mathbf{p})}\widetilde{\psi}_E(\theta) = e^{-i\sqrt{2mE}(a_1 \cos\theta + a_2 \sin\theta)}\widetilde{\psi}_E(\theta) \tag{17.3}$$

and rotations acting by rotation in momentum space

$$\widetilde{u}(\mathbf{0}, R(\phi))\widetilde{\psi}_E(\theta) = \widetilde{\psi}_E(\theta - \phi) \tag{17.4}$$

Although we won't prove it here, the representations constructed this way provide essentially all the unitary irreducible representations of $E(2)$, parametrized by a real number $E > 0$. The only other ones are those on which the translations act trivially, and $SO(2)$ acts as an irreducible representation. We have seen that such $SO(2)$ representations are one-dimensional, and characterized by an integer, the weight. These representations in some sense correspond to the case $E = 0$, but note that for non-zero weight they are something different than just that constant wavefunctions, using a non-trivial action of $SO(2)$ on the wavefunction value.

17.2 The case of $E(3)$

In the physical case of three spatial dimensions, the state space of the theory of a quantum free particle is again a Euclidean group representation, with the same

relationship to the Schrödinger representation as in two spatial dimensions. The main difference is that the rotation group is now three dimensional and non-commutative, so instead of the single Lie algebra basis element l we have three of them, satisfying Poisson bracket relations that are the Lie algebra relations of $\mathfrak{so}(3)$

$$\{l_1, l_2\} = l_3,\ \{l_2, l_3\} = l_1,\ \{l_3, l_1\} = l_2$$

The p_j give the other three basis elements of the Lie algebra of $E(3)$. They commute amongst themselves and the action of rotations on vectors provides the rest of the non-trivial Poisson bracket relations

$$\{l_1, p_2\} = p_3, \quad \{l_1, p_3\} = -p_2$$

$$\{l_2, p_1\} = -p_3, \quad \{l_2, p_3\} = p_1$$

$$\{l_3, p_1\} = p_2, \quad \{l_3, p_2\} = -p_1$$

An isomorphism of this Lie algebra with a Lie algebra of matrices is given by

$$l_1 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad l_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad l_3 \leftrightarrow \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$p_1 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad p_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad p_3 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The l_j are quadratic functions in the q_j, p_j, given by the classical mechanical expression for the angular momentum

$$\mathbf{l} = \mathbf{q} \times \mathbf{p}$$

or, in components

$$l_1 = q_2 p_3 - q_3 p_2, \quad l_2 = q_3 p_1 - q_1 p_3, \quad l_3 = q_1 p_2 - q_2 p_1$$

The Euclidean group $E(3)$ is a subgroup of the Jacobi group $G^J(3)$ in the same way as in two dimensions, and the Schrödinger representation Γ_S provides a representation of $E(3)$ with Lie algebra version

$$\Gamma'_S(l_1) = -iL_1 = -i(Q_2 P_3 - Q_3 P_2) = -(q_2 \frac{\partial}{\partial q_3} - q_3 \frac{\partial}{\partial q_2})$$

$$\Gamma'_S(l_2) = -iL_2 = -i(Q_3 P_1 - Q_1 P_3) = -(q_3 \frac{\partial}{\partial q_1} - q_1 \frac{\partial}{\partial q_3})$$

$$\Gamma'_S(l_3) = -iL_3 = -i(Q_1P_2 - Q_2P_1) = -(q_1\frac{\partial}{\partial q_2} - q_2\frac{\partial}{\partial q_1})$$

$$\Gamma'_S(p_j) = -iP_j = -\frac{\partial}{\partial q_j}$$

These are just the infinitesimal versions of the action of $E(3)$ on functions induced from its action on position space $\mathbf{R}^3$. Given an element $g = (\mathbf{a}, R) \in E(3) \subset G^J(3)$ we have a unitary transformation on wavefunctions

$$u(\mathbf{a}, R)\psi(\mathbf{q}) = \Gamma_S(g)\psi(\mathbf{q}) = \psi(g^{-1} \cdot \mathbf{q}) = \psi(R^{-1}(\mathbf{q} - \mathbf{a}))$$

These group elements will be a product of a translation and a rotation, and the unitary transformations u are exponentials of the Lie algebra actions above, with

$$u(\mathbf{a}, \mathbf{1})\psi(\mathbf{q}) = e^{-i(a_1P_1+a_2P_2+a_3P_3)}\psi(\mathbf{q}) = \psi(\mathbf{q} - \mathbf{a})$$

for a translation by $\mathbf{a}$, and

$$u(\mathbf{0}, R(\phi, \mathbf{e}_j))\psi(\mathbf{q}) = e^{-i\phi L_j}\psi(\mathbf{q}) = \psi(R(-\phi, \mathbf{e}_j)\mathbf{q})$$

for $R(\phi, \mathbf{e}_j)$ a rotation about the j-axis by angle ϕ.

This representation of $E(3)$ on wavefunctions is reducible, since in terms of momentum eigenstates, rotations will only take eigenstates with one value of the momentum to those with another value of the same length-squared. We can get an irreducible representation by using the Casimir operator $P_1^2+P_2^2+P_3^2$, which commutes with all elements in the Lie algebra of $E(3)$. The Casimir operator will act on an irreducible representation as a scalar, and the representation will be characterized by that scalar. The Casimir operator is just $2m$ times the Hamiltonian

$$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2)$$

and so the constant characterizing an irreducible will just be the energy $2mE$. Our irreducible representation will be on the space of solutions of the time-independent Schrödinger equation

$$\frac{1}{2m}(P_1^2 + P_2^2 + P_3^2)\psi(\mathbf{q}) = -\frac{1}{2m}(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} + \frac{\partial^2}{\partial q_3^2})\psi(\mathbf{q}) = E\psi(\mathbf{q})$$

Using the Fourier transform

$$\psi(\mathbf{q}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int_{\mathbf{R}^3} e^{i\mathbf{p}\cdot\mathbf{q}}\widetilde{\psi}(\mathbf{p})d^3\mathbf{p}$$

the time-independent Schrödinger equation becomes

$$(\frac{|\mathbf{p}|^2}{2m} - E)\widetilde{\psi}(\mathbf{p}) = 0$$

and we have distributional solutions

$$\widetilde{\psi}(\mathbf{p}) = \widetilde{\psi}_E(\mathbf{p})\delta(|\mathbf{p}|^2 - 2mE)$$

characterized by functions $\widetilde{\psi}_E(\mathbf{p})$ defined on the sphere $|\mathbf{p}|^2 = 2mE$.

Such complex-valued functions on the sphere of radius $\sqrt{2mE}$ provide a Fourier-transformed version $\widetilde{u}$ of the irreducible representation of $E(3)$. Here the action of the group $E(3)$ is by

$$\widetilde{u}(\mathbf{a}, \mathbf{1})\widetilde{\psi}_E(\mathbf{p}) = e^{-i(\mathbf{a}\cdot\mathbf{p})}\widetilde{\psi}_E(\mathbf{p})$$

for translations, by

$$\widetilde{u}(\mathbf{0}, R)\widetilde{\psi}_E(\mathbf{p}) = \widetilde{\psi}_E(R^{-1}\mathbf{p})$$

for rotations, and by

$$\widetilde{u}(\mathbf{a}, R)\widetilde{\psi}_E(\mathbf{p}) = \widetilde{u}(\mathbf{a}, \mathbf{1})\widetilde{u}(0, R)\widetilde{\psi}_E(\mathbf{p}) = e^{-i\mathbf{a}\cdot R^{-1}\mathbf{p}}\widetilde{\psi}_E(R^{-1}\mathbf{p})$$

for a general element.

17.3 Other representations of $E(3)$

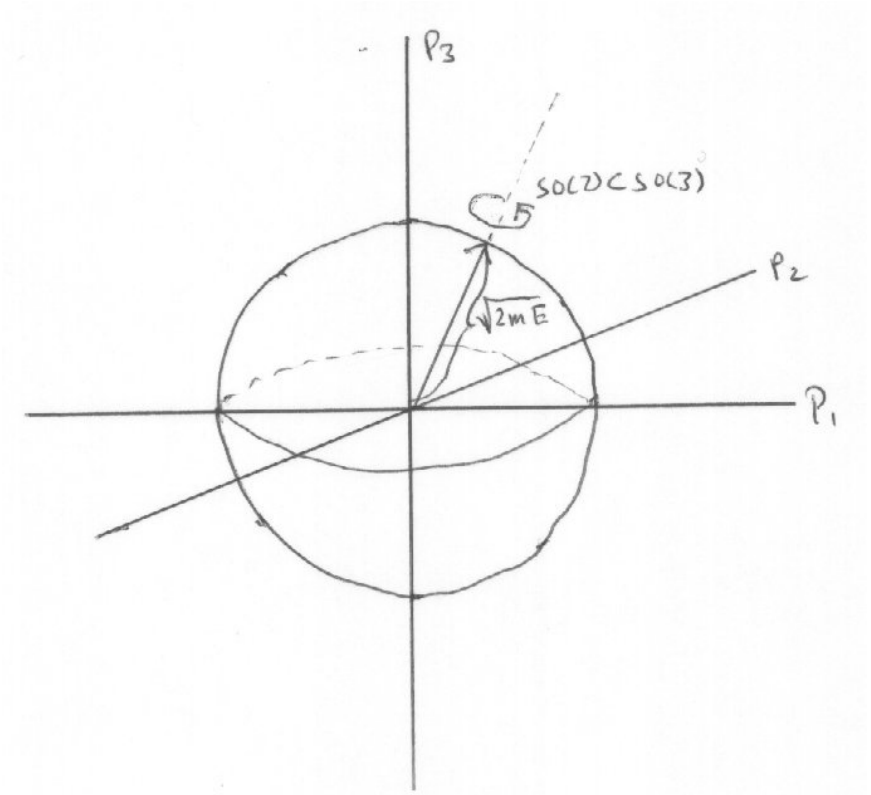
For the case of $E(3)$, besides the representations parametrized by $E > 0$ constructed above, as in the $E(2)$ case there are finite-dimensional representations where the translation subgroup of $E(3)$ acts trivially. Such irreducible representations are just the spin-s representations $(\rho_s, \mathbf{C}^{2s+1})$ of $SO(3)$ for $s = 0, 1, 2, \ldots$.

$E(3)$ has some structure not seen in the $E(2)$ case, which can be used to construct new classes of infinite-dimensional irreducible representations. This can be seen from two different points of view:

- There is a second Casimir operator which one can show commutes with the $E(3)$ action, given by

$$\mathbf{L} \cdot \mathbf{P} = L_1 P_1 + L_2 P_2 + L_3 P_3$$

- The group $SO(3)$ acts on momentum vectors by rotation, with orbit of the group action the sphere of momentum vectors of fixed energy $E > 0$. This is the sphere on which the Fourier transform of the wavefunctions in the representation is supported. Unlike the corresponding circle in the $E(2)$ case, here there is a non-trivial subgroup of the rotation group $SO(3)$ which leaves a given momentum vector invariant. This is just the $SO(2) \subset SO(3)$ subgroup of rotations about the axis determined by the momentum vector, and it is different for different points in momentum space.



For single-component wavefunctions, a straightforward computation shows that the second Casimir operator $\mathbf{L} \cdot \mathbf{P}$ acts as zero. By introducing wavefunctions with several components, together with an action of $SO(3)$ that mixes the components, it turns out that one can get new irreducible representations, with a non-zero value of the second Casimir corresponding to a non-trivial weight of the action of the $SO(2)$ of rotations about the momentum vector.

One can construct such multiple-component wavefunctions as representations of $E(3)$ by taking the tensor product of our irreducible representation on wavefunctions of energy E (call this $\mathcal{H}_E$) and the finite dimensional irreducible representation $\mathbf{C}^{2s+1}$

$$\mathcal{H}_E \otimes \mathbf{C}^{2s+1}$$

The Lie algebra representation operators for the translation part of $E(3)$ act as momentum operators on $\mathcal{H}_E$ and as 0 on $\mathbf{C}^{2s+1}$. For the $SO(3)$ part of $E(3)$, we get operators we can write as

$$J_j = L_j + S_j$$

where L_j acts on $\mathcal{H}_E$ and $S_j = \rho'(l_j)$ acts on $\mathbf{C}^{2s+1}$.

This tensor product representation will not be irreducible, but its irreducible components can be found by taking the eigenspaces of the second Casimir op-

erator, which will now be

$$\mathbf{J} \cdot \mathbf{P}$$

We will not work out the details of this here (although details can be found in chapter 31 for the case $s = \frac{1}{2}$, where $SO(3)$ is replaced by $Spin(3)$). What happens is that the tensor product breaks up into irreducibles as

$$\mathcal{H}_E \otimes \mathbf{C}^{2s+1} = \bigoplus_{n=-s}^{n=s} \mathcal{H}_{E,n}$$

where n is an integer taking values from $-s$ to s that is called the "helicity". $\mathcal{H}_{E,n}$ is the subspace of the tensor product on which the first Casimir $|\mathbf{P}|^2$ takes the value $2mE$, and the second Casimir $\mathbf{J} \cdot \mathbf{P}$ takes the value np, where $p = \sqrt{2mE}$. The physical interpretation of the helicity is that it is the component of angular momentum along the axis given by the momentum vector. The helicity can also be thought of as the weight of the action of the $SO(2)$ subgroup of $SO(3)$ corresponding to rotations about the axis of the momentum vector.

Choosing $E > 0$ and $n \in \mathbf{Z}$, the representations on $\mathcal{H}_{E,n}$ (which we have constructed using some s such that $|s| \geq n$) give all possible irreducible representations of $E(3)$. The representation spaces have a physical interpretation as the state space for a free quantum particle of energy E which carries an "internal" quantized angular momentum about its direction of motion, given by the helicity.

17.4 For further reading

The angular momentum operators are a standard topic in every quantum mechanics textbook, see for example chapter 12 of [57]. The characterization here of free-particle wavefunctions at fixed energy as giving irreducible representations of the Euclidean group is not so conventional, but it is just an example of a non-relativistic version of the conventional description of relativistic quantum particles in terms of representations of the Poincaré group (see chapter 39). In the Poincaré group case the analog of the $E(3)$ irreducible representations of non-zero helicity considered here will be irreducible representations labeled by a non-zero mass and an irreducible representation of $SO(3)$ (the spin). In that case for massless particles one will again see representations labeled by a helicity (an irreducible representation of $SO(2)$), but there is no analog of such massless particles in the $E(3)$ case.

For more details about representations of $E(2)$ and $E(3)$, see [66] or [69] (which is based on [65]).

Chapter 18

Representations of Semi-direct Products

In this chapter we will examine some aspects of representations of semi-direct products, in particular for the case of the Jacobi group and its Lie algebra, as well as the case of $N \rtimes K$, for N commutative.

The Schrödinger representation provides a unitary representation of the Heisenberg group, one that carries extra structure arising from the fact that the symplectic group acts on the Heisenberg group by automorphisms. Each element of the symplectic group takes a given construction of the Schrödinger representation to a unitarily equivalent one, providing an operator on the state space called an "intertwining operator". These intertwining operators will give (up to a phase factor), a representation of the symplectic group. Up to the problem of the phase factor, the Schrödinger representation in this way extends to a representation of the full Jacobi group. To explicitly find the phase factor, one can start with the Lie algebra representation, where the $\mathfrak{sp}(2d, \mathbf{R})$ action is given by quantizing quadratic functions on phase space. It turns out that, for a finite dimensional phase space, this gives a representation up to sign, which can be turned into a true representation by taking a double cover (called $Mp(2d, \mathbf{R})$) of $Sp(2d, \mathbf{R})$.

In later chapters, we will find that many actions of groups on quantum systems can be understood as subgroups of this $Mp(2d, \mathbf{R})$, with the corresponding observables arising as the quadratic combinations of momentum and position operators determined by the moment map.

The Euclidean group $E(d)$ is a subgroup of the Jacobi group and we saw in chapter 17 how some of its representations can be understood by restricting the Schrödinger representation to this subgroup. More generally, this is an example of a semi-direct product $N \rtimes K$ with N commutative. In such cases irreducible representations can be characterized in terms of the action of K on irreducible representations of N, and the irreducible representations of certain subgroups of K.

The reader should be warned that much of the material included in this chapter is not well-motivated by its applications to non-relativistic quantum mechanics, where it is not obviously needed. The motivation is rather provided by the more complicated case of relativistic quantum field theory, but it seems worthwhile to first see how things work in a simpler context. In particular, the discussion of representations of $N \rtimes K$ for M commutative is motivated by the case of the Poincaré group (see chapter 39), and that of intertwining operators by the case of symmetry groups acting on quantum fields (see chapter 36).

18.1 Intertwining operators and the metaplectic representation

For a general semi-direct product $N \rtimes K$ with non-commutative N, the representation theory can be quite complicated. For the Jacobi group case though, it turns out that things simplify dramatically because of the Stone-von Neumann theorem which says that, up to unitary equivalence, we only have one irreducible representation of $N = H_{2d+1}$.

In the general case, recall that for each $k \in K$ the definition of the semi-direct product comes with an automorphism $\phi_k : N \to N$ satisfying $\phi_{k_1 k_2} = \phi_{k_1}\phi_{k_2}$. Given a representation π of N, for each k we can define a new representation π_k of N by first acting with ϕ_k:

$$\pi_k(n) = \pi(\phi_k(n))$$

In the special case of the Heisenberg group and Schrödinger representation Γ_S, we can do this for each $k \in K = Sp(2d, \mathbf{R})$, defining a new represention by

$$\Gamma_{S,k}(n) = \Gamma_S(\phi_k(n))$$

The Stone-von Neumann theorem assures us that these must all be unitarily equivalent, so there must exist unitary operators U_k satisfying

$$\Gamma_{S,k} = U_k \Gamma_S U_k^{-1} = \Gamma_S(\phi_k(n)) \tag{18.1}$$

Operators like this that relate two representations are called "intertwining operators".

Definition (Intertwining operator)**.** *If $(\pi_1, V_1), (\pi_2, V_2)$ are two representations of a group G, an intertwining operator between these two representations is an operator U such that*

$$\pi_2(g)U = U\pi_1(g) \quad \forall g \in G$$

In our case $V_1 = V_2$ is the Schrödinger representation state space $\mathcal{H}$ and $U_k : \mathcal{H} \to \mathcal{H}$ is an intertwining operator between Γ_S and $\Gamma_{S,k}$ for each $k \in Sp(2d, \mathbf{R})$. Since

$$\Gamma_{S,k_1 k_2} = U_{k_1 k_2} \Gamma_S U_{k_1 k_2}^{-1}$$

the U_k should satisfy the group homomorphism property

$$U_{k_1 k_2} = U_{k_1} U_{k_2}$$

and give us a representation of the group $Sp(2d, \mathbf{R})$ on $\mathcal{H}$. This is what we expect on general principles: a group action on the classical phase space after quantization becomes a unitary representation on the quantum state space.

The problem with this argument is that the U_k are not uniquely defined. Schur's lemma tells us that since the representation on $\mathcal{H}$ is irreducible, the operators commuting with the representation operators are just the complex scalars. These give a phase ambiguity in the definition of the unitary operators U_k, which then give a representation of $Sp(2d, \mathbf{R})$ on $\mathcal{H}$ only up to a phase, i.e.

$$U_{k_1 k_2} = U_{k_1} U_{k_2} e^{i\varphi(k_1, k_2)}$$

for some real-valued function φ of pairs of group elements. In terms of corresponding Lie algebra representation operators U'_L, this ambiguity appears as an unknown constant times the identity operator.

The question then arises whether the phases of the U_k can be chosen so as to satisfy the homomorphism property (i.e. can one choose phases so that $\varphi(k_1, k_2) = N 2\pi$ for N integral?). It turns out that one can not quite do this, needing to allow N to be half-integral, so one gets the homomorphism property up to a sign. Just as in the $SO(d)$ case where a similar sign ambiguity showed the need to go to a double-cover $Spin(d)$ to get a true representation, here one also needs to go to a double cover of $Sp(2d, \mathbf{R})$, called the metaplectic group $Mp(2d, \mathbf{R})$. The nature of this sign ambiguity and double cover is subtle, for details see [39] or [25]. In section 18.2.1 we will show by computation one aspect of the double cover.

Since this is just a sign ambiguity, it does not appear infinitesimally: one can choose the ambiguous constants in the Lie algebra representation operators so that the Lie algebra homomorphism property is satisfied. However, this will no longer be true for infinite dimensional phase spaces, a situation that is described as an "anomaly" in the symmetry. This phenomenon will be examined in more detail in chapter 33.

In the finite dimensional case, we can construct the U_k explicitly, by exponentiating the Lie algebra representation operators U'_L, which are constructed by quantization of the homogeneous order-two polynomials that give the Lie algebra $\mathfrak{sp}(2d, \mathbf{R})$.

This quantization takes

$$\mu_L \in \mathfrak{sp}(2d, \mathbf{R}) \to U'_L$$

where μ_L is the polynomial corresponding to the matrix L to U'_L, which is the corresponding polynomial in operators Q_j, P_j, as determined by equation 15.1. This choice will satisfy the Lie algebra homomorphism property

$$[U'_{L_1}, U'_{L_2}] = U'_{[L_1, L_2]} \tag{18.2}$$

The Lie algebra relation (see 14.14)

$$\{\mu_L, \begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix}\} = L^T \begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix} \tag{18.3}$$

becomes after quantization

$$[U'_L, \begin{pmatrix}\mathbf{Q}\\ \mathbf{P}\end{pmatrix}] = L^T \begin{pmatrix}\mathbf{Q}\\ \mathbf{P}\end{pmatrix} \tag{18.4}$$

Exponentiating this U'_L will give us our U_k, and thus the operators we want.

Note that if we only need to satisfy equation 18.4 the U'_L can be changed by a constant times the identity operator, but such a change would be inconsistent with equation 18.2 (and thus called an "anomaly"). Equation 18.4 could be written

$$[U'_L, \Gamma'_S(X)] = \Gamma'_S(L \cdot X) \tag{18.5}$$

where

$$L \cdot X = \frac{d}{dt}\phi_{e^{tL}}(X)_{|t=0}$$

It is the infinitesimal expression of the intertwining property 18.1.

18.2 Some examples

As a balance to the abstract discussion so far in this chapter, in this section we'll work out a couple of the simplest possible examples in great detail. These examples will also make clear the conventions being chosen, and show the basic structure of what the quadratic operators corresponding to symmetries look like, a structure that will reappear in the much more complicated infinite-dimensional quantum field theory examples we will come to later.

18.2.1 The $SO(2)$ action on the $d = 1$ phase space

In the case $d = 1$ one has elements $g \in SO(2) \subset Sp(2, \mathbf{R})$ acting on $c_q q + c_p p \in \mathcal{M}$ by

$$\begin{pmatrix}c_q\\ c_p\end{pmatrix} \to g \begin{pmatrix}c_q\\ c_p\end{pmatrix} = \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix} \begin{pmatrix}c_q\\ c_p\end{pmatrix}$$

so

$$g = e^{\theta L}$$

where

$$L = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

To find the intertwining operators, we first find the quadratic function μ_L in q, p that satisfies

$$\{\mu_L, \begin{pmatrix}q\\ p\end{pmatrix}\} = L^T \begin{pmatrix}q\\ p\end{pmatrix} = \begin{pmatrix}-p\\ q\end{pmatrix}$$

By equation 14.5 this is

$$\mu_L = \frac{1}{2}\begin{pmatrix} q & p \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} = \frac{1}{2}(q^2 + p^2)$$

Quantizing μ_L using the Schrödinger representation Γ'_S, one has a unitary Lie algebra representation U' of $\mathfrak{so}(2)$ with

$$U'_L = -\frac{i}{2}(Q^2 + P^2)$$

satisfying

$$[U'_L, \begin{pmatrix} Q \\ P \end{pmatrix}] = \begin{pmatrix} -P \\ Q \end{pmatrix} \tag{18.6}$$

and intertwining operators

$$U_g = e^{\theta U'_L} = e^{-i\frac{\theta}{2}(Q^2+P^2)}$$

These give a representation of $SO(2)$ only up to a sign. To see the problem, consider the state $\psi(q) \subset \mathcal{H} = L^2(\mathbf{R})$ given by

$$\psi(q) = e^{-\frac{q^2}{2}}$$

One has

$$(Q^2 + P^2)\psi(q) = (q^2 - \frac{d^2}{dq^2})\psi(q) = \psi(q)$$

so $\psi(q)$ is an eigenvector of $Q^2 + P^2$ with eigenvalue 1. As one goes around the group $SO(2)$ once (taking θ from 0 to 2π), the representation acts by a phase that only goes from 0 to π, demonstrating the same problem that occurs in the case of the spinor representation.

Conjugating the Heisenberg Lie algebra representation operators by the unitary operators U_g intertwines the representations corresponding to rotations of the phase space plane by an angle θ.

$$e^{-i\frac{\theta}{2}(Q^2+P^2)}\begin{pmatrix} Q \\ P \end{pmatrix}e^{i\frac{\theta}{2}(Q^2+P^2)} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} Q \\ P \end{pmatrix} \tag{18.7}$$

Note that this is a quite different calculation than in the spin case where we also constructed a double cover of $SO(2)$. Despite the quite different context (rotations acting on an infinite dimensional state space), again one sees the double cover here, as either U_g or $-U_g$ will give the same rotation.

This example will be studied in much greater detail when we get to the theory of the quantum harmonic oscillator in chapter 20. Note that the $SO(2)$ group action here inherently requires using both coordinate and momentum variables, it is not a symmetry that can be seen just by looking at the problem in configuration space.

18.2.2 The $SO(2)$ action by rotations of the plane for $d = 2$

In the case $d = 2$ there is a another example of an $SO(2)$ group which is a subgroup of the symplectic group, here $Sp(4, \mathbf{R})$. This is the group of rotations of the configuration space $\mathbf{R}^2$, with a simultaneous rotation of the momentum space, leaving invariant the Poisson bracket. The group $SO(2)$ acts on $c_{q_1} q_1 + c_{q_2} q_2 + c_{p_1} p_1 + c_{p_2} p_2 \in \mathcal{M}$ by

$$\begin{pmatrix} c_{q_1} \\ c_{q_2} \\ c_{p_1} \\ c_{p_2} \end{pmatrix} \to g \begin{pmatrix} c_{q_1} \\ c_{q_2} \\ c_{p_1} \\ c_{p_2} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & \cos\theta & -\sin\theta \\ 0 & 0 & \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} c_{q_1} \\ c_{q_2} \\ c_{p_1} \\ c_{p_2} \end{pmatrix}$$

so $g = e^{\theta L}$ where $L \in \mathfrak{sp}(4, \mathbf{R})$ is given by

$$L = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

L acts on phase space coordinate functions by

$$\begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} \to L^T \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} q_2 \\ -q_1 \\ p_2 \\ -p_1 \end{pmatrix}$$

By equation 14.14, with

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad B = C = 0$$

the quadratic function μ_L that satisfies

$$\{\mu_L, \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix}\} = L^T \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} q_2 \\ -q_1 \\ p_2 \\ -p_1 \end{pmatrix}$$

is

$$\mu_L = -\mathbf{q} \cdot \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{p} = q_1 p_2 - q_2 p_1$$

This is just the formula for the angular momentum corresponding to rotation about an axis perpendicular to the $q_1 - q_2$ plane

$$l = q_1 p_2 - q_2 p_1$$

Quantization gives a representation of the Lie algebra $\mathfrak{so}(2)$ with

$$U'_L = -i(Q_1 P_2 - Q_2 P_1)$$

satisfying

$$[U'_L, \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}] = \begin{pmatrix} Q_2 \\ -Q_1 \end{pmatrix}, \quad [U'_L, \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}] = \begin{pmatrix} P_2 \\ -P_1 \end{pmatrix}$$

Exponentiating gives a representation of $SO(2)$

$$U_{e^{\theta L}} = e^{-i\theta(Q_1P_2 - Q_2P_1)}$$

with conjugation by $U_{e^{\theta L}}$ rotating linear combinations of the Q_1, Q_2 (or the P_1, P_2) each by an angle θ.

$$U_{e^{\theta L}}(c_{q_1}Q_1 + c_{q_2}Q_2)U^{-1}_{e^{\theta L}} = c'_{q_1}Q_1 + c'_{q_2}Q_2$$

where

$$\begin{pmatrix} c'_{q_1} \\ c'_{q_2} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} c_{q_1} \\ c_{q_2} \end{pmatrix}$$

Note that for this $SO(2)$ the double cover is trivial. As far as this subgroup of $Sp(4, \mathbf{R})$ is concerned, there is no need to consider the double cover $Mp(4, \mathbf{R})$ to get a well-defined representation.

Replacing the matrix L by

$$\begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & A \end{pmatrix}$$

for A any real 2 by 2 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

we get an action of the group $GL(2, \mathbf{R}) \subset Sp(4, \mathbf{R})$ on $\mathcal{M}$, and after quantization a Lie algebra representation

$$U'_A = i \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}$$

which will satisfy

$$[U'_A, \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}] = -A \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}, \quad [U'_A, \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}] = A^T \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}$$

Note that the action of A on the momentum operators is the dual of the action on the position operators. Only in the case of an orthogonal action (the $SO(2)$ earlier) are these the same, with $A^T = -A$.

18.3 Representations of $N \rtimes K$, N commutative

The representation theory of semi-direct products $N \rtimes K$ will in general be rather complicated. However, when N is commutative things simplify considerably, and in this section we'll survey some of the general features of this case. The

special cases of the Euclidean groups in 2 and 3 dimensions were covered in chapter 17 and the Poincaré group case will be discussed in chapter 39.

For a general commutative group N, one does not have the simplifying feature of the Heisenberg group, the uniqueness of its irreducible representation. For commuative groups on the other hand, while there are many irreducible representations, they are all one-dimensional. As a result, the set of representations of N acquires its own group structure, also commutative, and one can define

Definition (Character group)**.** *For N a commutative group, let $\widehat{N}$ be the set of characters of N, i.e. functions*

$$\alpha : N \to \mathbf{C}$$

that satisfy the homomorphism property

$$\alpha(n_1 n_2) = \alpha(n_1)\alpha(n_2)$$

The elements of $\widehat{N}$ form a group, with multiplication

$$(\alpha_1\alpha_2)(n) = \alpha_1(n)\alpha_2(n)$$

We only will actually need the case $N = \mathbf{R}^d$, where we have already seen that the differentiable irreducible representations are one-dimensional and given by

$$\alpha_{\mathbf{p}}(\mathbf{a}) = e^{i\mathbf{p}\cdot\mathbf{a}}$$

where $\mathbf{a} \in N$. So the character group in this case is $\widehat{N} = \mathbf{R}^d$, with elements labeled by the vector $\mathbf{p}$.

For a semidirect product $N \rtimes K$, we will have an automorphism ϕ_k of N for each $k \in K$. From this action on N, we get an induced action on functions on N, in particular on elements of $\widehat{N}$, by

$$\widehat{\phi}_k : \alpha \in \widehat{N} \to \widehat{\phi}_k(\alpha) \in \widehat{N}$$

where $\widehat{\phi}_k(\alpha)$ is the element of $\widehat{N}$ satisfying

$$\widehat{\phi}_k(\alpha)(n) = \alpha(\phi_k^{-1}(n))$$

For the case of $N = \mathbf{R}^d$, we have

$$\widehat{\phi}_k(\alpha_{\mathbf{p}})(\mathbf{a}) = e^{i\mathbf{p}\cdot\phi_k^{-1}(\mathbf{a})} = e^{i(((\phi_k^{-1})^T(\mathbf{p}))\cdot\mathbf{a}}$$

so

$$\widehat{\phi}_k(\alpha_{\mathbf{p}}) = \alpha_{(\phi_k^{-1})^T(\mathbf{p})}$$

When K acts by orthogonal transformations on $N = \mathbf{R}^d$, $\phi_k^T = \phi_k^{-1}$ so

$$\widehat{\phi}_k(\alpha_{\mathbf{p}}) = \alpha_{\phi_k(\mathbf{p})}$$

To analyze representations (π, V) of $N \rtimes K$, one can begin by restricting attention to the N action, decomposing V into subspaces V_α where N acts according to α. $v \in V$ is in the subspace V_α when

$$\pi(n, \mathbf{1})v = \alpha(n)v$$

Acting by K will take this subspace to another one according to

Theorem.

$$v \in V_\alpha \implies \pi(\mathbf{0}, k)v \in V_{\widehat{\phi}_k(\alpha)}$$

Proof. Using the definition of the semi-direct product in chapter 16 one can show that the group multiplication satisfies

$$(\mathbf{0}, k^{-1})(n, \mathbf{1})(\mathbf{0}, k) = (\phi_{k^{-1}}(n), \mathbf{1})$$

Using this, one has

$$\begin{aligned}
\pi(n, \mathbf{1})\pi(\mathbf{0}, k)v =& \pi(\mathbf{0}, k)\pi(\mathbf{0}, k^{-1})\pi(n, \mathbf{1})\pi(\mathbf{0}, k)v \\
=& \pi(\mathbf{0}, k)\pi(\phi_{k^{-1}}(n), \mathbf{1})v \\
=& \pi(\mathbf{0}, k)\alpha(\phi_{k^{-1}}(n))v \\
=& \widehat{\phi}_k(\alpha)(n)\pi(\mathbf{0}, k)v
\end{aligned}$$

□

For each $\alpha \in \widehat{N}$ one can look at its orbit under the action of K by $\widehat{\phi}_k$, which will give a subset $\mathcal{O}_\alpha \subset \widehat{N}$. From the above theorem, we see that if $V_\alpha \neq 0$, then we will also have $V_\beta \neq 0$ for $\beta \in \mathcal{O}_\alpha$, so one piece of information that characterizes a representation V is the set of orbits one gets in this way.

α also defines a subgroup $K_\alpha \subset K$ consisting of group elements whose action on $\widehat{N}$ leaves α invariant:

Definition (Stabilizer group or little group)**.** *The subgroup $K_\alpha \subset K$ of elements $k \in K$ such that*

$$\widehat{\phi}_k(\alpha) = \alpha$$

for a given $\alpha \in \widehat{N}$ is called the stabilizer subgroup (by mathematicians) or little subgroup (by physicists).

The group K_α will act on the subspace V_α, and this representation of K_α is a second piece of information one can use to characterize a representation.

In the case of the Euclidean group $E(2)$ we found that the non-zero orbits $\mathcal{O}_\alpha$ were circles and the groups K_α were trivial. For $E(3)$, the non-zero orbits were spheres, with K_α an $SO(2)$ subgroup of $SO(3)$ (one that varies with α). In these cases we found that our construction of representations of $E(2)$ or $E(3)$ on spaces of solutions of the single-component Schrödinger equation corresponded under Fourier transform to a representation on functions on the orbits $\mathcal{O}_\alpha$. We also found in the $E(3)$ case that using multiple-component wavefunctions

gave new representations corresponding to a choice of orbit $\mathcal{O}_\alpha$ and a choice of irreducible representation of $K_\alpha = SO(2)$. We did not show this, but this construction gives an irreducible representation when a single orbit $\mathcal{O}_\alpha$ occurs (with a transitive K action), with an irreducible representation of K_α on V_α.

We will not further pursue the general theory here, but one can show that distinct irreducible representations of $N \rtimes K$ will occur for each choice of an orbit $\mathcal{O}_\alpha$ and an irreducible representation of K_α. One way to construct these representations is as the solution space of an appropriate wave-equation, with the wave-equation corresponding to the eigenvalue equation for a Casimir operator. In general, other "subsidiary conditions" then need be imposed to pick out a subspace of solutions that give an representation of $N \rtimes K$, this corresponds to the existence of other Casimir operators.

18.4 For further reading

For more on representations of semi-direct products, see section 3.8 of [59], chapter 5 of [66], [8], and [26]. The general theory was developed by Mackey during the late 1940s and 1950s, and his lecture notes on representation theory [41] are a good source for the details of this. The point of view taken here, that emphasizes constructing representations as solutions spaces of differential equations, where the differential operators are Casimir operators, is explained in more detail in [33].

The conventional derivation found in most physics textbooks of the operators U'_L coming from an infinitesimal group action uses Lagrangian methods and Noether's theorem. The purely Hamiltonian method used here treats configuration and momentum variables on the same footing, and is useful especially in the case of group actions that mix them. For another treatment of these operators along the lines of this chapter, see section 14 of [25].

The issue of the phase factor in the intertwining operators and the metaplectic double cover will be discussed in later chapters using a different realization of the Heisenberg Lie algebra representation. For a discussion of this in terms of the Schrödinger representation, see part I of [39].

Chapter 19

Central Potentials and the Hydrogen Atom

When the Hamiltonian function is invariant under rotations, we then expect eigenspaces of the corresponding Hamiltonian operator to carry representations of $SO(3)$. These spaces of eigenfunctions of a given energy break up into irreducible representations of $SO(3)$, and we have seen that these are labeled by a integer $l = 0, 1, 2, \ldots$ and have dimension $2l + 1$. One can use this to find properties of the solutions of the Schrödinger equation whenever one has a rotation-invariant potential energy. We will work out what happens for the case of the Coulomb potential describing the hydrogen atom. This specific case is exactly solvable because it has a second not-so-obvious $SO(3)$ symmetry, in addition to the one coming from rotations of $\mathbf{R}^3$.

19.1 Quantum particle in a central potential

In classical physics, to describe not free particles, but particles experiencing some sort of force, one just needs to add a "potential energy" term to the kinetic energy term in the expression for the energy (the Hamiltonian function). In one dimension, for potential energies that just depend on position, one has

$$h = \frac{p^2}{2m} + V(q)$$

for some function $V(q)$. In the physical case of three dimensions, this will be

$$h = \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2) + V(q_1, q_2, q_3)$$

Quantizing and using the Schrödinger representation, the Hamiltonian op-

erator for a particle moving in a potential $V(q_1, q_2, q_3)$ will be

$$\begin{aligned} H =& \frac{1}{2m}(P_1^2 + P_2^2 + P_3^3) + V(Q_1, Q_2, Q_3) \\ =& \frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} + \frac{\partial^2}{\partial q_3^2}) + V(q_1, q_2, q_3) \\ =& \frac{-\hbar^2}{2m}\Delta + V(q_1, q_2, q_3) \end{aligned}$$

We will be interested in so-called "central potentials", potential functions that are functions only of $q_1^2 + q_2^2 + q_3^2$, and thus only depend upon r, the radial distance to the origin. For such V, both terms in the Hamiltonian will be $SO(3)$ invariant, and eigenspaces of H will be representations of $SO(3)$.

Using the expressions for the angular momentum operators in spherical coordinates derived in chapter 8 (including equation 8.8 for the Casimir operator L^2), one can show that the Laplacian has the following expression in spherical coordinates

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}L^2$$

The Casmir operator L^2 has eigenvalues $l(l+1)$ on irreducible representations of dimension $2l+1$ (integral spin l). So, restricted to such an irreducible representation, we have

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}$$

To solve the Schrödinger equation, we want to find the eigenfunctions of H. The space of eigenfunctions of energy E will be a sum of of irreducible representations of $SO(3)$, with the $SO(3)$ acting on the angular coordinates of the wavefunctions, leaving the radial coordinate invariant. We have seen in chapter 8 that such representations on functions of angular coordinates can be explicitly expressed in terms of the spherical harmonic functions $Y_l^m(\theta, \phi)$. So, to find eigenfunctions of the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + V(r)$$

we want to find functions $g_{lE}(r)$ depending on $l = 0, 1, 2, \ldots$ and the energy eigenvalue E satisfying

$$(\frac{-\hbar^2}{2m}(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}) + V(r))g_{lE}(r) = Eg_{lE}(r)$$

Given such a $g_{lE}(r)$ we will have

$$Hg_{lE}(r)Y_l^m(\theta, \phi) = Eg_{lE}(r)Y_l^m(\theta, \phi)$$

and the

$$\psi(r, \theta, \phi) = g_{lE}(r)Y_l^m(\theta, \phi)$$

will span a $2l+1$ dimensional (since $m = -l, -l+1, \ldots, l-1, l$) space of energy eigenfunctions for H of eigenvalue E.

For a general potential function $V(r)$, exact solutions for the eigenvalues E and corresponding functions $g_{lE}(r)$ cannot be found in closed form. One special case where we can find such solutions is for the three-dimensional harmonic oscillator, where $V(r) = \frac{1}{2}m\omega^2 r^2$. These are much more easily found though using the creation and annihilation operator techniques to be discussed in chapter 20.

The other well-known and physically very important case is the case of a $\frac{1}{r}$ potential, called the Coulomb potential. This describes a light charged particle moving in the potential due to the electric field of a much heavier charged particle, a situation that corresponds closely to that of a hydrogen atom. In this case we have

$$V = -\frac{e^2}{r}$$

where e is the charge of the electron, so we are looking for solutions to

$$(\frac{-\hbar^2}{2m}(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}) - \frac{e^2}{r})g_{lE}(r) = Eg_{lE}(r)$$

Since having

$$\frac{d^2}{dr^2}(rg) = Erg$$

is equivalent to

$$(\frac{d^2}{dr^2} + \frac{2}{r})g = Eg$$

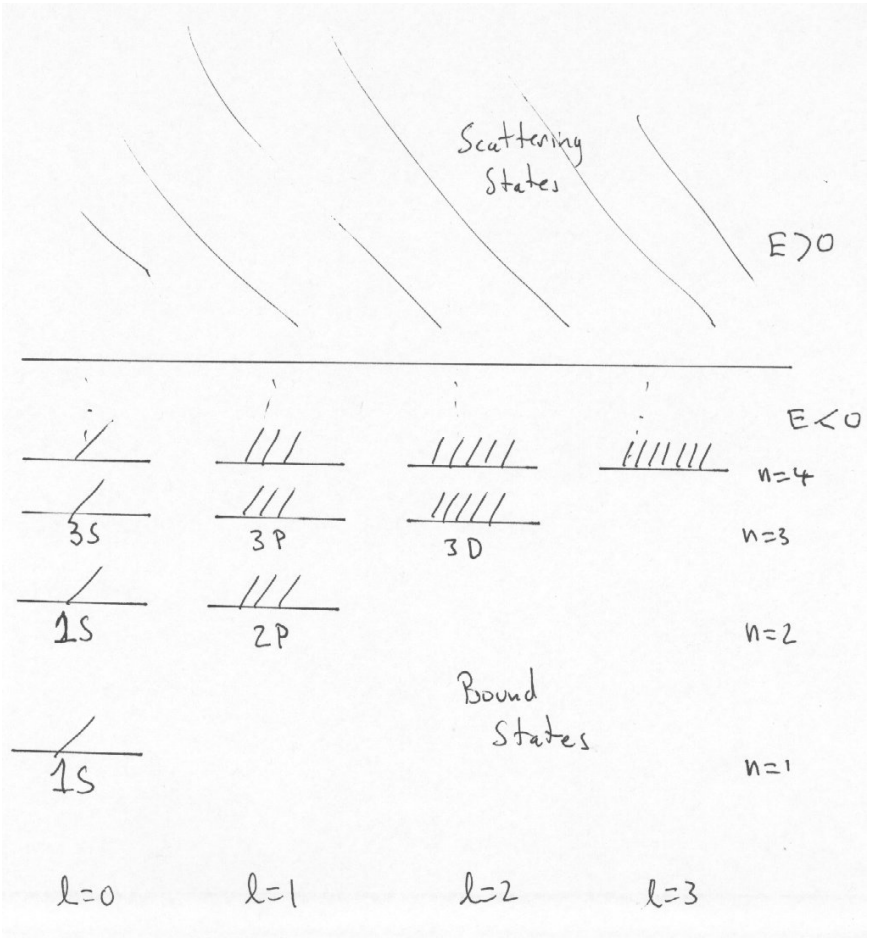
for any function g, $g_{lE}(r)$ will satisfy

$$(\frac{-\hbar^2}{2m}(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}) - \frac{e^2}{r})rg_{lE}(r) = Erg_{lE}(r)$$

The solutions to this equation can be found through a rather elaborate process described in most quantum mechanics textbooks, which involves looking for a power series solution. For $E \geq 0$ there are non-normalizable solutions that describe scattering phenomena that we won't study here. For $E < 0$ solutions correspond to an integer $n = 1, 2, 3, \ldots$, with $n \geq l+1$. So, for each n we get n solutions, with $l = 0, 1, 2, \ldots, n-1$, all with the same energy

$$E_n = -\frac{me^4}{2\hbar^2 n^2}$$

A plot of the different energy eigenstates looks like this:



The degeneracy in the energy values leads one to suspect that there is some extra group action in the problem commuting with the Hamiltonian. If so, the eigenspaces of energy eigenfunctions will come in irreducible representations of some larger group than $SO(3)$. If the representation of the larger group is reducible when one restricts to the $SO(3)$ subgroup, giving n copies of our $SO(3)$ representation of spin l, that would explain the pattern observed here. In the next section we will see that this is the case, and there use representation theory to derive the above formula for E_n.

We won't go through the process of showing how to explicitly find the functions $g_{lE_n}(r)$ but just quote the result. Setting

$$a_0 = \frac{\hbar^2}{me^2}$$

(this has dimensions of length and is known as the "Bohr radius"), and defining

$g_{nl}(r) = g_{lE_n}(r)$ the solutions are of the form

$$g_{nl}(r) \propto e^{-\frac{r}{na_0}}(\frac{2r}{na_0})^l L_{n+l}^{2l+1}(\frac{2r}{na_0})$$

where the L_{n+l}^{2l+1} are certain polynomials known as associated Laguerre polynomials.

So, finally, we have found energy eigenfunctions

$$\psi_{nlm}(r,\theta,\phi) = g_{nl}(r)Y_l^m(\theta,\phi)$$

for

$$n = 1, 2, \dots$$

$$l = 0, 1, \dots, n-1$$

$$m = -l, -l+1, \dots, l-1, l$$

The first few of these, properly normalized, are

$$\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$$

(called the $1S$ state, "S" meaning $l = 0$)

$$\psi_{200} = \frac{1}{\sqrt{8\pi a_0^3}}(1 - \frac{r}{2a_0})e^{-\frac{r}{2a_0}}$$

(called the $2S$ state), and the three dimensional $l = 1$ (called $2P$, "P" meaning $l = 1$) states with basis elements

$$\psi_{211} = -\frac{1}{8\sqrt{\pi a_0^3}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \sin\theta e^{i\phi}$$

$$\psi_{211} = -\frac{1}{4\sqrt{2\pi a_0^3}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \cos\theta$$

$$\psi_{21-1} = \frac{1}{8\sqrt{\pi a_0^3}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \sin\theta e^{-i\phi}$$

19.2 $\mathfrak{so}(4)$ symmetry and the Coulomb potential

The Coulomb potential problem is very special in that it has an additional symmetry, of a non-obvious kind. This symmetry appears even in the classical problem, where it is responsible for the relatively simple solution one can find to the essentially identical Kepler problem. This is the problem of finding the classical trajectories for bodies orbiting around a central object exerting a gravitational force, which also has a $\frac{1}{r}$ potential. Kepler's second law for such

motion comes from conservation of angular momentum, which corresponds to the Poisson bracket relation

$$\{l_j, h\} = 0$$

Here we'll take the Coulomb version of the Hamiltonian that we need for the hydrogen atom problem

$$h = \frac{1}{2m}|\mathbf{p}|^2 - \frac{e^2}{r}$$

One can read the relation $\{l_j, h\} = 0$ in two ways:

- The hamiltonian h is invariant under the action of the group ($SO(3)$) whose infinitesimal generators are l_j.
- The components of the angular momentum (l_j) are invariant under the action of the group ($\mathbf{R}$ of time translations) whose infinitesimal generator is h, so the angular momentum is a conserved quantity.

Kepler's first and third laws have a different origin, coming from the existence of a new conserved quantity for this special choice of Hamiltonian. This quantity is, like the angular momentum, a vector, often called the Lenz (or sometimes Runge-Lenz, or even Laplace-Runge-Lenz) vector.

Definition (Lenz vector)**.** *The Lenz vector is the vector-valued function on the phase space* $\mathbf{R}^6$ *given by*

$$\mathbf{w} = \frac{1}{m}(\mathbf{l} \times \mathbf{p}) + e^2 \frac{\mathbf{q}}{|\mathbf{q}|}$$

Simple manipulations of the cross-product show that one has

$$\mathbf{l} \cdot \mathbf{w} = 0$$

We won't here explicitly calculate the various Poisson brackets involving the components w_j of $\mathbf{w}$, since this is a long and unilluminating calculation, but will just quote the results, which are

- $$\{w_j, h\} = 0$$

  This says that, like the angular momentum, the vector with components w_j is a conserved quantity under time evolution of the system, and its components generate symmetries of the classical system.

- $$\{l_j, w_k\} = \epsilon_{jkl} w_l$$

  These relations say that the generators of the $SO(3)$ symmetry act on w_j the way one would expect, since w_j is a vector.

- $$\{w_j, w_k\} = \epsilon_{jkl} l_l (\frac{-2h}{m})$$

  This is the most surprising relation, and it has no simple geometrical explanation (although one can change variables in the problem to try and give it one). It expresses a highly non-trivial relationship between the two sets of symmetries generated by the vectors $\mathbf{l}, \mathbf{w}$ and the Hamiltonian h.

The w_j are cubic in the q and p variables, so one would expect that the Groenewold-van Hove no-go theorem would tell one that there is no consistent way to quantize this system by finding operators W_j corresponding to the w_j that would satisfy the commutation relations corresponding to these Poisson brackets. It turns out though that this can be done, although not for functions defined over the entire phase-space. One gets around the no-go theorem by doing something that only works when the Hamiltonian h is negative (we'll be taking a square root of $-h$).

The choice of operators W_j that works is

$$\mathbf{W} = \frac{1}{2m}(\mathbf{L} \times \mathbf{P} - \mathbf{P} \times \mathbf{L}) + e^2 \frac{\mathbf{Q}}{|\mathbf{Q}|^2}$$

where the last term is the operator of multiplication by $e^2 q_j / |\mathbf{q}|^2$. By elaborate and unenlightening computations the W_j can be shown to satisfy the commutation relations corresponding to the Poisson bracket relations of the w_j:

$$[W_j, H] = 0$$

$$[L_j, W_k] = i\hbar \epsilon_{jkl} W_l$$

$$[W_j, W_k] = i\hbar \epsilon_{jkl} L_l (-\frac{2}{m} H)$$

as well as

$$\mathbf{L} \cdot \mathbf{W} = \mathbf{W} \cdot \mathbf{L} = 0$$

The first of these shows that energy eigenstates will be preserved not just by the angular momentum operators L_j, but by a new set of non-trivial operators, the W_j, so will be representations of a larger Lie algebra thatn $\mathfrak{so}(3)$.

In addition, one has the following relation between W^2, H and the Casimir operator L^2

$$W^2 = e^4 \mathbf{1} + \frac{2}{m} H (L^2 + \hbar^2 \mathbf{1})$$

and it is this which will allow us to find the eigenvalues of H, since we know those for L^2, and can find those of W^2 by changing variables to identify a second $\mathfrak{so}(3)$ Lie algebra.

To do this, first change normalization by defining

$$\mathbf{K} = \sqrt{\frac{-m}{2E}} \mathbf{W}$$

where E is the eigenvalue of the Hamiltonian that we are trying to solve for. Note that it is at this point that we violate the conditions of the no-go theorem, since we must have $E < 0$ to get a $\mathbf{K}$ with the right properties, and this restricts the validity of our calculations to a subset of the energy spectrum. For $E > 0$ one can proceed in a similar way, but the Lie algebra one gets is different ($\mathfrak{so}(3,1)$ instead of $\mathfrak{so}(4)$).

One then has the following relation between operators

$$2H(K^2 + L^2 + \hbar^2\mathbf{1}) = -me^4\mathbf{1}$$

and the following commutation relations

$$[L_j, L_k] = i\hbar\epsilon_{jkl}L_l$$

$$[L_j, K_k] = i\hbar\epsilon_{jkl}K_l$$

$$[K_j, K_k] = i\hbar\epsilon_{jkl}L_l$$

Defining

$$\mathbf{M} = \frac{1}{2}(\mathbf{L} + \mathbf{K}), \quad \mathbf{N} = \frac{1}{2}(\mathbf{L} - \mathbf{K})$$

one has

$$[M_j, M_k] = i\hbar\epsilon_{jkl}M_l$$

$$[N_j, N_k] = i\hbar\epsilon_{jkl}N_l$$

$$[M_j, N_k] = 0$$

This shows that we have two commuting copies of $\mathfrak{so}(3)$ acting on states, spanned respectively by the M_j and N_j, with two corresponding Casimir operators M^2 and N^2.

Using the fact that

$$\mathbf{L} \cdot \mathbf{K} = \mathbf{K} \cdot \mathbf{L} = 0$$

one finds that

$$M^2 = N^2$$

Recall from our discussion of rotations in three dimensions that representations of $\mathfrak{so}(3) = \mathfrak{su}(2)$ correspond to representations of $Spin(3) = SU(2)$, the double cover of $SO(3)$ and the irreducible ones have dimension $2l + 1$, with l half-integral. Only for l integral does one get representations of $SO(3)$, and it is these that occur in the $SO(3)$ representation on functions on $\mathbf{R}^3$. For four dimensions, we found that $Spin(4)$, the double cover of $SO(4)$, is $SU(2) \times SU(2)$, and one thus has $\mathfrak{spin}(4) = \mathfrak{so}(4) = \mathfrak{su}(2) \times \mathfrak{su}(2) = \mathfrak{so}(3) \times \mathfrak{so}(3)$. This is exactly the Lie algebra we have found here, so one can think of the Coulomb problem as having an $\mathfrak{so}(4)$ symmetry. The representations that will occur can include the half-integral ones, since neither $\mathfrak{so}(3)$ is the $\mathfrak{so}(3)$ of physical rotations in 3-space (those are generated by $\mathbf{L} = \mathbf{M} + \mathbf{N}$, which will have integral eigenvalues of l).

The relation between the Hamiltonian and the Casimir operators M^2 and N^2 is

$$2H(K^2 + L^2 + \hbar^2\mathbf{1}) = 2H(2M^2 + 2N^2 + \hbar^2\mathbf{1}) = 2H(4M^2 + \hbar^2\mathbf{1}) = -me^4\mathbf{1}$$

On irreducible representations of $\mathfrak{so}(3)$ of spin μ, we will have

$$M^2 = \mu(\mu+1)\mathbf{1}$$

for some half-integral μ, so we get the following equation for the energy eigenvalues

$$E = -\frac{-me^4}{2\hbar^2(4\mu(\mu+1)+1)} = -\frac{-me^4}{2\hbar^2(2\mu+1)^2}$$

Letting $n = 2\mu + 1$, for $\mu = 0, \frac{1}{2}, 1, \ldots$ we get $n = 1, 2, 3, \ldots$ and precisely the same equation for the eigenvalues described earlier

$$E_n = -\frac{me^4}{2\hbar^2 n^2}$$

It is not hard to show that the irreducible representations of a product like $\mathfrak{so}(3) \times \mathfrak{so}(3)$ are just tensor products of irreducibles, and in this case the two factors of the product are identical due to the equality of the Casimirs $M^2 = N^2$. The dimension of the $\mathfrak{so}(3) \times \mathfrak{so}(3)$ irreducibles is thus $(2\mu+1)^2 = n^2$, explaining the multiplicity of states one finds at energy eigenvalue E_n.

19.3 The hydrogen atom

The Coulomb potential problem provides a good description of the quantum physics of the hydrogen atom, but it is missing an important feature of that system, the fact that electrons are spin $\frac{1}{2}$ systems. To describe this, one really needs to take as space of states two-component wavefunctions

$$|\psi\rangle = \begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix}$$

(or, equivalently, replace our state space $\mathcal{H}$ of wavefunctions by the tensor product $\mathcal{H} \otimes \mathbf{C}^2$) in a way that we will examine in detail in chapter 31.

The Hamiltonian operator for the hydrogen atom acts trivially on the $\mathbf{C}^2$ factor, so the only effect of the additional wavefunction component is to double the number of energy eigenstates at each energy. Electrons are fermions, so antisymmetry of multi-particle wavefunctions implies the Pauli principle that states can only be occupied by a single particle. As a result, one finds that when adding electrons to an atom described by the Coulomb potential problem, the first two fill up the lowest Coulomb energy eigenstate (the ψ_{100} or $1S$ state at $n = 1$), the next eight fill up the $n = 2$ states (two each for $\psi_{200}, \psi_{211}, \psi_{210}, \psi_{21-1}$), etc. This goes a long ways towards explaining the structure of the periodic table of elements.

When one puts a hydrogen atom in a constant magnetic field B, the Hamiltonian acquires a term that acts only on the $\mathbf{C}^2$ factor, of the form

$$\frac{2e}{mc}\mathbf{B} \cdot \sigma$$

This is exactly the sort of Hamiltonian we began our study of quantum mechanics with for a simple two-state system. It causes a shift in energy eigenvalues proportional to $\pm|\mathbf{B}|$ for the two different components of the wavefunction, and the observation of this energy splitting makes clear the necessity of treating the electron using the two-component formalism.

19.4 For further reading

This is a standard topic in all quantum mechanics books. For example, see chapters 12 and 13 of [57]. The $\mathfrak{so}(4)$ calculation is not in [57], but is in some of the other such textbooks, a good example is chapter 7 of [4]. For extensive discussion of the symmetries of the $\frac{1}{r}$ potential problem, see [24] or [26].

Chapter 20

The Harmonic Oscillator

In this chapter we'll begin the study of the most important exactly solvable physical system, the harmonic oscillator. Later chapters will discuss extensions of the methods developed here to the case of fermionic oscillators, as well as free quantum field theories, which are harmonic oscillator systems with an infinite number of degrees of freedom.

For a finite number of degrees of freedom, the Stone-von Neumann theorem tells us that there is essentially just one way to non-trivially represent the (exponentiated) Heisenberg commutation relations as operators on a quantum mechanical state space. We have seen two unitarily equivalent constructions of these operators: the Schrödinger representation in terms of functions on either coordinate space or momentum space. It turns out that there is another class of quite different constructions of these operators, one that depends upon introducing complex coordinates on phase space and then using properties of holomorphic functions. We'll refer to this as the Bargmann-Fock representation, although quite a few mathematicians have had their name attached to it for one good reason or another (some of the other names one sees are Friedrichs, Segal, Shale, Weil, as well as the descriptive terms "holomorphic" and "oscillator").

Physically the importance of this representation is that it diagonalizes the Hamiltonian operator for a fundamental sort of quantum system: the harmonic oscillator. In the Bargmann-Fock representation the energy eigenstates of such a system are the simplest states and energy eigenvalues are just integers. These integers label the irreducible representations of the $U(1)$ symmetry generated by the Hamiltonian, and they can be interpreted as counting the number of "quanta" in the system. It is the ubiquity of this example that justifies the "quantum" in "quantum mechanics". The operators on the state space can be simply understood in terms of basic operators called annihilation and creation operators which increase or decrease by one the number of quanta.

20.1 The harmonic oscillator with one degree of freedom

An even simpler case of a particle in a potential than the Coulomb potential of the last chapter is the case of $V(q)$ quadratic in q. This is also the lowest-order approximation when one studies motion near a local minimum of an arbitrary $V(q)$, expanding $V(q)$ in a power series around this point. We'll write this as

$$h = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$$

with coefficients chosen so as to make ω the angular frequency of periodic motion of the classical trajectories. These satisfy Hamilton's equations

$$\dot{p} = -\frac{\partial V}{\partial q} = m\omega^2 q, \quad \dot{q} = \frac{p}{m}$$

so

$$\ddot{q} = -\omega^2 q$$

which will have solutions with periodic motion of angular frequency ω. These solutions can be written as

$$q(t) = c_+ e^{i\omega t} + c_- e^{-i\omega t}$$

for $c_+, c_- \in \mathbf{C}$ where, since $q(t)$ must be real, we have $c_- = \bar{c}_+$. The space of solutions of the equation of motion is thus two real-dimensional, and abstractly one can think of this as the phase space of the system.

More conventionally, one can parametrize the phase space by initial values that determine the classical trajectories, for instance by the position $q(0)$ and momentum $p(0)$ at an initial time $t(0)$. Since

$$p(t) = m\dot{q} = mc_+ i\omega e^{i\omega t} - mc_- i\omega e^{-i\omega t} = im\omega(c_+ e^{i\omega t} - \bar{c}_+ e^{-i\omega t})$$

we have

$$q(0) = c_+ + c_- = 2\,\mathrm{Re}(c+), \quad p(0) = im\omega(c_+ - c_-) = 2m\omega\,\mathrm{Im}(c_+)$$

so

$$c_+ = \frac{1}{2}q(0) + i\frac{1}{2m\omega}p(0)$$

The classical phase space trajectories are

$$q(t) = (\frac{1}{2}q(0) + i\frac{1}{2m\omega}p(0))e^{i\omega t} + (\frac{1}{2}q(0) - i\frac{1}{2m\omega}p(0))e^{-i\omega t}$$

$$p(t) = (\frac{im\omega}{2}q(0) - \frac{1}{2}p(0))e^{i\omega t} + (\frac{-im\omega}{2}q(0) + \frac{1}{2}p(0))e^{-i\omega t}$$

Instead of using two real coordinates to describe points in the phase space (and having to introduce a reality condition when using complex exponentials), one can instead use a single complex coordinate

$$z(t) = \frac{1}{\sqrt{2}}(q(t) - \frac{i}{m\omega}p(t))$$

Then the equation of motion is a first-order rather than second-order differential equation

$$\dot{z} = i\omega z$$

with solutions

$$z(t) = z(0)e^{i\omega t} \tag{20.1}$$

The classical trajectories are then realized as complex functions of t, and parametrized by the complex number

$$z(0) = \frac{1}{\sqrt{2}}(q(0) - \frac{i}{m\omega}p(0))$$

Since the Hamiltonian is just quadratic in the p and q, we have seen that we can construct the corresponding quantum operator uniquely using the Schrödinger representation. For $\mathcal{H} = L^2(\mathbf{R})$ we have a Hamiltonian operator

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 Q^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2$$

To find solutions of the Schrödinger equation, as with the free particle, one proceeds by first solving for eigenvectors of H with eigenvalue E, which means finding solutions to

$$H\psi_E = (-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2)\psi_E = E\psi_E$$

Solutions to the Schrödinger equation will then be linear combinations of the functions

$$\psi_E(q)e^{-\frac{i}{\hbar}Et}$$

Standard but somewhat intricate methods for solving differential equations like this show that one gets solutions for $E = E_n = (n + \frac{1}{2})\hbar\omega$, n a non-negative integer, and the normalized solution for a given n (which we'll denote ψ_n) will be

$$\psi_n(q) = (\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2})^{\frac{1}{4}} H_n(\sqrt{\frac{m\omega}{\hbar}}q)e^{-\frac{m\omega}{2\hbar}q^2} \tag{20.2}$$

where H_n is a family of polynomials called the Hermite polynomials. The ψ_n provide an orthonormal basis for $\mathcal{H}$ (one does not need to consider non-normalizable wavefunctions as in the free particle case), so any initial wavefunction $\psi(q, 0)$ can be written in the form

$$\psi(q, 0) = \sum_{n=0}^{\infty} c_n \psi_n(q)$$

with

$$c_n = \int_{-\infty}^{+\infty} \psi_n(q)\psi(q,0)dq$$

(note that the ψ_n are real-valued). At later times, the wavefunction will be

$$\psi(q,t) = \sum_{n=0}^{\infty} c_n \psi_n(q) e^{-\frac{i}{\hbar}E_n t} = \sum_{n=0}^{\infty} c_n \psi_n(q) e^{-i(n+\frac{1}{2})\omega t}$$

20.2 Creation and annihilation operators

It turns out that there is a quite easy method which allows one to explicitly find eigenfunctions and eigenvalues of the harmonic oscillator Hamiltonian (although it's harder to show it gives all of them). This also leads to a new representation of the Heisenberg group (of course unitarily equivalent to the Schrödinger one by the Stone-von Neumann theorem). Instead of working with the self-adjoint operators Q and P that satisfy the commutation relation

$$[Q,P] = i\hbar\mathbf{1}$$

we define

$$a = \sqrt{\frac{m\omega}{2\hbar}}Q + i\sqrt{\frac{1}{2m\omega\hbar}}P, \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}Q - i\sqrt{\frac{1}{2m\omega\hbar}}P$$

which satisfy the commutation relation

$$[a, a^\dagger] = \mathbf{1}$$

To simplify calculations, from now on we will set $\hbar = m = \omega = 1$. This corresponds to a specific choice of units for energy, distance and time, and the general case of arbitrary constants can be recovered by rescaling the results of our calculations. So, now

$$a = \frac{1}{\sqrt{2}}(Q + iP), \quad a^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$

and

$$Q = \frac{1}{\sqrt{2}}(a + a^\dagger), \quad P = \frac{1}{i\sqrt{2}}(a - a^\dagger)$$

The Hamiltonian operator is

$$\begin{aligned} H = \frac{1}{2}(Q^2 + P^2) =& \frac{1}{2}(\frac{1}{2}(a + a^\dagger)^2 - \frac{1}{2}(a - a^\dagger)^2) \\ =& \frac{1}{2}(aa^\dagger + a^\dagger a) \\ =& a^\dagger a + \frac{1}{2} \end{aligned}$$

Up to the constant $\frac{1}{2}$, H is given by the operator

$$N = a^\dagger a$$

which satisfies the commutation relations

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a$$

and

$$[N, a^\dagger] = a^\dagger$$

If $|c\rangle$ is a normalized eigenvector of N with eigenvalue c, one has

$$c = \langle c|a^\dagger a|c\rangle = |a|c\rangle|^2 \geq 0$$

so eigenvalues of N must be non-negative. Using the commutation relations of $N, a, a^\dagger$ gives

$$Na|c\rangle = ([N, a] + aN)|c\rangle = a(N-1)|c\rangle = (c-1)a|c\rangle$$

and

$$Na^\dagger|c\rangle = ([N, a^\dagger] + a^\dagger N)|c\rangle = a^\dagger(N+1)|c\rangle = (c+1)a^\dagger|c\rangle$$

This shows that $a|c\rangle$ will have eigenvalue $c-1$ for N, and a normalized eigenfunction for N will be

$$|c-1\rangle = \frac{1}{\sqrt{c}}a|c\rangle$$

Similarly, since

$$|a^\dagger|c\rangle|^2 = \langle c|aa^\dagger|c\rangle = \langle c|(N+1)|c\rangle = c+1$$

we have

$$|c+1\rangle = \frac{1}{\sqrt{c+1}}a^\dagger|c\rangle$$

We can find eigenfunctions for H by first solving

$$a|0\rangle = 0$$

for $|0\rangle$ (the lowest energy or "vacuum" state) which will have energy eigenvalue $\frac{1}{2}$, then acting by $a^\dagger$ n-times on $|0\rangle$ to get states with energy eigenvalue $n + \frac{1}{2}$. The equation for $|0\rangle$ is thus

$$a|0\rangle = \frac{1}{\sqrt{2}}(Q + iP)\psi_0(q) = \frac{1}{\sqrt{2}}(q + \frac{d}{dq})\psi_0(q) = 0$$

One can check that all solutions to this are all of the form

$$\psi_0(q) = Ce^{-\frac{q^2}{2}}$$

so there is a unique normalized lowest-energy eigenfunction

$$\psi_0(q) = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{q^2}{2}}$$

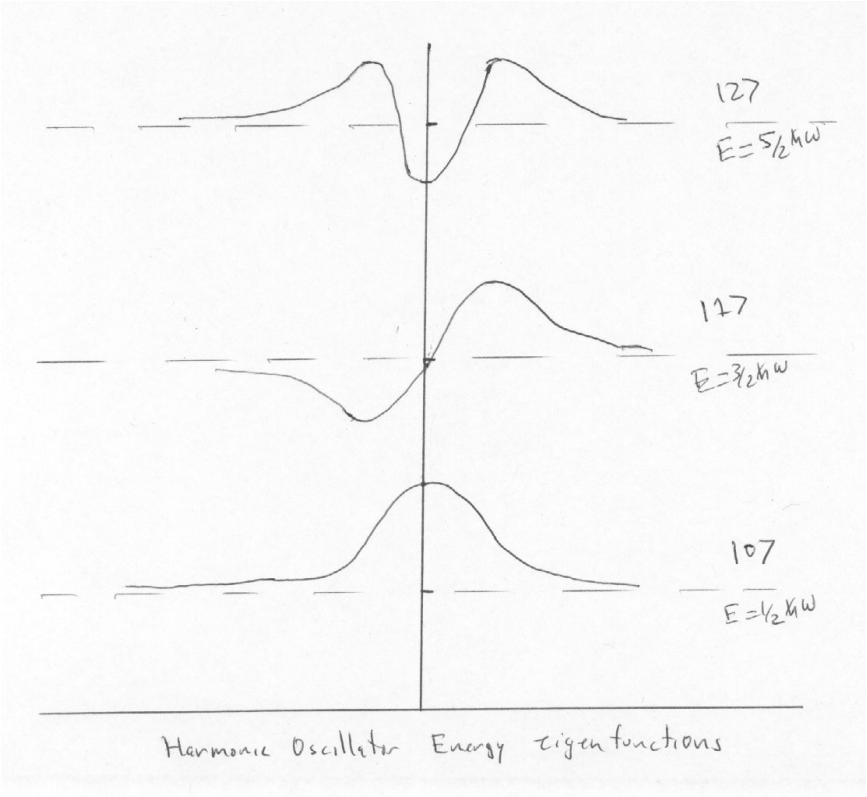
The rest of the energy eigenfunctions can be found by computing

$$|n\rangle = \frac{a^\dagger}{\sqrt{n}} \cdots \frac{a^\dagger}{\sqrt{2}} \frac{a^\dagger}{\sqrt{1}} |0\rangle = \frac{1}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} (q - \frac{d}{dq})^n e^{-\frac{q^2}{2}}$$

which (after putting back in constants and consulting the definition of a Hermite polynomial) can be shown to give the eigenfunctions claimed earlier in equation 20.2.

In the physical interpretation of this quantum system, the state $|n\rangle$, with energy $\hbar\omega(n + \frac{1}{2})$ is thought of as a state describing n "quanta". The state $|0\rangle$ is the "vacuum state" with zero quanta, but still carrying a "zero-point" energy of $\frac{1}{2}\hbar\omega$. The operators $a^\dagger$ and a have somewhat similar properties to the raising and lowering operators we used for $SU(2)$ but their commutator is different (just the identity operator), leading to simpler behavior. In this case they are called "creation" and "annihilation" operators respectively, due to the way they change the number of quanta. The relation of such quanta to physical particles like the photon is that quantization of the electromagnetic field involves quantization of an infinite collection of oscillators, with the quantum of an oscillator corresponding physically to a photon with a specific momentum and polarization. This leads to a well-known problem of how to handle the infinite vacuum energy corresponding to adding up $\frac{1}{2}\hbar\omega$ for each oscillator.

The first few eigenfunctions are plotted below. The lowest energy eigenstate is a Gaussian centered at $q = 0$, with a Fourier transform that is also a Gaussian centered at $p = 0$. Classically the lowest energy solution is an oscillator at rest at its equilibrium point ($q = p = 0$), but for a quantum oscillator one cannot have such a state with a well-defined position and momentum. Note that the plot gives the wavefunctions, which in this case are real and can be negative. The square of this function is what has an intepretation as the probability density for measuring a given position.



20.3 The Bargmann-Fock representation

Working with the operators a and $a^\dagger$ and their commutation relation

$$[a, a^\dagger] = \mathbf{1}$$

makes it clear that there is a simpler way to represent these operators than the Schrödinger representation as operators on position space functions that we have been using, while the Stone-von Neumann theorem assures us that this will be unitarily equivalent to the Schrödinger representation. This representation appears in the literature under a large number of different names, depending on the context, all of which refer to the same representation:

Definition (Bargmann-Fock or oscillator or holomorphic or Segal-Shale-Weil representation)**.** *The Bargmann-Fock (etc.) representation is given by taking as state space $\mathcal{H} = \mathcal{F}$, where $\mathcal{F}$ is the space of holomorphic functions on $\mathbf{C}$ with finite norm in the inner product*

$$\langle \psi_1 | \psi_2 \rangle = \frac{1}{\pi} \int_{\mathbf{C}} \overline{\psi_1(w)} \psi_2(w) e^{-|w|^2} du dv \tag{20.3}$$

where $w = u + iv$. We define the following two operators acting on this space:

$$a = \frac{d}{dw}, \quad a^\dagger = w$$

One has

$$[a, a^\dagger]w^n = \frac{d}{dw}(ww^n) - w\frac{d}{dw}w^n = (n + 1 - n)w^n = w^n$$

so this commutator is the identity operator on polynomials

$$[a, a^\dagger] = \mathbf{1}$$

and

Theorem. *The Bargmann-Fock representation has the following properties*

- *The elements*
$$\frac{w^n}{\sqrt{n!}}$$
of $\mathcal{F}$ for $n = 0, 1, 2, \ldots$ are orthornormal.
- *The operators a and $a^\dagger$ are adjoints with respect to the given inner product on $\mathcal{F}$.*
- *The basis*
$$\frac{w^n}{\sqrt{n!}}$$
of $\mathcal{F}$ for $n = 0, 1, 2, \ldots$ is complete.

Proof. The proofs of the above statements are not difficult, in outline they are

- For orthonormality one can just compute the integrals
$$\int_{\mathbf{C}} \overline{w}^m w^n e^{-|w|^2} du dv$$
in polar coordinates.
- To show that w and $\frac{d}{dw}$ are adjoint operators, use integration by parts.
- For completeness, assume $\langle n|\psi\rangle = 0$ for all n. The expression for the $|n\rangle$ as Hermite polynomials times a Gaussian implies that
$$\int F(q)e^{-\frac{q^2}{2}}\psi(q)dq = 0$$
for all polynomials $F(q)$. Computing the Fourier transform of $\psi(q)e^{-\frac{q^2}{2}}$ gives
$$\int e^{-ikq}e^{-\frac{q^2}{2}}\psi(q)dq = \int \sum_{j=0}^{\infty} \frac{(-ikq)^j}{j!}e^{-\frac{q^2}{2}}\psi(q)dq = 0$$
So $\psi(q)e^{-\frac{q^2}{2}}$ has Fourier transform 0 and must be 0 itself. Alternatively, one can invoke the spectral theorem for the self-adjoint operator H, which guarantees that its eigenvectors form a complete and orthonormal set.

□

Since in this representation the number operator $N = a^\dagger a$ satisfies

$$Nw^n = w\frac{d}{dw}w^n = nw^n$$

the monomials in w diagonalize the number and energy operators, so one has

$$|n\rangle = \frac{w^n}{\sqrt{n!}}$$

for the normalized energy eigenstate of energy $\hbar\omega(n + \frac{1}{2})$.

Note that we are here taking the state space $\mathcal{F}$ to include infinite linear combinations of the states $|n\rangle$, as long as the Bargmann-Fock norm is finite. We will sometimes want to restrict to the subspace of finite linear combinations of the $|n\rangle$, which we will sometimes denote $\mathcal{F}^{fin}$. This is just the space $\mathbf{C}[w]$ of polynomials.

20.4 The Bargmann transform

The Stone von-Neumann theorem implies the existence of

Definition. *Bargmann transform*
There is a unitary map called the Bargmann transform

$$\mathcal{B} : \mathcal{H}_{BF} \to \mathcal{H}_S$$

between the Bargmann-Fock and Schrödinger representations, with operators satisfying the relation

$$\Gamma'_{BF}(X) = \mathcal{B}^{-1}\Gamma'_S(X)\mathcal{B}$$

for $X \in \mathfrak{h}_{2d+1}$.

In practice, knowing $\mathcal{B}$ explicitly is often not needed, since one can use the representation independent relation

$$a_j = \frac{1}{\sqrt{2}}(Q_j + iP_j)$$

to express operators either purely in terms of a_j and $a_j^\dagger$, which have a simple expression

$$a_j = \frac{\partial}{\partial w_j}, \quad a_j^\dagger = w_j$$

in the Bargmann-Fock representation, or purely in terms of Q_j and P_j which have a simple expression

$$Q_j = q_j, \quad P_j = -i\frac{\partial}{\partial q_j}$$

in the Schrödinger representation.

To give an idea of what the Bargmann transform looks like explicitly, we'll just give the formula for the $d = 1$ case here, without proof. If $\psi(q)$ is a state in $\mathcal{H}_S = L^2(\mathbf{R})$, then

$$(\mathcal{B}\psi)(z) = \frac{1}{\pi^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-z^2 - \frac{q^2}{2} + 2qz} \psi(q) dq$$

One can check this equation for the case of the lowest energy state in the Schrödinger representation, where $|0\rangle$ has coordinate space representation

$$\psi(q) = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{q^2}{2}}$$

and

$$\begin{aligned}
(\mathcal{B}\psi)(z) =& \frac{1}{\pi^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-z^2 - \frac{q^2}{2} + 2qz} \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{q^2}{2}} dq \\
=& \frac{1}{\pi^{\frac{1}{2}}} \int_{-\infty}^{+\infty} e^{-z^2 - q^2 + 2qz} dq \\
=& \frac{1}{\pi^{\frac{1}{2}}} \int_{-\infty}^{+\infty} e^{-(q-z)^2} dq \\
=& \frac{1}{\pi^{\frac{1}{2}}} \int_{-\infty}^{+\infty} e^{-q^2} dq \\
=& 1
\end{aligned}$$

which is the expression for the state $|0\rangle$ in the Bargmann-Fock representation.

20.5 Multiple degrees of freedom

Up until now we have been working with the simple case of one physical degree of freedom, i.e. one pair (Q, P) of position and momentum operators satisfying the Heisenberg relation $[Q, P] = i\mathbf{1}$, or one pair of adjoint operators $a, a^\dagger$ satisfying $[a, a^\dagger] = \mathbf{1}$. We can easily extend this to any number d of degrees of freedom by taking tensor products of our state space $\mathcal{F}$, and d copies of our operators, acting on each factor of the tensor product. Our new state space will be

$$\mathcal{H} = \mathcal{F}_d = \underbrace{\mathcal{F} \otimes \cdots \otimes \mathcal{F}}_{\text{d times}}$$

and we will have operators

$$Q_j, P_j \quad j = 1, \ldots d$$

satisfying

$$[Q_j, P_k] = i\delta_{jk}\mathbf{1}, \quad [Q_j, Q_k] = [P_j, P_k] = 0$$

where Q_j and P_j just act on the j'th term of the tensor product in the usual way.

We can now define annihilation and creation operators in the general case:

Definition (Annihilation and creation operators)**.** *The $2d$ operators*

$$a_j = \frac{1}{\sqrt{2}}(Q_j + iP_j), \quad a_j^\dagger = \frac{1}{\sqrt{2}}(Q_j - iP_j), \quad j = 1, \ldots, d$$

are called annihilation (the a_j) and creation (the $a_j^\dagger$) operators.

One can easily check that these satisfy:

Definition (Canonical commutation relations)**.** *The canonical commutation relations (often abbreviated CCR) are*

$$[a_j, a_k^\dagger] = \delta_{jk}\mathbf{1}, \quad [a_j, a_k] = [a_j^\dagger, a_k^\dagger] = 0$$

Using the fact that tensor products of function spaces correspond to functions on the product space, in the Schrödinger representation we have

$$\mathcal{H} = L^2(\mathbf{R}^d)$$

and in the Bargmann-Fock representation $\mathcal{H} = \mathcal{F}_d$ is the space of holomorphic functions in d complex variables (with finite norm in the d-dimensional version of 20.3).

The harmonic oscillator Hamiltonian for d degrees of freedom will be

$$H = \frac{1}{2}\sum_{j=1}^{d}(P_j^2 + Q_j^2) = \sum_{j=1}^{d}(a_j^\dagger a_j + \frac{1}{2})$$

where one should keep in mind that one can rescale each degree of freedom separately, allowing different parameters ω_j for the different degrees of freedom. The energy and number operator eigenstates will be written

$$|n_1, \ldots, n_d\rangle$$

where

$$a_j^\dagger a_j |n_1, \ldots, n_d\rangle = N_j |n_1, \ldots, n_d\rangle = n_j |n_1, \ldots, n_d\rangle$$

Note that for $d = 3$ the harmonic oscillator problem is an example of the central potential problems described in chapter 19. It has an $SO(3)$ symmetry, with angular momentum operators that commute with the Hamiltonian, and space of energy eigenstates that can be organized into irreducible $SO(3)$ representations. In the Schrödinger representation states are in $\mathcal{H} = L^2(\mathbf{R}^3)$, decribed by wavefunctions that can be written in rectangular or spherical coordinates, and the Hamiltonian is a second order differential operator. In the Bargmann-Fock representation, states in $\mathcal{F}_3$ are described by holomorphic functions of 3 complex variables, with operators given in terms of products of annihilation

and creation operators. The Hamiltonian is, up to a constant, just the number operator, with energy eigenstates homogeneous polynomials (with eigenvalue of the number operator their degree).

Either the P_j, Q_k or the $a_j, a_k^\dagger$ together with the identity operator will give a representation of the Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$ on $\mathcal{H}$, and by exponentiation a representation of the Heisenberg group H_{2d+1}. Quadratic combinations of these operators will give a representation of $\mathfrak{sp}(2d, \mathbf{R})$, the Lie algebra of $Sp(2d, \mathbf{R})$. In the next chapters we will study these and other aspects of the quantum harmonic oscillator as a unitary representation.

20.6 For further reading

All quantum mechanics books should have a similar discussion of the harmonic oscillator, with a good example the detailed one in chapter 7 of Shankar [57]. One source for a detailed treatment of the Bargmann-Fock representation and Bargmann transform is [19].

Chapter 21

The Harmonic Oscillator as a Representation of the Heisenberg Group

The quantum harmonic oscillator explicitly constructed in the previous chapter provides new insight into the representation theory of the Heisenberg and metaplectic groups, using the existence of not just the Schrödinger representation Γ_S, but the unitarily equivalent Bargmann-Fock version. In this chapter we'll examine various aspects of the Heisenberg group H_{2d+1} part of this story that the formalism of annihilation and creation operators illuminates, going beyond the understanding of this representation one gets from the use of position space wavefunctions and the Schrödinger representation.

The Schrödinger representation Γ_S of H_{2d+1} uses a specific choice of extra structure on classical phase space: a decomposition of its coordinates into positions q_j and momenta p_j. For the unitarily equivalent Bargmann-Fock representation a different sort of extra structure is needed, a decomposition of coordinates on phase space into complex coordinates z_j and their complex conjugates $\overline{z}_j$. Such a decomposition is called a "complex structure" J, and will correspond after quantization to a choice that distinguishes annihilation and creation operators. This choice has physical significance, it is equivalent to a specification of the lowest energy state $|0\rangle \in \mathcal{H}$ (since this by definition is the state satisfying $a_j|0\rangle = 0$ for all annihilation operators a_j). In chapter 20 we used one particular standard choice of J. For other choices one gets different eigenstates of the number operator, known to physicists as "squeezed states". In later chapters on relativistic quantum field theory, we will see that the phenomenon of anti-particles is best understood in terms of a new possibility for the choice of J that appears in that case.

The Heisenberg group representation constructed in this way is denoted Γ_J. It does not commute with the Hamiltonian H, so it is not a symmetry, which would take states to other states with the same energy. While it doesn't com-

mute with the Hamiltonian, it does have physically important aspects. In particular it takes the state $|0\rangle$ to a distinguished set of states known as "coherent states". These states are labeled by points of the phase space $\mathbf{R}^{2d}$ and provide the closest analog possible in the quantum system of classical states (i.e. those with a well-defined value of position and momentum variables).

21.1 Complex structures and phase space

Quantization of phase space $M = \mathbf{R}^{2d}$ using the Schrödinger representation gives a unitary Lie algebra representation Γ'_S of the Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$ which takes the q_j and p_j coordinate functions on phase space to operators Q_j and P_j on $\mathcal{H}_S = L^2(\mathbf{R}^d)$. This involves a choice, that of taking states to be functions of the q_j, or (using the Fourier transform) of the p_j. It turns out to be a general phenomenon that quantization involves choosing some extra structure on phase space, beyond the Poisson bracket.

For the case of the harmonic oscillator, we found in chapter 20 that quantization was most conveniently performed using annihilation and creation operators, which involve a different sort of choice of extra structure on phase space. There we introduced complex coordinates on phase space, making the choice

$$z_j = \frac{1}{\sqrt{2}}(q_j - ip_j), \quad \overline{z}_j = \frac{1}{\sqrt{2}}(q_j + ip_j)$$

The z_j were then quantized using creation operators $a_j^\dagger$, the $\overline{z}_j$ using annihilation operators a_j. In the Bargmann-Fock representation, where the state space is a space of functions of complex variables w_j, we have

$$a_j = \frac{\partial}{\partial w_j}, \quad a_j^\dagger = w_j$$

and there is a distinguished state, the constant function, which is annihilated by all the a_j.

In this section we'll introduce the notion of a complex structure on a real vector space, with such structures characterizing the possible ways of introducing complex coordinates $z_j, \overline{z}_j$ and thus annihilation and creation operators. The abstract notion of a complex structure can be formalized as follows. Given any real vector space $V = \mathbf{R}^n$, we have seen that taking complex linear combinations of vectors in V gives a complex vector space $V \otimes \mathbf{C}$, the complexification of V, and this can be identified with $\mathbf{C}^n$, a real vector space of twice the dimension. When $n = 2d$ is even, one can get a complex vector space out of $V = \mathbf{R}^{2d}$ in a different way, but to do this one needs the following additional piece of information:

Definition (Complex structure)**.** *A complex structure on a real vector space V is a linear operator*

$$J : V \to V$$

such that

$$J^2 = -\mathbf{1}$$

Given such a pair $(V = \mathbf{R}^{2d}, J)$, one can break up complex linear combinations of vectors in V into those on which J acts as i and those on which it acts as $-i$ (since $J^2 = -\mathbf{1}$, its eigenvalues must be $\pm i$). Note that we have extended the action of J on V to an action on $V \otimes \mathbf{C}$ using complex linearity. One has

$$V \otimes \mathbf{C} = V_J^+ \oplus V_J^-$$

where V_J^+ is the $+i$ eigenspace of the operator J on $V \otimes \mathbf{C}$ and V_J^- is the $-i$ eigenspace. Complex conjugation takes elements of V_J^+ to V_J^- and vice-versa. The choice of J has thus given us two complex vector spaces of complex dimension d, V_J^+ and V_J^-, related by this complex conjugation.

Since

$$J(v - iJv) = i(v - iJv)$$

for any $v \in V$, one can identify the real vector space V with the complex vector space V_J^+ by the map

$$v \in V \to \frac{1}{\sqrt{2}}(v - iJv) \in V_J^+ \tag{21.1}$$

This allows one to think of the pair (V, J) as giving V the structure of a complex vector space, with J providing multiplication by i. Similarly, taking

$$v \in V \to \frac{1}{\sqrt{2}}(v + iJv) \in V_J^-$$

identifies V with V_J^-.

The real vector space we want to choose a complex structure on is the dual phase space $\mathcal{M} = M^*$. There will then be a decomposition

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$$

and quantization will take elements of $\mathcal{M}_J^+$ to linear combinations of creation operators, $\mathcal{M}_J^-$ to linear combinations of annihilation operators. Note that, as in earlier chapters, it is elements not of M but of the dual phase space $\mathcal{M}$ that we want to work with, since it is these that have a Lie algebra structure, and become operators after quantization.

The standard choice of complex structure is to take $J = J_0$, where J_0 is the linear operator that acts on basis vectors q_j, p_j of $\mathcal{M}$ by

$$J_0 q_j = p_j, \quad J_0 p_j = -q_j$$

One can take as basis elements of $\mathcal{M}_{J_0}^+$, the $+i$ eigenspace of J_0, the complex coordinate functions in $\mathcal{M} \otimes \mathbf{C}$ given by

$$z_j = \frac{1}{\sqrt{2}}(q_j - ip_j)$$

since one has

$$J_0 z_j = \frac{1}{\sqrt{2}}(p_j + iq_j) = iz_j$$

Basis elements of $\mathcal{M}^-_{J_0}$ are the complex conjugates

$$\overline{z}_j = \frac{1}{\sqrt{2}}(q_j + ip_j)$$

With respect to the chosen basis q_j, p_j, one can write a complex structure as a matrix. For the case of J_0 and for $d = 1$, on an arbitrary element of $\mathcal{M}$ one has

$$J_0(c_q q + c_p p) = c_q p - c_p q$$

so J_0 in matrix form with respect to the basis (q, p) is

$$J_0 \begin{pmatrix} c_q \\ c_p \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_q \\ c_p \end{pmatrix} = \begin{pmatrix} -c_p \\ c_q \end{pmatrix} \tag{21.2}$$

21.2 Complex structures and quantization

Recall that the Heisenberg Lie algebra is just the Lie algebra of linear and constant functions on M, so can be thought of as

$$\mathfrak{h}_{2d+1} = \mathcal{M} \oplus \mathbf{R}$$

where the $\mathbf{R}$ component is the constant functions. The Lie bracket is just the Poisson bracket. Complexifying this, one has

$$\mathfrak{h}_{2d+1} \otimes \mathbf{C} = (\mathcal{M} \oplus \mathbf{R}) \otimes \mathbf{C} = (\mathcal{M} \otimes \mathbf{C}) \oplus \mathbf{C} = \mathcal{M}^+_J \oplus \mathcal{M}^-_J \oplus \mathbf{C}$$

so one can write elements of $\mathfrak{h}_{2d+1} \otimes \mathbf{C}$ as pairs $(u, c) = (u^+ + u^-, c)$ where

$$u \in \mathcal{M} \otimes \mathbf{C}, \quad u^+ \in \mathcal{M}^+_J, \quad u^- \in \mathcal{M}^-_J, \quad c \in \mathbf{C}$$

This complexified Lie algebra is still a Lie algebra, with the Lie bracket relations extended from the real Lie algebra by complex linearity. One has

$$[(u_1, c_1), (u_2, c_2)] = (0, \Omega(u_1, u_2))$$

where Ω is the antisymmetric bilinear form on $\mathcal{M}$ given by the Poisson bracket on linear functions (extended by complex linearity to a bilinear form on $\mathcal{M} \otimes \mathbf{C}$).

For each J, we would like to find a quantization that takes elements of $\mathcal{M}^+_J$ to linear combinations of creation operators, $\mathcal{M}^-_J$ to linear combinations of annihilation operators. This will give a representation of the complexified Lie algebra

$$\Gamma'_J : (u, c) \in \mathfrak{h}_{2d+1} \otimes \mathbf{C} \to \Gamma'_J(u, c)$$

which must satisfy the Lie algebra homomorphism property

$$[\Gamma'_J(u_1, c_1), \Gamma'_J(u_2, c_2)] = \Gamma'_J([(u_1, c_1), (u_2, c_2)]) = \Gamma'_J(0, \Omega(u_1, u_2)) \tag{21.3}$$

Note that Γ'_J will only be a unitary representation (with $\Gamma'_J(u,c)$ skew-adjoint operators) for (u,c) in the real Lie subalgebra $\mathfrak{h}_{2d+1}$ (meaning $u \in \mathcal{M},\ c \in \mathbf{R}$).

Since we can write

$$(u,c) = (u^+,0) + (u^-,0) + (0,c)$$

where $u^+ \in \mathcal{M}^+_J$ and $u^- \in \mathcal{M}^-_J$, we have

$$\Gamma'_J(u,c) = \Gamma'_J(u^+,0) + \Gamma'_J(u^-,0) + \Gamma'_J(0,c)$$

The last term must be

$$\Gamma'_J(0,c) = -ic\mathbf{1}$$

which is chosen so that for c real one has a skew-adjoint transformation and thus a unitary representation.

We would like to construct $\Gamma'_J(u^+,0)$ as a linear combination of creation operators and $\Gamma'_J(u^-,0)$ as a linear combination of annihilation operators. For this to be possible, we need two conditions on J. The first is a compatibility condition between Ω and J: for all $v_1, v_2 \in \mathcal{M}$

$$\Omega(Jv_1, Jv_2) = \Omega(v_1, v_2) \tag{21.4}$$

From the definition of the symplectic group in chapter 14, this condition just says that $J \in Sp(2d, \mathbf{R})$. Since we are extending the action of J to $\mathcal{M} \otimes \mathbf{C}$ by complex linearity, this condition will remain true for $u_1, u_2 \in \mathcal{M} \otimes \mathbf{C}$. Given this condition, the $\Gamma'_J(u^+,0)$ will commute, since if $u_1^+, u_2^+ \in \mathcal{M}^+_J$, by 21.3 we have

$$[\Gamma'_J(u_1^+,0), \Gamma'_J(u_2^+,0)] = \Gamma'_J(0, \Omega(u_1^+, u_2^+))$$

and

$$\Omega(u_1^+, u_2^+) = \Omega(Ju_1^+, Ju_2^+) = \Omega(iu_1^+, iu_2^+) = -\Omega(u_1^+, u_2^+) = 0$$

The $\Gamma'_J(u^-,0)$ will commute with each other by essentially the same argument.

For the case of the standard complex structure $J = J_0$, one can check this compatibility condition by computing (treating the $d = 1$ case, which generalizes easily, and using equations 14.1 and 21.2)

$$\begin{aligned}
\Omega(J_0(c_q q + c_p p), J_0(c'_q q + c'_p p)) =& (\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_q \\ c_p \end{pmatrix})^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c'_q \\ c'_p \end{pmatrix}) \\
=& \begin{pmatrix} c_q & c_p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c'_q \\ c'_p \end{pmatrix} \\
=& \begin{pmatrix} c_q & c_p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} c'_q \\ c'_p \end{pmatrix} \\
=& \Omega(c_q q + c_p p, c'_q q + c'_p p)
\end{aligned}$$

More simply of course, one could just note that $J_0 \in SL(2, \mathbf{R}) = Sp(2, \mathbf{R})$.

For the case of $J = J_0$ and arbitrary values of d, one can write out explicitly Ω on basis elements

$$z_j \in \mathcal{M}^+_{J_0}, \quad \overline{z}_j \in \mathcal{M}^-_{J_0}$$

as

$$\Omega(z_j, z_k) = \{z_j, z_k\} = \{\frac{1}{\sqrt{2}}(q_j - ip_j), \frac{1}{\sqrt{2}}(q_j - ip_j)\} = 0$$

$$\Omega(\overline{z}_j, \overline{z}_k) = (\{\overline{z}_j, \overline{z}_k\} = \{\frac{1}{\sqrt{2}}(q_j + ip_j), \frac{1}{\sqrt{2}}(q_j + ip_j)\} = 0$$

$$\Omega(z_j, \overline{z}_k) = \{z_j, \overline{z}_k\} = \{\frac{1}{\sqrt{2}}(q_j - ip_j), \frac{1}{\sqrt{2}}(q_j + ip_j)\} = i\delta_{jk}$$

or

$$\{z_j, -i\overline{z}_k\} = \delta_{jk}$$

Note that here the conjugate variable to z_j with respect to the Poisson bracket is $-i\overline{z}_k$.

The Lie algebra representation is given in this case by

$$\Gamma'_{J_0}(z_j, 0) = -ia_j^\dagger = -iw_j, \quad \Gamma'_{J_0}(\overline{z}_j, 0) = -ia_j = -i\frac{\partial}{\partial w_j}, \quad \Gamma'_{J_0}(0, 1) = -i\mathbf{1}$$

Note that this is precisely the Bargmann-Fock representation, i.e. we have shown that $\Gamma'_{J_0} = \Gamma'_{BF}$.

To check that Γ'_{J_0} is a Lie algebra homomorphism, compute

$$\begin{aligned}[\Gamma'_{J_0}(z_j, 0), \Gamma'_{J_0}(\overline{z}_k, 0)] =& [-ia_j^\dagger, -ia_k] = -[a_j^\dagger, a_k] \\ =& \delta_{jk}\mathbf{1} = \delta_{jk}\Gamma'_{J_0}(0, i)\end{aligned}$$

which is correct since

$$[(z_j, 0), (\overline{z}_k, 0)] = (0, \{z_j, \overline{z}_k\}) = (0, i\delta_{jk})$$

Note that the operators a_j and $a_j^\dagger$ are not skew-adjoint, so Γ'_{J_0} is not unitary on the full Lie algebra $\mathfrak{h}_{2d+1} \otimes \mathbf{C}$, but only on the real subspace $\mathfrak{h}_{2d+1}$ of real linear combinations of $q_j, p_j, 1$.

21.3 The positivity condition on J

We still need a second condition on J, a positivity condition. Recall that the annihilation and creation operators satisfy (for $d = 1$)

$$[a, a^\dagger] = \mathbf{1}$$

This condition on the commutator corresponds to the following condition on the representation, for $J = J_0$

$$[\Gamma'_{J_0}(z, 0), \Gamma'_{J_0}(\overline{z}, 0)] = [-ia^\dagger, -ia] = \mathbf{1}$$

By the homomorphism property 21.3 we have

$$[\Gamma'_{J_0}(z, 0), \Gamma'_{J_0}(\overline{z}, 0)] = \Gamma'_{J_0}(0, \Omega(z, \overline{z})) = -i\Omega(z, \overline{z})\mathbf{1}$$

so positivity here corresponds to the fact that

$$-i\Omega(z,\overline{z}) = 1 > 0$$

Use of the opposite sign for the commutator

$$[a, a^\dagger] = -\mathbf{1}$$

would correspond to interchanging the role of a and $a^\dagger$, with the lowest energy state now satisfying $a^\dagger|0\rangle = 0$ and no state in the state space satisfying $a|0\rangle = 0$. This is equivalent to a change of sign of J, interchanging $\mathcal{M}_J^+$ and $\mathcal{M}_J^-$. For the $d = 1$ case with the wrong sign, one can just make this interchange to construct the state space, but in higher dimensions one needs to have the same sign for all $[a_j, a_j^\dagger]$. In order to have a state $|0\rangle$ that is annihilated by all annihilation operators, we need all the commutators $[a_j, a_j^\dagger]$ to have the positive sign.

For the case of general J and arbitrary d, to get operators $\Gamma'_J(u, 0)$ with the right positivity properties, we will need the condition

$$-i\Omega(u,\overline{u}) > 0$$

for non-zero $u \in \mathcal{M}_J^+$. Only if this condition is satisfied will we be able to construct Γ'_J in terms of conventional annihilation and creation operators for basis elements of $\mathcal{M}_J^+$ and $\mathcal{M}_J^-$. Using the identification 21.1 of $\mathcal{M}$ and $\mathcal{M}_J^+$, $u \in \mathcal{M}_J^+$ can be written as

$$u = \frac{1}{\sqrt{2}}(v - iJv)$$

for some non-zero $v \in \mathcal{M}$. So another way to write the positivity condition is as

$$\begin{aligned}
-i\Omega(u,\overline{u}) =& -i\frac{1}{2}\Omega(v - iJv, v + iJv) \\
=& \frac{1}{2}(-i\Omega(v,v) - i\Omega(Jv,Jv) + \Omega(v,Jv) - \Omega(Jv,v)) \\
=& \Omega(v,Jv) > 0
\end{aligned}$$

For the standard complex structure J_0, we can check this using the matrix expressions for Ω and J_0

$$\begin{aligned}
\Omega(c_q q + c_p p, J_0(c_q q + c_p p)) &= \begin{pmatrix} c_q & c_p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_q \\ c_p \end{pmatrix} \\
&= \begin{pmatrix} c_q & c_p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} c_q \\ c_p \end{pmatrix} \\
&= c_q^2 + c_p^2
\end{aligned}$$

Note that $\Omega(v, Jv)$ thus gives a positive-definite quadratic function on $\mathcal{M}$. Using the isomorphism $\mathcal{M} = M$ provided by Ω, this corresponds to a positive-definite

quadratic function on the phase space itself. For J_0 this is just (twice) the standard harmonic oscillator Hamiltonian function. One application of more general J is to the case of more general quadratic (but still positive-definite) Hamiltonian functions.

We can give a name to the class of J for which we will have a formalism of annihilation and creation operators:

Definition (Positive compatible complex structures)**.** *A complex structure J on $\mathcal{M}$ is said to be positive and compatible with Ω if it satisfies the compatibility condition 21.4 (i.e. is in $Sp(2d, \mathbf{R})$) and either of the equivalent positivity conditions*

- $$-i\Omega(u, \overline{u}) > 0$$

  for non-zero $u \in \mathcal{M}^+_J$.

- $$\Omega(v, Jv) > 0$$

  for non-zero $v \in \mathcal{M}$.

Given such a complex structure, we have:

Theorem. *Given a positive compatible complex structure J on $\mathcal{M}$, one can find a basis z^J_j of $\mathcal{M}^+_J$ such that a representation of $\mathfrak{h}_{2d+1} \otimes \mathbf{C}$, unitary for the real subalgebra $\mathfrak{h}_{2d+1}$, is given by*

$$\Gamma'_J(z^J_j, 0) = -ia^\dagger_j, \quad \Gamma'_J(\overline{z}^J_j, 0) = -ia_j, \quad \Gamma'_J(0, c) = -ic\mathbf{1}$$

where $a_j, a^\dagger_k$ satisfy the conventional commutation relations, and $\overline{z}^J_j$ is the complex conjugate of z^J_j.

Proof. An outline of the construction goes as follows:

1. Define a norm on $\mathcal{M}$ by $|v|^2 = \Omega(v, Jv)$. One then has a positive inner product $\langle \cdot, \cdot \rangle_J$ on $\mathcal{M}$ and by Gram-Schmidt orthornormalization can find a basis of $\text{span}\{q_j\} \subset \mathcal{M}$ consisting of d vectors q^J_j satisfying

   $$\langle q^J_j, q^J_k \rangle_J = \delta_{jk}$$

2. The vectors Jq^J_j will also be orthonormal since

   $$\langle Jq^J_j, Jq^J_k \rangle_J = \Omega(Jq^J_j, J^2 q^J_j) = \Omega(q^J_j, Jq^J_j) = \langle q^J_j, q^J_k \rangle_J$$

   They will be orthogonal to the q^J_j since

   $$\langle q^J_j, Jq^J_k \rangle_J = \Omega(q^J_j, J^2 q^J_k) = -\Omega(q^J_j, q^J_k) = 0$$

3. Define

$$z_j^J = \frac{1}{\sqrt{2}}(q_j^J - iJq_j^J)$$

The z_j^J give a complex basis of $\mathcal{M}_J^+$, their complex conjugates $\overline{z}_j^J$ a complex basis of $\mathcal{M}_J^-$.

4. One can check that

$$\Gamma'_J(z_j^J, 0) = -ia_j^\dagger = -iw_j, \quad \Gamma'_J(\overline{z}_j^J, 0) = -ia_j = -i\frac{\partial}{\partial w_j}$$

satisfy the desired commutation relations and give a unitary representation on linear combinations of the $(z_j^J, 0)$ and $(\overline{z}_j^J, 0)$ in the real subalgebra $\mathfrak{h}_{2d+1}$.

□

21.4 Complex structures for $d = 1$ and squeezed states

To get a better understanding of what happens for other complex structures than J_0, in this section we'll see explicitly what happens when $d = 1$. We can generalize the case $J = J_0$, where a basis of $\mathcal{M}_{J_0}^+$ is given by

$$z = \frac{1}{\sqrt{2}}(q - ip)$$

by replacing the i by an arbitrary complex number τ. Then the condition that $q - \tau p$ be in $\mathcal{M}_J^+$ and its conjugate in $\mathcal{M}_J^-$ is

$$J(q - \tau p) = J(q) - \tau J(p) = i(q - \tau p)$$

$$J(q - \overline{\tau} p) = J(q) - \overline{\tau} J(p) = -i(q - \overline{\tau} p)$$

Subtracting the two equations one finds

$$J(p) = -\frac{1}{\mathrm{Im}(\tau)}q + \frac{\mathrm{Re}(\tau)}{\mathrm{Im}(\tau)}p$$

and adding them gives

$$J(q) = -\frac{\mathrm{Re}(\tau)}{\mathrm{Im}(\tau)}q + (\mathrm{Im}(\tau) + \frac{(\mathrm{Re}(\tau))^2}{\mathrm{Im}(\tau)})p$$

With respect to the basis (q, p) the matrix for J is

$$J = \begin{pmatrix} -\frac{\mathrm{Re}(\tau)}{\mathrm{Im}(\tau)} & -\frac{1}{\mathrm{Im}(\tau)} \\ \mathrm{Im}(\tau) + \frac{(\mathrm{Re}(\tau))^2}{\mathrm{Im}(\tau)} & \frac{\mathrm{Re}(\tau)}{\mathrm{Im}(\tau)} \end{pmatrix} = \frac{1}{\mathrm{Im}(\tau)} \begin{pmatrix} -\mathrm{Re}(\tau) & -1 \\ |\tau|^2 & \mathrm{Re}(\tau) \end{pmatrix} \tag{21.5}$$

One can easily check that $\det J = 1$, so $J \in SL(2, \mathbf{R})$ and is compatible with Ω.

The positivity condition here is that the matrix

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} J = \frac{1}{\mathrm{Im}(\tau)} \begin{pmatrix} |\tau|^2 & -\mathrm{Re}(\tau) \\ \mathrm{Re}(\tau) & 1 \end{pmatrix}$$

give a positive quadratic form. This will be the case when $\mathrm{Im}(\tau) > 0$. We have thus constructed a set of J that are positive, compatible with Ω, and parametrized by an element τ of the upper half-plane, with J_0 corresponding to $\tau = i$.

To construct annihilation and creation operators satisfying the standard commutation relations

$$[a_\tau, a_\tau] = [a_\tau^\dagger, a_\tau^\dagger] = 0, \quad [a_\tau, a_\tau^\dagger] = \mathbf{1}$$

set

$$a_\tau = \frac{1}{\sqrt{2\,\mathrm{Im}(\tau)}}(Q - \overline{\tau}P), \quad a_\tau^\dagger = \frac{1}{\sqrt{2\,\mathrm{Im}(\tau)}}(Q - \tau P)$$

The Hamiltonian with eigenvalues $n + \frac{1}{2}$ for $n = 0, 1, 2, \cdots$ will be

$$H_\tau = \frac{1}{2}(a_\tau a_\tau^\dagger + a_\tau^\dagger a_\tau) = \frac{1}{2\,\mathrm{Im}(\tau)}(Q^2 + |\tau|^2 P^2 - \mathrm{Re}(\tau)(QP + PQ)) \tag{21.6}$$

The lowest energy state will satisfy

$$a_\tau |0\rangle_\tau = 0$$

which in the Schrödinger representation is the differential equation

$$(Q - \overline{\tau}P)\psi(q) = (q + i\overline{\tau}\frac{d}{dq})\psi(q) = 0$$

which has as solutions

$$\psi(q) \propto e^{i\frac{\tau}{2|\tau|^2}q^2} \tag{21.7}$$

This will be a normalizable state for $\mathrm{Im}(\tau) > 0$, again showing the necessity of the positivity condition.

Eigenstates of H_τ for general τ are known as "squeezed states" in physics. Note that for τ pure imaginary, they correspond just to a rescaling of variables

$$q \to \frac{1}{\sqrt{\mathrm{Im}(\tau)}}q, \quad p \to \sqrt{\mathrm{Im}(\tau)}p$$

Such states are "squeezed" in the sense that for $\mathrm{Im}(\tau)$ large the position uncertainty in the state $|0\rangle_\tau$ will become small (while the momentum uncertainty becomes large).

The construction for $d = 1$ can be generalized to arbitrary d, with complex structures J now parametrized by a d-dimensional complex matrix τ which must be symmetric (to be compatible with Ω), and such that $\mathrm{Im}(\tau)$ is a positive-definite matrix. The space of such complex structures is known as the Siegel upper half-space.

21.5 Coherent states and the Heisenberg group action

Since the Hamiltonian for the harmonic oscillator does not commute with the operators a_j or $a_j^\dagger$ which give the representation of the Lie algebra $\mathfrak{h}_{2d+1}$ on the state space $\mathcal{H}_{BF}$, the Heisenberg Lie group and its Lie algebra are not symmetries of the system. Energy eigenstates do not break up into irreducible representations of the group but rather the entire state space makes up such an irreducible representation. The state space for the harmonic oscillator does however have a distinguished state, the lowest energy state $|0\rangle$, and one can ask what happens to this state under the Heisenberg group action. We'll study this question for the simplest case of $d = 1$ and the standard complex structure J_0.

Considering the basis of operators for the Lie algebra representation $\mathbf{1}, a, a^\dagger$, we see that the first acts as a constant on $|0\rangle$, generating a phase tranformation of the state, while the second annihilates $|0\rangle$, so generates group transformations that leave the state invariant. It is only the third operator $a^\dagger$, that takes $|0\rangle$ to other non-zero states, and one could consider the family of states

$$e^{\alpha a^\dagger}|0\rangle$$

for $\alpha \in \mathbf{C}$. The transformations $e^{\alpha a^\dagger}$ are not unitary since $\alpha a^\dagger$ is not skew adjoint. It is better to fix this by replacing $\alpha a^\dagger$ with the skew-adjoint combination $\alpha a^\dagger - \overline{\alpha} a$, defining

Definition (Coherent states)**.** *The coherent states in $\mathcal{H}$ are the states*

$$|\alpha\rangle = e^{\alpha a^\dagger - \overline{\alpha} a}|0\rangle$$

where $\alpha \in \mathbf{C}$.

Since $e^{\alpha a^\dagger - \overline{\alpha} a}$ is unitary, the $|\alpha\rangle$ will be a family of distinct normalized states in $\mathcal{H}$, with $\alpha = 0$ corresponding to the lowest energy state $|0\rangle$. These are, up to phase transformation, precisely the states one gets by acting on $|0\rangle$ with arbitrary elements of the Heisenberg group H_3.

Using the Baker-Campbell-Hausdorff formula gives

$$|\alpha\rangle = e^{\alpha a^\dagger - \overline{\alpha} a}|0\rangle = e^{\alpha a^\dagger} e^{-\overline{\alpha} a} e^{-\frac{|\alpha|^2}{2}}|0\rangle$$

and since $a|0\rangle = 0$ one has

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} e^{\alpha a^\dagger}|0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{21.8}$$

Since $a|n\rangle = \sqrt{n}|n-1\rangle$ one finds

$$a|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{(n-1)!}}|n-1\rangle = \alpha|\alpha\rangle$$

and this property could be used as an equivalent definition of coherent states.

Note that coherent states are superpositions of different states $|n\rangle$, so are not eigenvectors of the number operator N. They are eigenvectors of

$$a = \frac{1}{\sqrt{2}}(Q + iP)$$

with eigenvalue α so one can try and think of α as a complex number whose real part gives the position and imaginary part the momentum. This does not lead to a violation of the Heisenberg uncertainty principle since this is not a self-adjoint operator, and thus not an observable. Such states are however very useful for describing certain sorts of physical phenomena, for instance the state of a laser beam, where (for each momentum component of the electromagnetic field) one does not have a definite number of photons, but does have a definite amplitude and phase.

One thing coherent states do provide is an alternate complete set of norm one vectors in $\mathcal{H}$, so any state can be written in terms of them. However, these states are not orthogonal (they are eigenvectors of a non-self-adjoint operator so the spectral theorem for self-adjoint operators does not apply). One can easily compute that

$$|\langle\beta|\alpha\rangle|^2 = e^{-|\alpha-\beta|^2}$$

One possible reason these states are given the name "coherent" is that they remain coherent states as they evolve in time (for the harmonic oscillator Hamiltonian), with α evolving in time along a classical phase space trajectory. If the state at $t = 0$ is a coherent state labeled by α_0 ($|\psi(0)\rangle = |\alpha_0\rangle$), by 21.8, at later times one has (here $\hbar = \omega = 1$)

$$\begin{aligned}
|\psi(t)\rangle =& e^{-iHt}|\alpha_0\rangle \\
=& e^{-iHt}e^{-\frac{|\alpha_0|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle \\
=& e^{-i(n+\frac{1}{2})t}e^{-\frac{|\alpha_0|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle \\
=& e^{-i\frac{1}{2}t}e^{-\frac{|e^{-it}\alpha_0|^2}{2}}\sum_{n=0}^{\infty}\frac{(e^{-it}\alpha_0)^n}{\sqrt{n!}}|n\rangle \\
=& e^{-i\frac{1}{2}t}|e^{-it}\alpha_0\rangle
\end{aligned}$$

Up to the phase factor $e^{-i\frac{1}{2}t}$, this remains a coherent state, with label α given by the classical time-dependence of the complex coordinate $\overline{z}(t) = \frac{1}{\sqrt{2}}(q(t) + ip(t))$ for the harmonic oscillator (see 20.1) with $\overline{z}(0) = \alpha_0$.

Digression (Spin coherent states)**.** *One can perform a similar construction replacing the group H_3 by the group $SU(2)$, and the state $|0\rangle$ by a highest weight vector of an irreducible representation $(\pi_n, V^n = \mathbf{C}^{n+1})$ of spin $\frac{n}{2}$. Writing $|\frac{n}{2}\rangle$*

for a highest weight vector, we have

$$\pi'_n(S_3)|\frac{n}{2}\rangle = \frac{n}{2}, \quad \pi'_n(S_+)|\frac{n}{2}\rangle = 0$$

and we can create a family of spin coherent states by acting on $|\frac{n}{2}\rangle$ *by elements of* $SU(2)$*. If we identify states in this family that differ just by a phase, the states are parametrized by a sphere.*

By analogy with the Heisenberg group coherent states, with $\pi'_n(S_+)$ *playing the role of the annihilation operator* a *and* $\pi'_n(S_-)$ *playing the role of the creation operator* $a^\dagger$*, we can define a skew-adjoint transformation*

$$\frac{1}{2}\theta e^{i\phi}\pi'_n(S_-) - \frac{1}{2}\theta e^{-i\phi}\pi'_n(S_+)$$

and exponentiate to get a family of unitary transformations parametrized by (θ, ϕ)*. Acting on the highest weight state we get a definition of the family of spin coherent states as*

$$|\theta, \phi\rangle = e^{\frac{1}{2}\theta e^{i\phi}\pi'_n(S_-) - \frac{1}{2}\theta e^{-i\phi}\pi'_n(S_+)}|\frac{n}{2}\rangle$$

One can show that the $SU(2)$ *group element used here corresponds, in terms of its action on vectors, to a rotation by an angle* θ *about the axis* $(\sin\phi, -\cos\phi, 0)$*, so one can associate the state* $|\theta, \phi\rangle$ *to the unit vector along the* z*-axis, rotated by this transformation.*

21.6 For further reading

For more about complex structures symplectic vector spaces, including a discussion of the Siegel upper half-space of (positive compatible complex structures for arbitrary d), see chapter 1.4 of [7]. Coherent states and spin coherent states are discussed in chapter 21 of [57]. Few quantum mechanics textbooks discuss squeezed states, for one that does, see chapter 12 of [78].

Chapter 22

The Harmonic Oscillator and the Metaplectic Representation, $d = 1$

In the last chapter we examined those aspects of the harmonic oscillator quantum system and the Bargmann-Fock representation that correspond to quantization of phase space functions of order less than or equal to one, finding a unitary representation Γ_J of the Heisenberg group H_{2d+1} for each positive compatible complex structure J on the dual phase space $\mathcal{M}$. We'll now turn to what happens for order two functions, which will give a representation of $Mp(2d, \mathbf{R})$ on the harmonic oscillator state space, extending Γ_J to a representation of the full Jacobi group. In this chapter we will see what happens in some detail for the $d = 1$ case, where the symplectic group is just $SL(2, \mathbf{R})$.

The choice of complex structure J corresponds not only to a choice of $|0\rangle_J$ (since J determines which operators are annihilation operators), but also to that of a specific subgroup $U(1) \subset SL(2, \mathbf{R})$. The nature of the double-cover needed for Γ_J to be a true representation (not just a representation up to sign) is best seen by considering the action of this $U(1)$ on the harmonic oscillator state space. The Lie algebra of this $U(1)$ acts on energy eigenstates with an extra $\frac{1}{2}$ term, well-known to physicists as the non-zero energy of the vacuum state, and this shows the need for the double-cover.

22.1 The metaplectic representation for $d = 1$

In the last chapter we saw that choosing a complex structure J on the dual phase space $\mathcal{M} = \mathbf{R}^{2d}$ allows one to break up complex linear combinations of the Q_j, P_j into annihilation and creation operators, giving a unitary representation Γ'_J of $\mathfrak{h}_{2d+1}$ on the Fock space $\mathcal{F}_d$. For the standard choice of complex structure $J = J_0$ we have $\Gamma'_{J_0} = \Gamma'_{BF}$ and this representation is the one used in

the standard description in terms of annihilation and creation operators of the quantum harmonic oscillator system with d degrees of freedom.

Recall from our discussion of the Schrödinger representation Γ'_S in section 18 that we can extend that representation from $\mathfrak{h}_{2d+1}$ to include quadratic combinations of the q_j, p_j, getting a unitary representation of the semi-direct product $\mathfrak{h}_{2d+1} \rtimes \mathfrak{sp}(2d, \mathbf{R})$. Restricting attention to the $\mathfrak{sp}(2d, \mathbf{R})$ factor, we get the metaplectic representation, and it is this that we will construct explicitly using Γ'_{BF} instead of Γ'_S. In this chapter, we'll start with the case $d = 1$, where $\mathfrak{sp}(2, \mathbf{R}) = \mathfrak{sl}(2, \mathbf{R})$.

One can readily compute the Poisson brackets of order two of z and $\overline{z}$ using the basic relation $\{z, \overline{z}\} = i$ and the Leibniz rule, finding the following for the non-zero cases

$$\{z\overline{z}, z^2\} = -2iz^2, \quad \{z\overline{z}, \overline{z}^2\} = 2i\overline{z}^2, \quad \{z^2, \overline{z}^2\} = 4iz\overline{z}$$

In the case of the Schrödinger representation, our quadratic combinations of p and q were real, and we could identify the Lie algebra they generated with the Lie algebra $\mathfrak{sl}(2, \mathbf{R})$ of traceless 2 by 2 real matrices with basis

$$E = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad F = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad G = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Since we have complexified, our quadratic combinations of z and $\overline{z}$ are in the complexification of $\mathfrak{sl}(2, \mathbf{R})$, the Lie algebra $\mathfrak{sl}(2, \mathbf{C})$ of traceless 2 by 2 complex matrices. We can take as a basis of $\mathfrak{sl}(2, \mathbf{C})$ over the complex numbers

$$Z = E - F, \; X_\pm = \frac{1}{2}(G \pm i(E + F))$$

which satisfy

$$[Z, X_-] = -2iX_-, \quad [Z, X_+] = 2iX_+, \quad [X_+, X_-] = -iZ$$

and then use as our isomorphism between quadratics in $z, \overline{z}$ and $\mathfrak{sl}(2, \mathbf{C})$

$$\frac{z^2}{2} \leftrightarrow X_-, \quad \frac{\overline{z}^2}{2} \leftrightarrow X_+, \quad z\overline{z} \leftrightarrow Z$$

The element

$$z\overline{z} = \frac{1}{2}(q^2 + p^2) \leftrightarrow Z = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

exponentiates to give a $SO(2) = U(1)$ subgroup of $SL(2, \mathbf{R})$ with elements of the form

$$e^{\theta Z} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

Note that $h = \frac{1}{2}(p^2 + q^2) = z\overline{z}$ is the classical Hamiltonian function for the harmonic oscillator.

We can now quantize quadratics in z and $\overline{z}$ using annihilation and creation operators acting on the Fock space $\mathcal{F}$. There is no operator ordering ambiguity for

$$z^2 \to (a^\dagger)^2 = w^2, \quad \overline{z}^2 \to a^2 = \frac{d^2}{dw^2}$$

For the case of $z\overline{z}$ (which is real), in order to get the $\mathfrak{sl}(2,\mathbf{R})$ commutation relations to come out right (in particular, the Poisson bracket $\{z^2, \overline{z}^2\} = 4iz\overline{z}$), we must take the symmetric combination

$$z\overline{z} \to \frac{1}{2}(aa^\dagger + a^\dagger a) = a^\dagger a + \frac{1}{2} = w\frac{d}{dw} + \frac{1}{2}$$

(which of course is just the standard Hamiltonian for the quantum harmonic oscillator).

Multiplying as usual by $-i$ one can now define an extension of the Bargmann-Fock representation to an $\mathfrak{sl}(2,\mathbf{C})$ representation by taking

$$\Gamma'_{BF}(X_+) = -\frac{i}{2}a^2, \quad \Gamma'_{BF}(X_-) = -\frac{i}{2}(a^\dagger)^2, \quad \Gamma'_{BF}(Z) = -i\frac{1}{2}(a^\dagger a + aa^\dagger)$$

One can check that we have made the right choice of $\Gamma'_{BF}(Z)$ to get an $\mathfrak{sl}(2,\mathbf{C})$ representation by computing

$$\begin{aligned}[\Gamma'_{BF}(X_+), \Gamma'_{BF}(X_-)] =& [-\frac{i}{2}a^2, -\frac{i}{2}(a^\dagger)^2] = -\frac{1}{2}(aa^\dagger + a^\dagger a) \\ =& -i\Gamma'_{BF}(Z) = \Gamma'_{BF}([X_+, X_-])\end{aligned}$$

As a representation of the real sub-Lie algebra $\mathfrak{sl}(2,\mathbf{R})$ of $\mathfrak{sl}(2,\mathbf{C})$, one has (using the fact that $G, E+F, E-F$ is a real basis of $\mathfrak{sl}(2,\mathbf{R})$):

Definition (Metaplectic representation of $\mathfrak{sl}(2,\mathbf{R})$)**.** *The representation Γ'_{BF} on $\mathcal{F}$ given by*

$$\Gamma'_{BF}(G) = \Gamma'_{BF}(X_+ + X_-) = -\frac{i}{2}((a^\dagger)^2 + a^2)$$

$$\Gamma'_{BF}(E+F) = \Gamma'_{BF}(-i(X_+ - X_-)) = -\frac{1}{2}((a^\dagger)^2 - a^2) \tag{22.1}$$

$$\Gamma'_{BF}(E-F) = \Gamma'_{BF}(Z) = -i\frac{1}{2}(a^\dagger a + aa^\dagger)$$

is a representation of $\mathfrak{sl}(2,\mathbf{R})$ called the metaplectic representation.

Note that one can explicitly see from these expressions that this is a unitary representation, since all the operators are skew-adjoint (using the fact that a and $a^\dagger$ are each other's adjoints).

This representation Γ'_{BF} will be unitarily equivalent to the Schrödinger version Γ'_S found earlier when quantizing q^2, p^2, pq as operators on $\mathcal{H} = L^2(\mathbf{R})$. It is however much easier to work with since it can be studied as the state

space of the quantum harmonic oscillator, with the Lie algebra acting simply by quadratic expressions in the annihilation and creation operators.

One thing that can now easily be seen is that this representation Γ'_{BF} does not integrate to give a representation of the group $SL(2,\mathbf{R})$. If the Lie algebra representation Γ'_{BF} comes from a Lie group representation Γ_{BF} of $SL(2,\mathbf{R})$, we have

$$\Gamma_{BF}(e^{\theta Z}) = e^{\theta\Gamma'_{BF}(Z)}$$

where

$$\Gamma'_{BF}(Z) = -i(a^\dagger a + \frac{1}{2}) = -i(N + \frac{1}{2})$$

so

$$\Gamma_{BF}(e^{\theta Z})|n\rangle = e^{-i\theta(n+\frac{1}{2})}|n\rangle$$

Taking $\theta = 2\pi$, this gives an inconsistency

$$\Gamma_{BF}(\mathbf{1})|n\rangle = -|n\rangle$$

which has its origin in the physical phenomenon that the energy of the lowest energy eigenstate $|0\rangle$ is $\frac{1}{2}$ rather than 0, so not an integer.

This is precisely the same sort of problem we found when studying the spinor representation of the Lie algebra $\mathfrak{so}(3)$. Just as in that case, the problem indicates that we need to consider not the group $SL(2,\mathbf{R})$, but a double cover, the metaplectic group $Mp(2,\mathbf{R})$. The behavior here is quite a bit more subtle than in the $Spin(3)$ double cover case, where $Spin(3)$ was just the group $SU(2)$, and topologically the only non-trivial cover of $SO(3)$ was the $Spin(3)$ one since $\pi_1(SO(3)) = \mathbf{Z}_2$. Here one has $\pi_1(SL(2,\mathbf{Z})) = \mathbf{Z}$, and each extra time one goes around the $U(1)$ subgroup we are looking at one gets a topologically different non-contractible loop in the group. As a result, $SL(2,\mathbf{R})$ has lots of non-trivial covering groups, of which only one interests us, the double cover $Mp(2,\mathbf{R})$. In particular, there is an infinite-sheeted universal cover $\widetilde{SL(2,\mathbf{R})}$, but that plays no role here.

Digression. *This group $Mp(2,\mathbf{R})$ is quite unusual in that it is a finite-dimensional Lie group, but does not have any sort of description as a group of finite-dimensional matrices. This is related to the fact that its only interesting irreducible representation is the infinite-dimensional one we are studying. The lack of any significant irreducible finite-dimensional representations corresponds to its not having a matrix description, which would give such a representation. Note that the lack of a matrix description means that this is a case where the definition we gave of a Lie algebra in terms of the matrix exponential does not apply. The more general geometric definition of the Lie algebra of a group in terms of the tangent space at the identity of the group does apply, although to do this one really needs a construction of the double cover $Mp(2,\mathbf{R})$, which is quite non-trivial. This is not actually a problem for purely Lie algebra calculations, since the Lie algebras of $Mp(2,\mathbf{R})$ and $SL(2,\mathbf{R})$ can be identified.*

Another aspect of the metaplectic representation that is relatively easy to see in the Bargmann-Fock construction is that the state space $\mathcal{F}$ is not an irreducible representation, but is the sum of two irreducible representations

$$\mathcal{F} = \mathcal{F}_{even} \oplus \mathcal{F}_{odd}$$

where $\mathcal{F}_{even}$ consists of the even functions, $\mathcal{F}_{odd}$ of odd functions. On the subspace $\mathcal{F}^{fin} \subset \mathcal{F}$ of finite sums of the number eigenstates, these are just the even and odd degree polynomials. Since the generators of the Lie algebra representation are degree two combinations of annihilation and creation operators, they will take even functions to even functions and odd to odd. The separate irreducibility of these two pieces is due to the fact that (when $n = m(2)$), one can get from state $|n\rangle$ to any another $|m\rangle$ by repeated application of the Lie algebra representation operators.

22.2 Complex structures and the $SL(2, \mathbf{R})$ action on $\mathcal{M}$

Recall from the discussion in chapter 18 that the existence of the metaplectic representation can be understood in terms of the fact that the action of $SL(2, \mathbf{R})$ on $\mathcal{M}$ implies an action by automorphisms on the Heisenberg group H_3, together with the uniqueness (up unitary equivalence) of the irreducible representation of H_3. This $SL(2, \mathbf{R})$ action on H_3 was studied in section 14.2 where we saw that it was given infinitesimally by Poisson brackets between order two ($\mathfrak{sl}(2, \mathbf{R})$) and linear ($\mathfrak{h}_3$) polynomials (see equation 14.8).

The Bargmann-Fock construction above of the metaplectic representation depends on an extra choice, one that is not invariant under the $SL(2, \mathbf{R})$ action. This is the choice of a complex structure J_0 to provide the splitting $\mathcal{M} \otimes \mathbf{C} = \mathcal{M}^+_{J_0} \oplus \mathcal{M}^-_{J_0}$ into $\pm i$ eigenspaces of J_0. Recall that the group $SL(2, \mathbf{R})$ acts on $\mathcal{M}$ by matrices

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

satisfying $\alpha\delta - \beta\gamma = 1$ (with respect to the choice of a basis $\{q, p\}$). Only a subgroup of $SL(2, \mathbf{R})$ will respect the splitting provided by J_0: the subgroup of matrices commuting with J_0. This will be this subgroup of $SL(2, \mathbf{R})$ that acts on $\mathcal{M} \otimes \mathbf{C}$ (extending the action on $\mathcal{M}$ by complex linearity) taking $\mathcal{M}^+_{J_0}$ to $\mathcal{M}^+_{J_0}$ and $\mathcal{M}^-_{J_0}$ to $\mathcal{M}^-_{J_0}$.

This commutativity condition is explicitly

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

so

$$\begin{pmatrix} \beta & -\alpha \\ \delta & -\gamma \end{pmatrix} = \begin{pmatrix} -\gamma & -\delta \\ \alpha & \beta \end{pmatrix}$$

which implies $\beta = -\gamma$ and $\alpha = \delta$. The elements of $SL(2, \mathbf{R})$ that we want will be of the form

$$\begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}$$

with unit determinant, so $\alpha^2 + \beta^2 = 1$. This is the $U(1) = SO(2)$ subgroup of $SL(2, \mathbf{R})$ of matrices of the form

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = e^{\theta Z}$$

The metaplectic representation restricted to this subgroup was studied using the Schrödinger representation in 18.2.1, and its role in showing the necessity of the metaplectic double cover was seen in the last section. Here we'll study the representation on the same subgroup, but in the Bargmann-Fock version using annihilation and creation operators.

Introducing the complex structure J_0 and thus coordinates $z, \overline{z}$ on the complexification $\mathcal{M} \otimes \mathbf{C}$, the Poisson bracket relations 14.8 after complexification break up into two sorts: those that preserve the complex structure and those that don't. The ones that preserve the complex structure will be

$$\{z\overline{z}, z\} = -iz, \quad \{z\overline{z}, \overline{z}\} = i\overline{z} \tag{22.2}$$

since it is $z\overline{z}$ that corresponds to Z according to our isomorphism of order two polynomials and $\mathfrak{sl}(2, \mathbf{R})$. Note that this could be written as

$$\{z\overline{z}, \begin{pmatrix} z \\ \overline{z} \end{pmatrix}\} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} z \\ \overline{z} \end{pmatrix}$$

which is a (complexified) example of equation 14.14 since $\mu_Z = z\overline{z}$ and $Z = -J_0$ acts as $-i$ on the coordinate function z, and i on the coordinate function $\overline{z}$.

Quantization by the metaplectic representation gives (see 22.1)

$$\Gamma'_{BF}(z\overline{z}) = \Gamma'_{BF}(Z) = -\frac{i}{2}(aa^\dagger + a^\dagger a)$$

and the quantized analogs of 22.2 are

$$[-\frac{i}{2}(aa^\dagger + a^\dagger a), a^\dagger] = -ia^\dagger, \quad [-\frac{i}{2}(aa^\dagger + a^\dagger a), a] = ia \tag{22.3}$$

Exponentiating, one has $g = e^{\theta Z} \in U(1) \subset SL(2, \mathbf{R})$ and unitary operators

$$U_g = \Gamma_{BF}(e^{\theta Z}) = e^{-i\frac{\theta}{2}(aa^\dagger + a^\dagger a)}$$

which satisfy

$$U_g a^\dagger U_g^{-1} = e^{-i\theta} a^\dagger, \quad U_g a U_g^{-1} = e^{i\theta} a \tag{22.4}$$

Note that, using equation 5.1 one has

$$\frac{d}{d\theta}(U_g a^\dagger U_g^{-1})_{|\theta=0} = [-\frac{i}{2}(aa^\dagger + a^\dagger a), a^\dagger]$$

so equation 22.3 is just the derivative at the identity of equation 22.4. Also note that

We see that, on operators, conjugation by the action of the $U(1)$ subgroup of $SL(2,\mathbf{R})$ does not mix creation and annihilation operators. On the distinguished state $|0\rangle$, U_g acts as the phase transformation

$$U_g|0\rangle = e^{-i\frac{1}{2}\theta}|0\rangle$$

Besides 22.2, there are also Poisson bracket relations corresponding to infinitesimal $\mathfrak{sl}(2,\mathbf{R})$ transformations that do not preserve the complex structure. They are

$$\{z^2, \overline{z}\} = 2iz, \quad \{z^2, z\} = 0, \quad \{\overline{z}^2, z\} = -2i\overline{z}, \quad \{\overline{z}^2, \overline{z}\} = 0 \tag{22.5}$$

As an example of $SL(2,\mathbf{R})$ transformations that change the complex structure, consider the subgroup of elements of the form

$$g_\alpha = \begin{pmatrix} e^\alpha & 0 \\ 0 & e^{-\alpha} \end{pmatrix}$$

For $\alpha > 0$ these are "squeezing" transformations which expand vectors in the q direction in $\mathcal{M}$, and contract them in the p direction. One can think of these as a change of basis in $\mathcal{M}$, with the complex structure in the new basis

$$J_\alpha = g_\alpha J_0 g_\alpha^{-1} = \begin{pmatrix} e^\alpha & 0 \\ 0 & e^{-\alpha} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-\alpha} & 0 \\ 0 & e^\alpha \end{pmatrix} = \begin{pmatrix} 0 & e^{2\alpha} \\ e^{-2\alpha} & 0 \end{pmatrix}$$

Comparing to equation 21.5 we find that J_α is the positive compatible complex structure with parameter $\tau = ie^{2\alpha}$.

The relations 22.5 correspond to the following relations of annihilation and creation operators:

$$[(a^\dagger)^2, a] = -2a^\dagger, \quad [(a^\dagger)^2, a^\dagger] = 0, \quad [a^2, a^\dagger] = 2a, \quad [a^2, a] = 0$$

and one sees that conjugation by exponentials of linear combinations of a^2 and $(a^\dagger)^2$ will mix annihilation and creation operators (unlike the $U(1) \subset SL(2,\mathbf{R})$ case of equations 22.3 and 22.4). For the example above

$$g_\alpha = e^{\alpha G}$$

and we find

$$\Gamma_{BF}(g_\alpha) = \Gamma_{BF}(e^{\alpha G}) = e^{\alpha \Gamma'_{BF}(G)} = e^{-\alpha \frac{i}{2}((a^\dagger)^2 + a^2)}$$

by 22.1.

The $\Gamma_{BF}(g_\alpha)$ are unitary operators (since exponentials of skew-adjoint operators) on the Fock space $\mathcal{F}$ that take $|0\rangle$ to a different state $|0\rangle_\alpha$, not proportional to $|0\rangle$. This state $|0\rangle_\alpha$ can be used to characterize the complex structure J_α, as the one corresponding to the change of variables that takes the annihilation operator a to the linear combination of annihilation and creation operators that annihilates $|0\rangle_\alpha$. One can generalize this for arbitrary positive compatible complex structures, and get a map that take τ in the upper half-plane to vectors in $\mathcal{F}$ (modulo scalar multiplication of the vectors). This map turns out to be quite useful in algebraic geometry, providing an embedding of the upper half-plane in complex projective space (the same holds true for $d > 1$ for the Siegel upper half-space).

22.3 Normal Ordering

Whenever one has a product involving both z and $\overline{z}$ that one would like to quantize, the non-trivial commutation relation of a and $a^\dagger$ means that one has different inequivalent possibilities, depending on the order one chooses for the a and $a^\dagger$. In this case, we chose to quantize $h = z\overline{z}$ using the symmetric choice

$$H = \frac{1}{2}(aa^\dagger + a^\dagger a) = a^\dagger a + \frac{1}{2}$$

because quantization of order two polynomials then gave a representation of $\mathfrak{sl}(2, \mathbf{R})$. We could instead have chosen to use $a^\dagger a$, which is an example of a "normal-ordered" product.

Definition. *Normal-ordered product*

Given any product P of the a and $a^\dagger$ operators, the normal ordered product of P, written $:P:$ is given by re-ordering the product so that all factors $a^\dagger$ are on the left, all factors a on the right, for example

$$:a^2a^\dagger a(a^\dagger)^3: = (a^\dagger)^4a^3$$

The advantage of working with the normal-ordered choice

$$a^\dagger a = :\frac{1}{2}(aa^\dagger + a^\dagger a):$$

is that it acts trivially on $|0\rangle$ and has integer rather than half-integer eigenvalues on $\mathcal{F}$. There is then no need to invoke a double-covering. The disadvantage is that one gets a representation of $\mathfrak{u}(1)$ that does not extend to $\mathfrak{sl}(2, \mathbf{R})$. One also needs to keep in mind that the definition of normal-ordering depends upon the choice of J, or equivalently, the choice of distinguished state $|0\rangle$ annihilated by the annihilation operators. A better notation would be something like $:P:_J$ rather than just $:P:$.

We have now seen that the necessary choice of a complex structure J in a Bargmann-Fock type quantization shows up in the following distinguished features of the representation:

- The choice of the decomposition $\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$. After quantization this determines which operators are linear combinations of annihilation operators and which are linear combinations of creation operators.

- The choice of normal-ordering prescription. $SL(2, \mathbf{R})$ transformations that mix annihilation and creation operators change the definition of the normal ordering symbol : :.

- The choice (up to a scalar factor) of a distinguished state $|0\rangle \in \mathcal{H}$, the state annihilated by annihilation operators. Equation 21.7 gives this state explicitly in the Schrödinger representation, showing how it depends on the complex structure τ.

- The choice of quadratic Hamiltonian as half the symmetrized product of annihilation and creation operators, and thus with energy eigenstates given by applying creation operators to $|0\rangle$. See equation 21.6 for the explicit form of this as a function of τ.

- The choice of a distinguished subgroup $U(1) \subset SL(2, \mathbf{R})$, the subgroup that commutes with J.

We saw in chapter 21 that the space of positive, compatible complex structures can be parametrized by the upper half-plane. An alternate way of characterizing this space is as the quotient space $SL(2, \mathbf{R})/U(1)$, since $SL(2, \mathbf{R})$ acts transitively on the complex structures (by conjugation of the matrix for J), with the stabilizer of J a subgroup $U(1) \subset SL(2, \mathbf{R})$.

$SL(2, \mathbf{R})$ transformations that do not commute with the complex structure are known in the physics literature as "Bogoliubov transformations". Instead of describing such transformations as we have done, in terms of real matrices and the basis q, p of $\mathcal{M}$, one can instead use complex matrices and the basis $z, \overline{z}$ of $\mathcal{M} \otimes \mathbf{C}$. Transformations that preserve the Poisson brackets (and, after quantization, the commutation relations of annihilation and creation operators) are given by complex matrices of the form

$$\begin{pmatrix} \alpha & \beta \\ \overline{\beta} & \overline{\alpha} \end{pmatrix}, \quad |\alpha|^2 - |\beta|^2 = 1$$

The group of such matrices is called $SU(1, 1)$ and is isomorphic to $SL(2, \mathbf{R})$.

22.4 For further reading

The metaplectic representation is not usually mentioned in the physics literature, and the discussions in the mathematical literature tend to be aimed at an advanced audience. Two good examples of such detailed discussions can be found in [19] and chapters 1 and 11 of [66]. For an example of the use of Bogoliubov transformations (change of complex structure) in the theory of superfluidity, see chapter 10.3 of [61].

Chapter 23

The Harmonic Oscillator as a Representation of $U(d)$

As a representation of $Mp(2d, \mathbf{R})$, Γ_{BF} is unitarily equivalent (by the Bargmann transform) to Γ_S, the Schrödinger representation studied earlier. The Bargmann-Fock version though makes some aspects of the representation easier to study; in particular it makes clear the nature of the double-cover that appears. A subtle aspect of the Bargmann-Fock construction is that it depends on a specific choice of complex structure J, a choice which corresponds to a choice of a distinguished state $|0\rangle$. This same choice picks out a subgroup $U(d) \subset Sp(2d, \mathbf{R})$ of transformations which commute with J, and the harmonic oscillator state space gives one a representation of a double-cover of this group. We will see that normal-ordering the products of annihilation and creation operators turns this into a representation of $U(d)$ itself. In this way, a $U(d)$ action on the finite-dimensional phase space gives operators that provide an infinite dimensional representation of $U(d)$ on the harmonic oscillator state space $\mathcal{H}$. This method for turning symmetries of the classical phase space into unitary representations of the symmetry group on a quantum state space is elaborated in great detail here not just because of its application to these simple quantum systems, but because it will turn out to be fundamental in our later study of quantum field theories.

We will see in detail how in the case $d = 2$ the group $U(2) \subset Sp(4, \mathbf{R})$ commutes with the Hamiltonian, so acts as symmetries preserving energy eigenspaces on the harmonic oscillator state space. This gives the same construction of all $SU(2) \subset U(2)$ irreducible representations that we studied in chapter 8. The case $d = 3$ corresponds to the physical example of a quadratic central potential in three dimensions, with the rotation group acting on the state space as an $SO(3)$ subgroup of the subgroup $U(3) \subset Sp(6, \mathbf{R})$ of symmetries commuting with the Hamiltonian.

23.1 Complex structures and the $Sp(2d, \mathbf{R})$ action on $\mathcal{M}$

We saw in chapter 21 that a generalization of the Bargmann-Fock representation can be defined for any choice of a positive compatible complex structure J on $\mathcal{M} = \mathbf{R}^{2d}$. J provides a decomposition

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$$

One can choose complex coordinates $z_j,\ j = 1, \cdots, d$ which will be basis elements in $\mathcal{M}_J^+$, while the $\overline{z}_j,\ j = 1, \cdots, d$ are basis elements in $\mathcal{M}^-$. The standard choice of complex structure $J = J_0$ corresponds to the choice

$$z_j = \frac{1}{\sqrt{2}}(q_j - ip_j), \quad \overline{z}_j = \frac{1}{\sqrt{2}}(q_j + ip_j)$$

with more general choices of complex structures given by the linear combinations of q_j, p_j described in detail for the $d = 1$ case in section 21.4. For the calculations of this chapter, one can assume unless otherwise stated that either the choice $J = J_0$ has been made, or the choice of complex structure does not matter.

The choice of complexified coordinate functions $z_j, \overline{z}_j$ gives a decomposition of the complexified Lie algebra $\mathfrak{sp}(2d, \mathbf{C})$ into three sub-algebras as follows:

- A Lie subalgebra with basis elements $z_j z_k$ (as usual, the Lie bracket is the Poisson bracket). There are $\frac{1}{2}(d^2 + d)$ distinct such basis elements. This is a commutative Lie subalgebra, since the Poisson bracket of any two basis elements is zero.

- A Lie subalgebra with basis elements $\overline{z}_j \overline{z}_k$. Again, it has dimension $\frac{1}{2}(d^2 + d)$ and is a commutative Lie subalgebra.

- A Lie subalgebra with basis elements $z_j \overline{z}_k$, which has dimension d^2. Computing Poisson brackets one finds

$$\begin{aligned} \{z_j \overline{z}_k, z_l \overline{z}_m\} =& z_j \{\overline{z}_k, z_l \overline{z}_m\} + \overline{z}_k \{z_j, z_l \overline{z}_m\} \\ =& -i z_j \overline{z}_m \delta_{kl} + i z_l \overline{z}_k \delta_{jm} \end{aligned} \tag{23.1}$$

The first two subalgebras correspond to complexified infinitesimal $Sp(2, \mathbf{R})$ transformations that do not preserve the decomposition

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_{J_0}^+ \oplus \mathcal{M}_{J_0}^-$$

These are the analogs for arbitrary d of the Bogoliubov transformations studied in the case $d = 1$, but we will not further discuss their properties in the general case. The last subalgebra is the one we will mostly be interested in since it turns out that quantization of elements of this subalgebra produces the operators of most physical interest.

Taking all complex linear combinations, this subalgebra can be identified with the Lie algebra $\mathfrak{gl}(d, \mathbf{C})$ of all d by d complex matrices, since if E_{jk} is the matrix with 1 at the j-th row and k-th column, zeros elsewhere, one has

$$[E_{jk}, E_{lm}] = E_{jm}\delta_{kl} - E_{lk}\delta_{jm}$$

and these provide a basis of $\mathfrak{gl}(d, \mathbf{C})$. Identifying bases by

$$iz_j\overline{z}_k \leftrightarrow E_{jk}$$

gives the isomorphism of Lie algebras. This $\mathfrak{gl}(d, \mathbf{C})$ is the complexification of $\mathfrak{u}(d)$, the Lie algebra of the unitary group $U(d)$. Elements of $\mathfrak{u}(d)$ will correspond to skew-adjoint matrices so real linear combinations of the real quadratic functions

$$z_j\overline{z}_k + \overline{z}_j z_k, \quad i(z_j\overline{z}_k - \overline{z}_j z_k)$$

on $\mathcal{M}$.

The moment map here is

$$A \in \mathfrak{gl}(d, \mathbf{C}) \to \mu_A = i\sum_{j,k} z_j A_{jk}\overline{z}_k$$

and we have

Theorem 23.1. *One has the Poisson bracket relation*

$$\{\mu_A, \mu_{A'}\} = \mu_{[A,A']}$$

so the moment map is a Lie algebra homomorphism.

One also has (for column vectors $\mathbf{z}$ *with components* $z_1, \ldots, z_d$*)*

$$\{\mu_A, \mathbf{z}\} = A^T\mathbf{z}, \quad \{\mu_A, \overline{\mathbf{z}}\} = -A\overline{\mathbf{z}} \tag{23.2}$$

Proof. Using 23.1 one has

$$\begin{aligned}
\{\mu_A, \mu_{A'}\} &= -\sum_{j,k,l,m} \{z_j A_{jk}\overline{z}_k, z_l A'_{lm}\overline{z}_m\} \\
&= -\sum_{j,k,l,m} A_{jk}A'_{lm}\{z_j\overline{z}_k, z_l\overline{z}_m\} \\
&= i\sum_{j,k,l,m} A_{jk}A'_{lm}(z_j\overline{z}_m\delta_{kl} - z_l\overline{z}_k\delta_{jm}) \\
&= i\sum_{j,k} z_j[A, A']_{jk}\overline{z}_k = \mu_{[A,A']}
\end{aligned}$$

To show 23.2, compute

$$\begin{aligned}
\{\mu_A, z_l\} =& \{i\sum_{j,k} z_j A_{jk}\overline{z}_k, z_l\} = i\sum_{j,k} z_j A_{jk}\{\overline{z}_k, z_l\} \\
=& \sum_j z_j A_{jl}
\end{aligned}$$

and

$$\begin{aligned}\{\mu_A, \overline{z}_l\} =& \{i \sum_{j,k} z_j A_{jk} \overline{z}_k, \overline{z}_l\} = i \sum_{j,k} A_{jk} \{z_j, \overline{z}_l\} \overline{z}_k \\ =& -\sum_k A_{lk} \overline{z}_k\end{aligned}$$

□

Note that here we have written formulas for $A \in \mathfrak{gl}(d, \mathbf{C})$, an arbitrary complex d by d matrix. It is only for $A \in \mathfrak{u}(d)$, the skew-adjoint ($\overline{A^T} = -A$) matrices, that μ_A will be a real-valued moment map, lying in the real lie algebra $sp(2d, \mathbf{R})$, and giving a unitary representation on the state space after quantization. For such A we can write the relations 23.2 as a (complexified) example of 14.14

$$\{\mu_A, \begin{pmatrix} \mathbf{z} \\ \overline{\mathbf{z}} \end{pmatrix}\} = \begin{pmatrix} A^T & \mathbf{0} \\ \mathbf{0} & \overline{A^T} \end{pmatrix} \begin{pmatrix} \mathbf{z} \\ \overline{\mathbf{z}} \end{pmatrix}$$

Recall that in chapter 14 we found the moment map $\mu_L = -\mathbf{q} \cdot A\mathbf{p}$ for elements $L \in \mathfrak{sp}(2d, \mathbf{R})$ of the block-diagonal form

$$\begin{pmatrix} A & \mathbf{0} \\ \mathbf{0} & -A^T \end{pmatrix}$$

where A is a real d by d matrix and so in $\mathfrak{gl}(d, \mathbf{R})$. That block decomposition corresponded to the decomposition of basis vectors of $\mathcal{M}$ into the sets q_j and p_j. Here we have complexified, and are working with respect to a different decomposition, that of $\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$. The matrices A in this case are complex, skew-adjoint, and in a different Lie subalgebra, $\mathfrak{u}(d) \subset \mathfrak{sp}(2d, \mathbf{R})$.

The standard Hamiltonian

$$h = \sum_{j=1}^{d} z_j \overline{z}_j$$

lies in this sub-algebra (it is the case $A = -i\mathbf{1}$), and one can show that its Poisson brackets with the rest of the sub-algebra are zero. It gives a basis element of the one-dimensional $\mathfrak{u}(1)$ subalgebra that commutes with the rest of the $\mathfrak{u}(d)$ subalgebra.

In section 22.2, for the case $d = 1$ and $J = J_0$, we found that there was a $U(1) \subset SL(2, \mathbf{R})$ group acting on $\mathcal{M}$ preserving Ω, and commuting with J_0. Complexifying $\mathcal{M}$ this $U(1)$ acted separately on $\mathcal{M}_{J_0}^+$ and $\mathcal{M}_{J_0}^-$, and there was a moment map taking $Z = -J_0$ to the function $\mu_Z = z\overline{z}$ on M. Here we have a $U(d) \subset Sp(2d, \mathbf{R})$, again acting on $\mathcal{M}$ preserving Ω, and commuting with J, so also acting separately on $\mathcal{M}_J^+$ and $\mathcal{M}_J^-$ after complexification.

23.2 The metaplectic representation and $U(d) \subset Sp(2d, \mathbf{R})$

Turning to the quantization problem, we would like to extend the quantization of linear functions of $z_j, \overline{z}_j$ of chapter 21 to quadratic functions, using annihilation and creation operators. For any j, k one can take

$$z_j z_k \to -i a_j^\dagger a_k^\dagger, \quad \overline{z}_j \overline{z}_k \to -i a_j a_k$$

There is no ambiguity in the quantization of the two subalgebras given by pairs of the z coordinates or pairs of the $\overline{z}$ coordinates since creation operators commute with each other, and annihilation operators commute with each other.

If $j \neq k$ one can take

$$z_j \overline{z}_k \to -i a_j^\dagger a_k = -i a_k a_j^\dagger$$

and there is again no ordering ambiguity. If $j = k$, as in the $d = 1$ case there is a choice to be made. One possibility is to take

$$z_j \overline{z}_j \to -i \frac{1}{2}(a_j a_j^\dagger + a_j^\dagger a_j) = -i(a_j^\dagger a_j + \frac{1}{2})$$

which will have the proper $\mathfrak{sp}(2d, \mathbf{R})$ commutation relations (in particular for commutators of a_j^2 with $(a_j^\dagger)^2$), but require going to a double cover to get a true representation of the group. The Bargmann-Fock construction thus gives us a unitary representation of $\mathfrak{u}(d)$ on Fock space $\mathcal{F}_d$, but after exponentiation this is a representation not of the group $U(d)$, but of a double cover we call $\widetilde{U(d)}$.

One could instead quantize using normal-ordered operators, taking

$$z_j \overline{z}_j \to -i a_j^\dagger a_j$$

The definition of normal ordering generalizes simply, since the order of annihilation and creation operators with different values of j is immaterial. If one uses this normal-ordered choice, one has shifted the usual quantized operators of the Bargmann-Fock representation by a scalar $\frac{1}{2}$ for each j, and after exponentiation the state space $\mathcal{H} = \mathcal{F}_d$ provides a representation of $U(d)$, with no need for a double cover. As a $\mathfrak{u}(d)$ representation however, this does not extend to a representation of $\mathfrak{sp}(2d, \mathbf{R})$, since commutation of a_j^2 with $(a_j^\dagger)^2$ can land one on the unshifted operators.

We saw above that the infinitesimal action of $\mathfrak{u}(d) \subset \mathfrak{sp}(2d, \mathbf{R})$ preserves the decomposition of $\mathcal{M} \otimes \mathbf{C} = \mathcal{M}^+ \oplus \mathcal{M}^-$, and this will be true after exponentiating for $U(d) \subset Sp(2d, \mathbf{R})$. We won't show this here, but $U(d)$ is the maximal subgroup that preserves this decomposition. The analog of the $d = 1$ parametrization of possible distinguished states $|0\rangle$ by $SL(2, \mathbf{R})/U(1)$ here would be a parametrization of such states (or, equivalently, of possible choices of J) by the space $Sp(2d, \mathbf{R})/U(d)$, the Siegel upper half-space.

Since the normal-ordering doesn't change the commutation relations obeyed by products of the form $a_j^\dagger a_k$, one can quantize the quadratic expression for

μ_A and get quadratic combinations of the $a_j, a_k^\dagger$ with the same commutation relations as in theorem 23.1. Letting

$$U'_A = \sum_{j,k} a_j^\dagger A_{jk} a_k$$

we have

Theorem 23.2. *For $A \in \mathfrak{gl}(d, \mathbf{C})$ a d by d complex matrix one has*

$$[U'_A, U'_{A'}] = U_{[A,A']}$$

So

$$A \in \mathfrak{gl}(d, \mathbf{C}) \to U'_A$$

is a Lie algebra representation of $\mathfrak{gl}(d, \mathbf{C})$ on $\mathcal{H} = \mathbf{C}[w_1, \ldots, w_d]$, the harmonic oscillator state space in d degrees of freedom.

One also has (for column vectors $\mathbf{a}$ with components $a_1, \ldots, a_d$)

$$[U'_A, \mathbf{a}^\dagger] = A^T \mathbf{a}^\dagger, \quad [U'_A, \mathbf{a}] = -A\mathbf{a} \tag{23.3}$$

Proof. Essentially the same proof as 23.1. □

For $A \in \mathfrak{u}(d)$ the Lie algebra representation U'_A of $\mathfrak{u}(d)$ exponentiates to give a representation of $U(d)$ on $\mathcal{H} = \mathbf{C}[w_1, \ldots, w_d]$ by operators

$$U_{e^A} = e^{U'_A}$$

These satisfy

$$U_{e^A} \mathbf{a}^\dagger (U_{e^A})^{-1} = e^{A^T} \mathbf{a}^\dagger, \quad U_{e^A} \mathbf{a} (U_{e^A})^{-1} = e^{\overline{A^T}} \mathbf{a} \tag{23.4}$$

(the relations 24.1 are the derivative of these). This shows that the U_{e^A} are intertwining operators for a $U(d)$ action on annihilation and creation operators that preserves the canonical commutation relations (the relations that say the $a_j, a_j^\dagger$ give a representation of the complexified Heisenberg Lie algebra). Here the use of normal-ordered operators means that U'_A is a representation of $\mathfrak{u}(d)$ that differs by a constant from the metaplectic representation, and U_{e^A} differs by a phase-factor. This does not affect the commutation relations with U'_A or the conjugation action of U_{e^A}. The representation one gets this way differs in two ways from the metaplectic representation. It acts on the same space $\mathcal{H} = \mathcal{F}_d$, but it is a true representation of $U(d)$, no double-cover is needed. It also does not extend to a representation of the larger group $Sp(2d, \mathbf{R})$.

The operators U'_A and U_{e^A} commute with the Hamiltonian operator. From the physics point of view, this is useful, as it provides a decomposition of energy eigenstates into irreducible representations of $U(d)$. From the mathematics point of view, the quantum harmonic oscillator state space provides a construction of a large class of irreducible representations of $U(d)$ (the energy eigenstates of a given energy).

23.3 Examples in $d = 2$ and 3

23.3.1 Two degrees of freedom and $SU(2)$

In the case $d = 2$, the group $U(2) \subset Sp(4, \mathbf{R})$ preserving the complex structure J_0 commutes with the standard harmonic oscillator Hamiltonian and so acts as symmetries on the quantum state space, preserving energy eigenspaces. Restricting to the subgroup $SU(2) \subset U(2)$, we can recover our earlier construction of $SU(2)$ representations in terms of homogeneous polynomials, in a new context. This use of the energy eigenstates of a two-dimensional harmonic oscillator appears in the physics literature as the "Schwinger boson method" for studying representations of $SU(2)$.

The state space for the $d = 2$ Bargmann-Fock representation, restricting to finite linear combinations of energy eigenstates, is

$$\mathcal{H} = \mathcal{F}_2^{fin} = \mathbf{C}[w_1, w_2]$$

the polynomials in two complex variables w_1, w_2. Recall from our $SU(2)$ discussion that it was useful to organize these polynomials into finite dimensional sets of homogeneous polynomials of degree n for $n = 0, 1, 2, \ldots$

$$\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2 \oplus \cdots$$

There are four annihilation or creation operators

$$a_1^\dagger = w_1,\ a_2^\dagger = w_2,\ a_1 = \frac{\partial}{\partial w_1},\ a_2 = \frac{\partial}{\partial w_2}$$

acting on $\mathcal{H}$. These are the quantizations of complexified phase space coordinates $z_1, z_2, \overline{z}_1, \overline{z}_2$ with quantization just the Bargmann-Fock construction of the representation Γ'_{BF} of $\mathfrak{h}_{2d}$

$$\Gamma'_{BF}(1) = -i\mathbf{1},\quad \Gamma'_{BF}(z_j) = -ia_j^\dagger,\quad \Gamma'_{BF}(\overline{z}_j) = -ia_j$$

Our original dual phase space was $\mathcal{M} = \mathbf{R}^4$, with a group $Sp(4, \mathbf{R})$ acting on it, preserving the antisymmetric bilinear form Ω. When picking the coordinates z_1, z_2, we made a standard choice of complex structure J_0 on $\mathcal{M}$. Complexifying, we have

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}^+_{J_0} \oplus \mathcal{M}^-_{J_0} = \mathbf{C}^2 \oplus \mathbf{C}^2$$

where z_1, z_2 are coordinates on $\mathcal{M}^+_{J_0}$, $\overline{z}_1, \overline{z}_2$ are coordinates on $\mathcal{M}^-_{J_0}$. This choice of $J = J_0$ picks out a distinguished subgroup $U(2) \subset Sp(4, \mathbf{R})$.

The quadratic combinations of the creation and annihilation operators give representations on $\mathcal{H}$ of three subalgebras of the complexification $\mathfrak{sp}(4, \mathbf{C})$ of $\mathfrak{sp}(4, \mathbf{R})$:

- A three dimensional commutative Lie sub-algebra spanned by $z_1 z_2, z_1^2, z_2^2$, with quantization

$$\Gamma'_{BF}(z_1 z_2) = -ia_1^\dagger a_2^\dagger,\quad \Gamma'_{BF}(z_1^2) = -i(a_1^\dagger)^2,\quad \Gamma'_{BF}(z_2^2) = -i(a_2^\dagger)^2$$

- A three dimensional commutative Lie sub-algebra spanned by $\overline{z}_1\overline{z}_2, \overline{z}_1^2, \overline{z}_2^2$, with quantization

$$\Gamma'_{BF}(\overline{z}_1\overline{z}_2) = -ia_1a_2, \quad \Gamma'_{BF}(\overline{z}_1^2) = -ia_1^2, \quad \Gamma'_{BF}(\overline{z}_2^2) = -ia_2^2$$

- A four dimensional Lie subalgebra isomorphic to $\mathfrak{gl}(2, \mathbf{C})$ with basis

$$z_1\overline{z}_1, z_2\overline{z}_2, z_1\overline{z}_2, \overline{z}_1 z_2$$

and quantization

$$\Gamma'_{BF}(z_1\overline{z}_1) = -\frac{i}{2}(a_1^\dagger a_1 + a_1 a_1^\dagger), \quad \Gamma'_{BF}(z_2\overline{z}_2) = -\frac{i}{2}(a_2^\dagger a_2 + a_2 a_2^\dagger)$$

$$\Gamma'_{BF}(\overline{z}_1 z_2) = -ia_1 a_2^\dagger, \quad \Gamma'_{BF}(z_1\overline{z}_2) = -ia_2 a_1^\dagger$$

Real linear combinations of

$$z_1\overline{z}_1, \quad z_2\overline{z}_2, \quad z_1\overline{z}_2 + z_2\overline{z}_1, \quad i(z_1\overline{z}_2 - z_2\overline{z}_1)$$

span the Lie algebra $\mathfrak{u}(2) \subset \mathfrak{sp}(4, \mathbf{R})$, and Γ'_{BF} applied to these gives a unitary Lie algebra representation by skew-adjoint operators.

Inside this last subalgebra, there is a distinguished element $h = z_1\overline{z}_1 + z_2\overline{z}_2$ that Poisson-commutes with the rest of the subalgebra (but not with elements in the first two subalgebras). Quantization of h gives the Hamiltonian operator

$$H = \frac{1}{2}(a_1 a_1^\dagger + a_1^\dagger a_1 + a_2 a_2^\dagger + a_2^\dagger a_2) = N_1 + \frac{1}{2} + N_2 + \frac{1}{2} = w_1\frac{\partial}{\partial w_1} + w_2\frac{\partial}{\partial w_2} + 1$$

This operator will just multiply a homogeneous polynomial by its degree plus one, so it acts just by multiplication by $n+1$ on $\mathcal{H}^n$. Exponentiating this operator (multiplied by $-i$) one gets a representation of a $U(1)$ subgroup of the metaplectic cover $Mp(4, \mathbf{R})$. Taking instead the normal-ordered version

$$:H: = a_1^\dagger a_1 + a_2^\dagger a_2 = N_1 + N_2 = w_1\frac{\partial}{\partial w_1} + w_2\frac{\partial}{\partial w_2}$$

one gets a representation of a $U(1)$ subroup of $Sp(4, \mathbf{R})$. Neither H nor $:H:$ commutes with operators coming from quantization of the first two subalgebras. These change the eigenvalue of H or $:H:$ by ± 2 so take

$$\mathcal{H}^n \to \mathcal{H}^{n\pm 2}$$

in particular taking $|0\rangle$ to either 0 or a state in $\mathcal{H}^2$.

h is a basis element for the $\mathfrak{u}(1)$ in $\mathfrak{u}(2) = \mathfrak{u}(1) \oplus \mathfrak{su}(2)$. For the $\mathfrak{su}(2)$ part a correspondence to our basis $X_j = -i\frac{\sigma_j}{2}$ in terms of 2 by 2 matrices is

$$X_1 \leftrightarrow \frac{1}{2}(z_1\overline{z}_2 + z_2\overline{z}_1), \quad X_2 \leftrightarrow \frac{i}{2}(z_2\overline{z}_1 - z_1\overline{z}_2), \quad X_3 \leftrightarrow \frac{1}{2}(z_1\overline{z}_1 - z_2\overline{z}_2)$$

This relates two different but isomorphic ways of describing $\mathfrak{su}(2)$: as 2 by 2 matrices with Lie bracket the commutator, or as quadratic polynomials, with Lie bracket the Poisson bracket.

Quantizing using normal-ordering of operators give a representation of $\mathfrak{su}(2)$ on $\mathcal{H}$

$$\Gamma'(X_1) = -\frac{i}{2}(a_1^\dagger a_2 + a_2^\dagger a_1), \quad \Gamma'(X_2) = \frac{1}{2}(a_2^\dagger a_1 - a_1^\dagger a_2)$$

$$\Gamma'(X_3) = -\frac{i}{2}(a_1^\dagger a_1 - a_2^\dagger a_2)$$

Comparing this to the representation π' of $\mathfrak{su}(2)$ on homogeneous polynomials discussed in chapter 8, one finds that they are isomorphic, although they act on dual spaces, so $\Gamma'(X) = \pi'(-X^T)$ for all $X \in \mathfrak{su}(2)$.

We see that, up to this change from a vector space to its dual, and the normal-ordering (which only affects the $\mathfrak{u}(1)$ factor, shifting the Hamiltonian by a constant), the Bargmann-Fock representation on polynomials and the $SU(2)$ representation on homogeneous polynomials are identical. The inner product that makes the representation unitary is the one of equation 8.2. The Bargmann-Fock representation extends this $SU(2)$ representation as a unitary representation to a much larger group ($H_5 \rtimes Mp(4, \mathbf{R})$), with all polynomials in w_1, w_2 now making up a single irreducible representation.

The fact that we have an $SU(2)$ group acting on the state space of the $d = 2$ harmonic oscillator and commuting with the action of the Hamiltonian H means that energy eigenstates can be organized as irreducible representations of $SU(2)$. In particular, one sees that the space $\mathcal{H}^n$ of energy eigenstates of energy $n + 1$ will be a single irreducible $SU(2)$ representation, the spin $\frac{n}{2}$ representation of dimension $n + 1$ (so $n + 1$ will be the multiplicity of energy eigenstates of that energy).

Another physically interesting subgroup here is the $SO(2) \subset SU(2) \subset Sp(4, \mathbf{R})$ consisting of simultaneous rotations in the position and momentum planes, which was studied in detail using the coordinates q_1, q_2, p_1, p_2 in section 18.2.2. There we found that the moment map was given by

$$\mu_L = l = q_1 p_2 - q_2 p_1$$

and quantization by the Schrödinger representation gave a representation of the Lie algebra $\mathfrak{so}(2)$ with

$$U'_L = -i(Q_1 P_2 - Q_2 P_1)$$

Note that this is a different $SO(2)$ action than the one with moment map the Hamiltonian, it acts separately on positions and momenta rather than mixing them.

To see what happens if one instead uses the Bargmann-Fock representation, note that

$$q_j = \frac{1}{\sqrt{2}}(z_j + \overline{z}_j), \quad p_j = i\frac{1}{\sqrt{2}}(z_j - \overline{z}_j)$$

so the moment map is

$$\begin{aligned}\mu_L =& \frac{i}{2}((z_1+\overline{z}_1)(z_2-\overline{z}_2)-(z_2+\overline{z}_2)(z_1-\overline{z}_1)) \\ =& i(z_2\overline{z}_1 - z_1\overline{z}_2)\end{aligned}$$

Quantizing, Bargmann-Fock gives a unitary representation of $\mathfrak{so}(2)$

$$U'_L = a_2^\dagger a_1 - a_1^\dagger a_2$$

which is $\Gamma'(2X_2)$. The factor of two here reflects the fact that exponentiation gives a representation of $SO(2) \subset Sp(4,\mathbf{R})$, with no need for a double cover.

23.3.2 Three degrees of freedom and $SO(3)$

The case $d = 3$ corresponds physically to the so-called isotropic quantum harmonic oscillator system, and it is an example of the sort of central potential problem we studied in chapter 19 (since the potential just depends on $r^2 = q_1^2 + q_2^2 + q_3^2$). For such problems, we saw that since the classical Hamiltonian is rotationally invariant, the quantum Hamiltonian will commute with the action of $SO(3)$ on wavefunctions and energy eigenstates can be decomposed into irreducible representations of $SO(3)$.

Here the Bargmann-Fock representation gives an action of $H_7 \rtimes Mp(6,\mathbf{R})$ on the state space, with a $U(3)$ subgroup commuting with the Hamiltonian (more precisely one has a double cover of $U(3)$, but by normal-ordering one can get an actual $U(3)$). The eigenvalue of the $U(1)$ corresponding to the Hamiltonian gives the energy of a state, and states of a given energy will be sums of irreducible representations of $SU(3)$. This works much like in the $d = 2$ case, although here our irreducible representations are the spaces $\mathcal{H}^n$ of homogeneous polynomials of degree n in three variables rather than two. These spaces have dimension $\frac{1}{2}(n+1)(n+2)$. A difference with the $SU(2)$ case is that one does not get all irreducible representations of $SU(3)$ this way.

The rotation group $SO(3)$ will be a subgroup of this $U(3)$ and one can ask how the $SU(3)$ irreducible $\mathcal{H}^n$ decomposes into a sum of irreducibles of the subgroup (which will be characterized by an integral spin $l = 0, 1, 2, \cdots$). One can show that for even n one gets all even values of l from 0 to n, and for odd n one gets all odd values of l from 1 to n. A derivation can be found in some quantum mechanics textbooks, see for example pgs. 456-460 of [43].

To construct the angular momentum operators in the Bargmann-Fock representation, recall that in the Schrödinger representation these were

$$L_1 = Q_2P_3 - Q_3P_2, \quad L_2 = Q_3P_1 - Q_1P_3, \quad L_3 = Q_1P_2 - Q_2P_1$$

and one can rewrite these operators in terms of annihilation and creation operators. Alternatively, one can use theoem 23.2, for Lie algebra basis elements $l_j \in \mathfrak{so}(3) \subset \mathfrak{u}(3) \subset \mathfrak{gl}(3,\mathbf{C})$ which are (see chapter 6)

$$l_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad l_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad l_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

to calculate

$$-iL_j = U'_{l_j} = \sum_{m,n=1}^{3} a_m^\dagger (l_j)_{mn} a_n$$

This gives

$$U'_{l_1} = a_3^\dagger a_2 - a_2^\dagger a_3, \quad U'_{l_2} = a_1^\dagger a_3 - a_3^\dagger a_1, \quad U'_{l_3} = a_2^\dagger a_1 - a_1^\dagger a_2$$

Exponentiating these operators gives a representation of the rotation group $SO(3)$ on the state space $\mathcal{F}_3$, commuting with the Hamiltonian, so acting on energy eigenspaces (which will be the homogeneous polynomials of fixed degree).

23.4 For further reading

The references from chapter 22 ([19], [66]) also contain the general case discussed here. The construction of the metaplectic representation restricted to $U(d) \subset Sp(2d, \mathbf{R})$ using annihilation and creation operators is a standard topic in quantum field theory textbooks, although there in an infinite rather than finite-dimensional context (and not explicitly in the language used here). We will encounter the quantum field theory version in later chapters.

Chapter 24

The Fermionic Oscillator

In this chapter we'll introduce a new quantum system by using a simple variation on techniques we used to study the harmonic oscillator, that of replacing commutators by anticommutators. This variant of the harmonic oscillator will be called a "fermionic oscillator", with the original sometimes called a "bosonic oscillator". The terminology of "boson" and "fermion" refers to the principle enunciated in chapter 9 that multiple identical particles are described by tensor product states that are either symmetric (bosons) or antisymmetric (fermions).

The bosonic and fermionic oscillator systems are single-particle systems, describing the energy states of a single particle, so the usage of the bosonic/fermionic terminology is not obviously relevant. In later chapters we will study quantum field theories, which can be treated as infinite-dimensional oscillator systems. In that context, multiple particle states will automatically be symmetric or antisymmetric, depending on whether the field theory is treated as a bosonic or fermionic oscillator system, thus justifying the terminology.

24.1 Canonical anticommutation relations and the fermionic oscillator

Recall that the Hamiltonian for the quantum harmonic oscillator system in d degrees of freedom (setting $\hbar = m = \omega = 1$) is

$$H = \sum_{j=1}^{d} \frac{1}{2}(Q_j^2 + P_j^2)$$

and that it can be diagonalized by introducing number operators $N_j = a_j^\dagger a_j$ defined in terms of operators

$$a_j = \frac{1}{\sqrt{2}}(Q_j + iP_j), \quad a_j^\dagger = \frac{1}{\sqrt{2}}(Q_j - iP_j)$$

that satisfy the so-called canonical commutation relations (CCR)

$$[a_j, a_k^\dagger] = \delta_{jk}\mathbf{1}, \quad [a_j, a_k] = [a_j^\dagger, a_k^\dagger] = 0$$

The simple change in the harmonic oscillator problem that takes one from bosons to fermions is the replacement of the bosonic annihilation and creation operators (which we'll now denote a_B and ${a_B}^\dagger$) by fermionic annihilation and creation operators called a_F and ${a_F}^\dagger$, and replacement of the commutator

$$[A, B] \equiv AB - BA$$

of operators by the anticommutator

$$[A, B]_+ \equiv AB + BA$$

The commutation relations are now

$$[a_F, a_F^\dagger]_+ = \mathbf{1}, \quad [a_F, a_F]_+ = 0, \quad [a_F^\dagger, a_F^\dagger]_+ = 0$$

with the last two relations implying that $a_F^2 = 0$ and $(a_F^\dagger)^2 = 0$

The fermionic number operator

$$N_F = a_F^\dagger a_F$$

now satisfies

$$N_F^2 = a_F^\dagger a_F a_F^\dagger a_F = a_F^\dagger(\mathbf{1} - a_F^\dagger a_F)a_F = N_F - {a_F^\dagger}^2 a_F^2 = N_F$$

(using the fact that $a_F^2 = {a_F^\dagger}^2 = 0$). So one has

$$N_F^2 - N_F = N_F(N_F - \mathbf{1}) = 0$$

which implies that the eigenvalues of N_F are just 0 and 1. We'll denote eigenvectors with such eigenvalues by $|0\rangle$ and $|1\rangle$. The simplest representation of the operators a_F and $a_F^\dagger$ on a complex vector space $\mathcal{H}_F$ will be on $\mathbf{C}^2$, and choosing the basis

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

the operators are represented as

$$a_F = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad a_F^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad N_F = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Since

$$H = \frac{1}{2}(a_F^\dagger a_F + a_F a_F^\dagger)$$

is just $\frac{1}{2}$ the identity operator, to get a non-trivial quantum system, instead we make a sign change and set

$$H = \frac{1}{2}(a_F^\dagger a_F - a_F a_F^\dagger) = N_F - \frac{1}{2}\mathbf{1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

The energies of the energy eigenstates $|0\rangle$ and $|1\rangle$ will then be $\pm\frac{1}{2}$ since

$$H|0\rangle = -\frac{1}{2}|0\rangle, \quad H|1\rangle = \frac{1}{2}|1\rangle$$

Note that the quantum system we have constructed here is nothing but our old friend the two-state system of chapter 3. Taking complex linear combinations of the operators

$$a_F, a_F^\dagger, N_F, \mathbf{1}$$

we get all linear transformations of $\mathcal{H}_F = \mathbf{C}^2$ (so this is an irreducible representation of the algebra of these operators). The relation to the Pauli matrices is just

$$a_F^\dagger = \frac{1}{2}(\sigma_1 + i\sigma_2), \quad a_F = \frac{1}{2}(\sigma_1 - i\sigma_2), \quad H = \frac{1}{2}\sigma_3$$

24.2 Multiple degrees of freedom

For the case of d degrees of freedom, one has this variant of the canonical commutation relations (CCR) amongst the bosonic annihilation and creation operators a_{Bj} and $a_{Bj}^\dagger$:

Definition (Canonical anticommutation relations)**.** *A set of* $2d$ *operators*

$$a_{Fj}, \ a_{Fj}^\dagger, \quad j = 1, \ldots, d$$

is said to satisfy the canonical anticommutation relations (CAR) when one has

$$[a_{Fj}, a_{Fk}^\dagger]_+ = \delta_{jk}\mathbf{1}, \quad [a_{Fj}, a_{Fk}]_+ = 0, \quad [a_{Fj}^\dagger, a_{Fk}^\dagger]_+ = 0$$

In this case one may choose as the state space the tensor product of N copies of the single fermionic oscillator state space

$$\mathcal{H}_F = (\mathbf{C}^2)^{\otimes d} = \underbrace{\mathbf{C}^2 \otimes \mathbf{C}^2 \otimes \cdots \otimes \mathbf{C}^2}_{d \text{ times}}$$

The dimension of $\mathcal{H}_F$ will be 2^d. On this space the operators a_{Fj} and $a_{Fj}^\dagger$ can be explicitly given by

$$a_{Fj} = \underbrace{\sigma_3 \otimes \sigma_3 \otimes \cdots \otimes \sigma_3}_{j-1 \text{ times}} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}$$

$$a_{Fj}^\dagger = \underbrace{\sigma_3 \otimes \sigma_3 \otimes \cdots \otimes \sigma_3}_{j-1 \text{ times}} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}$$

The factors of σ_3 ensure that the canonical anticommutation relations

$$[a_{Fj}, a_{Fk}]_+ = [a_{Fj}^\dagger, a_{Fk}^\dagger]_+ = [a_{Fj}, a_{Fk}^\dagger]_+ = 0$$

are satisfied for $j \neq k$ since in these cases one will get in the tensor product factors

$$[\sigma_3, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}]_+ = 0 \quad \text{or} \quad [\sigma_3, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}]_+ = 0$$

While this sort of tensor product construction is useful for discussing the physics of multiple qubits, in general it is easier to not work with large tensor products, and the Clifford algebra formalism we will describe in chapter 25 avoids this.

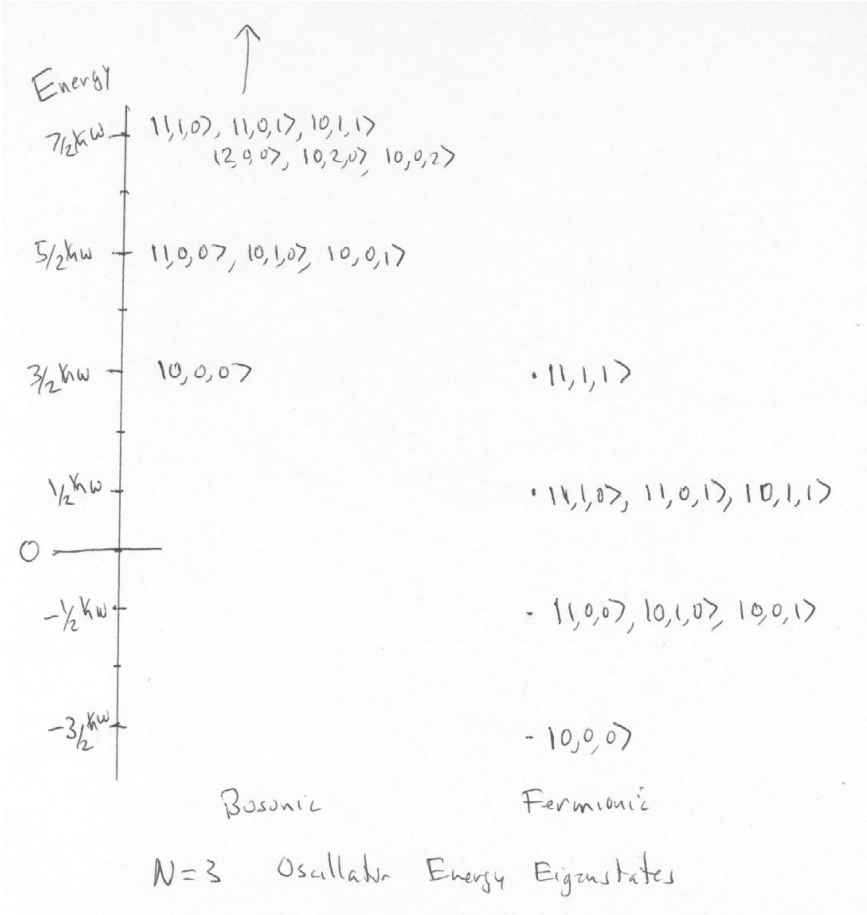
The number operators will be

$$N_{F\,j} = a_{F\,j}^\dagger a_{F\,j}$$

These will commute with each other, so can be simultaneously diagonalized, with eigenvalues $n_j = 0, 1$. One can take as an orthonormal basis of $\mathcal{H}_F$ the 2^d states

$$|n_1, n_2, \cdots, n_d\rangle$$

As an example, for the case $d = 3$ the pattern of states and their energy levels for the bosonic and fermionic cases looks like this



In the bosonic case the lowest energy state is at positive energy and there are an infinite number of states of ever increasing energy. In the fermionic case the lowest energy state is at negative energy, with the pattern of energy eigenvalues of the finite number of states symmetric about the zero energy level.

Just as in the bosonic case, we can consider quadratic combinations of creation and annihilation operators of the form

$$U'_A = \sum_{j,k} a^\dagger_{Fj} A_{jk} a_{Fk}$$

and we have

Theorem 24.1. *For $A \in \mathfrak{gl}(d, \mathbf{C})$ a d by d complex matrix one has*

$$[U'_A, U'_{A'}] = U_{[A,A']}$$

So

$$A \in \mathfrak{gl}(d, \mathbf{C}) \to U'_A$$

is a Lie algebra representation of $\mathfrak{gl}(d, \mathbf{C})$ on $\mathcal{H}_F$

One also has (for column vectors $\mathbf{a}_F$ with components $a_{F1}, \ldots, a_{Fd}$)

$$[U'_A, \mathbf{a}^\dagger_F] = A^T \mathbf{a}^\dagger_F, \quad [U'_A, \mathbf{a}_F] = -A\mathbf{a}_F \tag{24.1}$$

Proof. The proof is similar to that of 23.1, except besides the relation

$$[AB, C] = A[B, C] + [A, B]C$$

we also use the relation

$$[AB, C] = A[B, C]_+ - [A, B]_+ C$$

For example

$$\begin{aligned}
[U'_A, {a_F}^\dagger_l] &= \sum_{j,k} [{a_F}^\dagger_j A_{jk} a_{Fk}, {a_F}^\dagger_l] \\
&= \sum_{j,k} {a_F}^\dagger_j A_{jk} [a_{Fk}, {a_F}^\dagger_l]_+ \\
&= \sum_j {a_F}^\dagger_j A_{jl}
\end{aligned}$$

□

The Hamiltonian is

$$H = \sum_j (N_{Fj} - \frac{1}{2}\mathbf{1})$$

which (up to the constant $\frac{1}{2}$ that doesn't contribute to commutation relations) is just U'_B for the case $B = \mathbf{1}$. Since this commutes with all other d by d matrices, we have

$$[H, U'_A] = 0$$

for all $A \in \mathfrak{gl}(d, \mathbf{C})$, so these are symmetries and we have a representation of the Lie algebra $\mathfrak{gl}(d, \mathbf{C})$ on each energy eigenspace. Only for $A \in \mathfrak{u}(d)$ (A a skew-adjoint matrix) will the representation turn out to be unitary.

24.3 For further reading

Most quantum field theory books and a few quantum mechanics books contain some sort of discussion of the fermionic oscillator, see for example Chapter 21.3 of [57] or Chapter 5 of [10]. The standard discussion often starts with considering a form of classical analog using anticommuting "fermionic" variables and then quantization to get the fermionic oscillator. Here we are doing things in the opposite order, starting in this chapter with the quantized oscillator, then considering the classical analog in a later chapter.

Chapter 25

Weyl and Clifford Algebras

We have seen that just changing commutators to anticommutators takes the harmonic oscillator quantum system to a very different one (the fermionic oscillator), with this new system having in many ways a parallel structure. It turns out that this parallelism goes much deeper, with every aspect of the harmonic oscillator story having a fermionic analog. We'll begin in this chapter by studying the operators of the corresponding quantum systems.

25.1 The Complex Weyl and Clifford algebras

In mathematics, a "ring" is a set with addition and multiplication laws that are associative and distributive (but not necessarily commutative), and an "algebra" is a ring that is also a vector space over some field of scalars. The canonical commutation and anticommutation relations define interesting algebras, called the Weyl and Clifford algebras respectively. The case of complex numbers as scalars is simplest, so we'll start with that, before moving on to the real number case.

25.1.1 One degree of freedom, bosonic case

Starting with the one degree of freedom case (corresponding to two operators Q, P, which is why the notation will have a 2) we can define

Definition (Complex Weyl algebra, one degree of freedom)**.** *The complex Weyl algebra in the one degree of freedom case is the algebra Weyl*$(2, \mathbf{C})$ *generated by the elements* $1, a_B, a_B^\dagger$*, satisfying the canonical commutation relations:*

$$[a_B, a_B^\dagger] = 1, \quad [a_B, a_B] = [a_B^\dagger, a_B^\dagger] = 0$$

In other words, Weyl$(2, \mathbf{C})$ is the algebra one gets by taking arbitrary products and complex linear combinations of the generators. By repeated use of the commutation relation

$$a_B a_B^\dagger = 1 + a_B^\dagger a_B$$

any element of this algebra can be written as a sum of elements in normal order, of the form

$$c_{l,m}(a_B^\dagger)^l a_B^m$$

with all annihilation operators a_B on the right, for some complex constants $c_{l,m}$. As a vector space over $\mathbf{C}$, Weyl$(2,\mathbf{C})$ is infinite-dimensional, with a basis

$$1,\ a_B,\ a_B^\dagger,\ a_B^2,\ a_B^\dagger a_B,\ (a_B^\dagger)^2,\ a_B^3,\ a_B^\dagger a_B^2,\ (a_B^\dagger)^2 a_B,\ (a_B^\dagger)^3, \dots$$

This algebra is isomorphic to a more familiar one. Setting

$$a_B^\dagger = w, \quad a_B = \frac{\partial}{\partial w}$$

one sees that Weyl$(2,\mathbf{C})$ can be identified with the algebra of polynomial coefficient differential operators on functions of a complex variable w. As a complex vector space, the algebra is infinite dimensional, with a basis of elements

$$w^l \frac{\partial^m}{\partial w^m}$$

In our study of quantization and the harmonic oscillator we saw that the subset of such operators consisting of complex linear combinations of

$$1, \quad w, \quad \frac{\partial}{\partial w}, \quad w^2, \quad \frac{\partial^2}{\partial w^2}, \quad w\frac{\partial}{\partial w}$$

is closed under commutators, so it forms a Lie algebra of complex dimension 6. This Lie algebra includes as subalgebras the Heisenberg Lie algebra $\mathfrak{h}_3 \otimes \mathbf{C}$ (first three elements) and the Lie algebra $\mathfrak{sl}(2,\mathbf{C}) = \mathfrak{sl}(2,\mathbf{R}) \otimes \mathbf{C}$ (last three elements). Note that here we are allowing complex linear combinations, so we are getting the complexification of the real six-dimensional Lie algebra that appeared in our study of quantization.

Since the a_B and $a_B^\dagger$ are defined in terms of P and Q, one could of course also define the Weyl algebra as the one generated by $1, P, Q$, with the Heisenberg commutation relations, taking complex linear combinations of all products of these operators.

25.1.2 One degree of freedom, fermionic case

Changing commutators to anticommutators, one gets a different algebra, the Clifford algebra

Definition (Complex Clifford algebra, one degree of freedom)**.** *The complex Clifford algebra in the one degree of freedom case is the algebra Cliff$(2,\mathbf{C})$ generated by the elements $1, a_F, a_F^\dagger$, subject to the canonical anticommutation relations*

$$[a_F, a_F^\dagger]_+ = 1, \quad [a_F, a_F]_+ = [a_F^\dagger, a_F^\dagger]_+ = 0$$

This algebra is a four dimensional algebra over $\mathbf{C}$, with basis

$$1, \quad a_F, \quad a_F^\dagger, \quad a_F^\dagger a_F$$

since higher powers of the operators vanish, and one can use the anticommutation relation betwee a_F and $a_F^\dagger$ to normal order and put factors of a_F on the right. We saw in the last chapter that this algebra is isomorphic with the algebra $M(2, \mathbf{C})$ of 2 by 2 complex matrices, using

$$1 \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad a_F \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad a_F^\dagger \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a_F^\dagger a_F \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

We will see later on that there is also a way of identifying this algebra with "differential operators in fermionic variables", analogous to what happens in the bosonic (Weyl algebra) case.

Recall that the bosonic annihilation and creation operators were originally defined in term of the P and Q operators by

$$a_B = \frac{1}{\sqrt{2}}(Q + iP), \quad a_B^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$

Looking for the fermionic analogs of the operators Q and P, we use a slightly different normalization, and set

$$a_F = \frac{1}{2}(\gamma_1 + i\gamma_2), \quad a_F^\dagger = \frac{1}{2}(\gamma_1 - i\gamma_2)$$

so

$$\gamma_1 = a_F + a_F^\dagger, \quad \gamma_2 = \frac{1}{i}(a_F - a_F^\dagger)$$

and the CAR imply that the operators γ_j satisfy the anticommutation relations

$$[\gamma_1, \gamma_1]_+ = [a_F + a_F^\dagger, a_F + a_F^\dagger]_+ = 2$$

$$[\gamma_2, \gamma_2]_+ = -[a_F - a_F^\dagger, a_F - a_F^\dagger]_+ = 2$$

$$[\gamma_1, \gamma_2]_+ = \frac{1}{i}[a_F + a_F^\dagger, a_F - a_F^\dagger]_+ = 0$$

From this we see that

- One could alternatively have defined Cliff$(2, \mathbf{C})$ as the algebra generated by $1, \gamma_1, \gamma_2$, subject to the relations

  $$[\gamma_j, \gamma_k]_+ = 2\delta_{jk}$$

- Using just the generators 1 and γ_1, one gets an algebra Cliff$(1, \mathbf{C})$, generated by $1, \gamma_1$, with the relation

  $$\gamma_1^2 = 1$$

  This is a two-dimensional complex algebra, isomorphic to $\mathbf{C} \oplus \mathbf{C}$.

25.1.3 Multiple degrees of freedom

For a larger number of degrees of freedom, one can generalize the above and define Weyl and Clifford algebras as follows:

Definition (Complex Weyl algebras)**.** *The complex Weyl algebra for d degrees of freedom is the algebra Weyl$(2d, \mathbf{C})$ generated by the elements $1, a_{Bj}, a_{Bj}^\dagger$, $j = 1, \ldots, d$ satisfying the CCR*

$$[a_{Bj}, a_{Bk}^\dagger] = \delta_{jk} 1, \quad [a_{Bj}, a_{Bk}] = [a_{Bj}^\dagger, a_{Bk}^\dagger] = 0$$

Weyl$(2d, \mathbf{C})$ can be identified with the algebra of polynomial coefficient differential operators in m complex variables $w_1, w_2, \ldots, w_d$. The subspace of complex linear combinations of the elements

$$1, w_j, \frac{\partial}{\partial w_j}, w_j w_k, \frac{\partial^2}{\partial w_j \partial w_k}, w_j \frac{\partial}{\partial w_k}$$

is closed under commutators and is isomorphic to the complexification of the Lie algebra $\mathfrak{h}_{2d+1} \rtimes \mathfrak{sp}(2d, \mathbf{R})$ built out of the Heisenberg Lie algebra in $2d$ variables and the Lie algebra of the symplectic group $Sp(2d, \mathbf{R})$. Recall that this is the Lie algebra of polynomials of degree at most 2 on the phase space $\mathbf{R}^{2d}$, with the Poisson bracket as Lie bracket.

One could also define the complex Weyl algebra by taking complex linear combinations of products of generators $1, P_j, Q_j$, subject to the Heisenberg commutation relations.

For Clifford algebras one has

Definition (Complex Clifford algebras, using annilhilation and creation operators)**.** *The complex Clifford algebra for d degrees of freedom is the algebra Cliff$(2d, \mathbf{C})$ generated by $1, a_{Fj}, a_{Fj}^\dagger$ for $j = 1, 2, \ldots, d$ satisfying the CAR*

$$[a_{Fj}, a_{Fk}^\dagger]_+ = \delta_{jk} 1, \quad [a_{Fj}, a_{Fk}]_+ = [a_{Fj}^\dagger, a_{Fk}^\dagger]_+ = 0$$

or, alternatively, one has the following more general definition that also works in the odd-dimensional case

Definition (Complex Clifford algebras)**.** *The complex Clifford algebra in n variables is the algebra Cliff$(n, \mathbf{C})$ generated by $1, \gamma_j$ for $j = 1, 2, \ldots, n$ satisfying the relations*

$$[\gamma_j, \gamma_k]_+ = 2\delta_{jk}$$

We won't try and prove this here, but one can show that, abstractly as algebras, the complex Clifford algebras are something well-known. Generalizing the case $d = 1$ where we saw that Cliff$(2, \mathbf{C})$ was isomorphic to the algebra of 2 by 2 complex matrices, one has isomorphisms

$$\text{Cliff}(2d, \mathbf{C}) \leftrightarrow M(2^d, \mathbf{C})$$

in the even-dimensional case, and in the odd-dimensional case

$$\text{Cliff}(2d+1, \mathbf{C}) \leftrightarrow M(2^d, \mathbf{C}) \oplus M(2^d, \mathbf{C})$$

Two properties of $\text{Cliff}(n, \mathbf{C})$ are

- As a vector space over $\mathbf{C}$, a basis of $\text{Cliff}(n, \mathbf{C})$ is the set of elements

$$1, \quad \gamma_j, \quad \gamma_j\gamma_k, \quad \gamma_j\gamma_k\gamma_l, \ \ldots, \ \gamma_1\gamma_2\gamma_3\cdots\gamma_{n-1}\gamma_n$$

  for indices $j, k, l, \cdots \in 1, 2, \ldots, n$, with $j < k < l < \cdots$. To show this, consider all products of the generators, and use the commutation relations for the γ_j to identify any such product with an element of this basis. The relation $\gamma_j^2 = 1$ shows that one can remove repeated occurrences of a γ_j. The relation $\gamma_j\gamma_k = -\gamma_k\gamma_j$ can then be used to put elements of the product in the order of a basis element as above.

- As a vector space over $\mathbf{C}$, $\text{Cliff}(n, \mathbf{C})$ has dimension 2^n. One way to see this is to consider the product

$$(1+\gamma_1)(1+\gamma_2)\cdots(1+\gamma_n)$$

  which will have 2^n terms that are exactly those of the basis listed above.

25.2 Real Clifford algebras

We can define real Clifford algebras $\text{Cliff}(n, \mathbf{R})$ just as for the complex case, by taking only real linear combinations:

Definition (Real Clifford algebras)**.** *The real Clifford algebra in n variables is the algebra Cliff$(n, \mathbf{R})$ generated over the real numbers by $1, \gamma_j$ for $j = 1, 2, \ldots, n$ satisfying the relations*

$$[\gamma_j, \gamma_k]_+ = 2\delta_{jk}$$

For reasons that will be explained in the next chapter, it turns out that a more general definition is useful. We write the number of variables as $n = r + s$, for r, s non-negative integers, and now vary not just $r + s$, but also $r - s$, the so-called "signature".

Definition (Real Clifford algebras, arbitrary signature)**.** *The real Clifford algebra in $n = r + s$ variables is the algebra Cliff$(r, s, \mathbf{R})$ over the real numbers generated by $1, \gamma_j$ for $j = 1, 2, \ldots, n$ satisfying the relations*

$$[\gamma_j, \gamma_k]_+ = \pm 2\delta_{jk} 1$$

where we choose the $+$ sign when $j = k = 1, \ldots, r$ and the $-$ sign when $j = k = r+1, \ldots, n$.

In other words, as in the complex case different γ_j anticommute, but only the first r of them satisfy $\gamma_j^2 = 1$, with the other s of them satisfying $\gamma_j^2 = -1$.

Working out some of the low-dimensional examples, one finds:

- Cliff$(0, 1, \mathbf{R})$. This has generators 1 and γ_1, satisfying

  $$\gamma_1^2 = -1$$

  Taking real linear combinations of these two generators, the algebra one gets is just the algebra $\mathbf{C}$ of complex numbers, with γ_1 playing the role of $i = \sqrt{-1}$.

- Cliff$(0, 2, \mathbf{R})$. This has generators $1, \gamma_1, \gamma_2$ and a basis

  $$1, \quad \gamma_1, \quad \gamma_2, \quad \gamma_1\gamma_2$$

  with

  $$\gamma_1^2 = -1, \quad \gamma_2^2 = -1, \quad (\gamma_1\gamma_2)^2 = \gamma_1\gamma_2\gamma_1\gamma_2 = -\gamma_1^2\gamma_2^2 = -1$$

  This four-dimensional algebra over the real numbers can be identified with the algebra $\mathbf{H}$ of quaternions by taking

  $$\gamma_1 \leftrightarrow \mathbf{i}, \quad \gamma_2 \leftrightarrow \mathbf{j}, \quad \gamma_1\gamma_2 \leftrightarrow \mathbf{k}$$

- Cliff$(1, 1, \mathbf{R})$. This is the algebra $M(2, \mathbf{R})$ of 2 by 2 matrices, with one possible identification as follows

  $$1 \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \gamma_1 \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_2 \leftrightarrow \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_1\gamma_2 \leftrightarrow \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

  Note that one can construct this using the $a_F, a_F^\dagger$ for the complex case Cliff$(2, \mathbf{C})$

  $$\gamma_1 = a_F + a_F^\dagger, \quad \gamma_2 = a_F - a_F^\dagger$$

  since these are represented as real matrices.

It turns out that Cliff$(r, s, \mathbf{R})$ is always one or two copies of matrices of real, complex or quaternionic elements, of dimension a power of 2, but this requires a rather intricate algebraic argument that we will not enter into here. For the details of this and the resulting pattern of algebras one gets, see for instance [38]. One special case where the pattern is relatively simple is when one has $r = s$. Then $n = 2r$ is even-dimensional and one finds

$$\text{Cliff}(r, r, \mathbf{R}) = M(2^r, \mathbf{R})$$

We will see in the next chapter that just as quadratic elements of the Weyl algebra give a basis of the Lie algebra of the symplectic group, quadratic elements of the Clifford algebra give a basis of the Lie algebra of the orthogonal group.

25.3 For further reading

A good source for more details about Clifford algebras and spinors is Chapter 12 of the representation theory textbook [66]. For the details of what happens for all $\mathrm{Cliff}(r, s, \mathbf{R})$, another good source is Chapter 1 of [38].

Chapter 26

Clifford Algebras and Geometry

The definitions given in last chapter of Weyl and Clifford algebras were purely algebraic, based on a choice of generators. These definitions do though have a more geometrical formulation, with the definition in terms of generators corresponding to a specific choice of coordinates. For the Weyl algebra, the geometry involved is known as symplectic geometry, and we have already seen that in the bosonic case quantization of a phase space $\mathbf{R}^{2d}$ depends on the choice of a non-degenerate antisymmetric bilinear form Ω which determines the Poisson brackets and thus the Heisenberg commutation relations. Such a Ω also determines a group $Sp(2d, \mathbf{R})$, which is the group of linear transformations of $\mathbf{R}^{2d}$ preserving Ω. The Clifford algebra also has a coordinate invariant definition, based on a more well-known structure on a vector space $\mathbf{R}^n$, that of a non-degenerate symmetric bilinear form, i.e. an inner product. In this case the group that preserves the inner product is an orthogonal group. In the symplectic case antisymmetric forms require an even number of dimensions, but this is not true for symmetric forms, which also exist in odd dimensions.

26.1 Non-degenerate bilinear forms

In the case of $\mathcal{M} = \mathbf{R}^{2d}$, the dual phase space, for two vectors $u, u' \in \mathcal{M}$

$$u = c_{q_1} q_1 + c_{p_1} p_1 + \cdots + c_{q_d} q_d + c_{p_d} p_d \in \mathcal{M}$$

$$u' = c'_{q_1} q_1 + c'_{p_1} p_1 + \cdots + c'_{q_d} q_d + c'_{p_d} p_d \in \mathcal{M}$$

the Poisson bracket determines an antisymmetric bilinear form on $\mathcal{M}$, given explicitly by

$$\begin{aligned}\Omega(u,u') =& c_{q_1}c'_{p_1} - c_{p_1}c'_{q_1} + \cdots + c_{q_d}c'_{p_d} - c_{p_d}c'_{q_d} \\ =& \begin{pmatrix} c_{q_1} & c_{p_1} & \dots & c_{q_d} & c_{p_d} \end{pmatrix} \begin{pmatrix} 0 & 1 & \dots & 0 & 0 \\ -1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & -1 & 0 \end{pmatrix} \begin{pmatrix} c'_{q_1} \\ c'_{p_1} \\ \vdots \\ c'_{q_d} \\ c'_{p_d} \end{pmatrix}\end{aligned}$$

Matrices $g \in M(2d, \mathbf{R})$ such that

$$g^T \begin{pmatrix} 0 & 1 & \dots & 0 & 0 \\ -1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & -1 & 0 \end{pmatrix} g = \begin{pmatrix} 0 & 1 & \dots & 0 & 0 \\ -1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & -1 & 0 \end{pmatrix}$$

make up the group $Sp(2d, \mathbf{R})$ and preserve Ω, satisfying

$$\Omega(gu, gu') = \Omega(u, u')$$

This choice of Ω is much less arbitrary than it looks. One can show that given any non-degenerate antisymmetric bilinear form on $\mathbf{R}^{2d}$ a basis can be found with respect to which it will be the Ω given here (for a proof, see [7]). This is also true if one complexifies, taking $(\mathbf{q}, \mathbf{p}) \in \mathbf{C}^{2d}$ and using the same formula for Ω, which is now a bilinear form on $\mathbf{C}^{2d}$. In the real case the group that preserves Ω is called $Sp(2d, \mathbf{R})$, in the complex case $Sp(2d, \mathbf{C})$.

To get a fermionic analog of this, it turns out that all we need to do is replace "non-degenerate antisymmetric bilinear form $\Omega(\cdot, \cdot)$" with "non-degenerate symmetric bilinear form $\langle \cdot, \cdot \rangle$". Such a symmetric bilinear form is actually something much more familiar from geometry than the antisymmetric case analog: it is just a notion of inner product. Two things are different in the symmetric case:

- The underlying vector space does not have to be even dimensional, one can take $M = \mathbf{R}^n$ for any n, including n odd. To get a detailed analog of the bosonic case though, we will mostly consider the even case $n = 2d$.
- For a given dimension n, there is not just one possible choice of $\langle \cdot, \cdot \rangle$ up to change of basis, but one possible choice for each pair of integers r, s such that $r + s = n$. Given r, s, any choice of $\langle \cdot, \cdot \rangle$ can be put in the form

$$\begin{aligned}\langle \mathbf{u}, \mathbf{u}' \rangle =& u_1u'_1 + u_2u'_2 + \cdots u_ru'_r - u_{r+1}u'_{r+1} - \cdots - u_nu'_n \\ =& \begin{pmatrix} u_1 & \dots & u_n \end{pmatrix} \underbrace{\begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 0 \\ 0 & 0 & \dots & 0 & -1 \end{pmatrix}}_{r \text{ + signs, } s \text{ - signs}} \begin{pmatrix} u'_1 \\ u'_2 \\ \vdots \\ u'_{n-1} \\ u'_n \end{pmatrix}\end{aligned}$$

For a proof by Gram-Schmidt orthogonalization, see [7].

We can thus extend our definition of the orthogonal group as the group of transformations g preserving an inner product

$$\langle gu, gu' \rangle = \langle u, u' \rangle$$

to the case r, s arbitrary by

Definition (Orthogonal group $O(r, s, \mathbf{R})$)**.** *The group $O(r, s, \mathbf{R})$ is the group of real $r + s$ by $r + s$ matrices g that satisfy*

$$g^T \underbrace{\begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 0 \\ 0 & 0 & \dots & 0 & -1 \end{pmatrix}}_{r \text{ + signs, } s \text{ - signs}} g = \underbrace{\begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 0 \\ 0 & 0 & \dots & 0 & -1 \end{pmatrix}}_{r \text{ + signs, } s \text{ - signs}}$$

$SO(r, s, \mathbf{R}) \subset O(r, s, \mathbf{R})$ is the subgroup of matrices of determinant $+1$.

If one complexifies, taking components of vectors to be in $\mathbf{C}^n$, using the same formula for $\langle \cdot, \cdot \rangle$, one can change basis by multiplying the s basis elements by a factor of i, and in this new basis all basis vectors e_j satisfy $\langle e_j, e_j \rangle = 1$. One thus sees that on $\mathbf{C}^n$, as in the symplectic case, up to change of basis there is only one non-degenerate bilinear form. The group preserving this is called $O(n, \mathbf{C})$. Note that on $\mathbf{C}^n$ $\langle \cdot, \cdot \rangle$ is not the Hermitian inner product (which is antilinear on the first variable), and it is not positive definite.

26.2 Clifford algebras and geometry

As defined by generators in the last chapter, Clifford algebras have no obvious geometrical significance. It turns out however that they are powerful tools in the study of the geometry of linear spaces with an inner product, including especially the study of linear transformations that preserve the inner product, i.e. rotations. To see the relation between Clifford algebras and geometry, consider first the positive definite case $\text{Cliff}(n, \mathbf{R})$. To an arbitrary vector

$$\mathbf{v} = (v_1, v_2, \dots, v_n) \in \mathbf{R}^n$$

we associate the Clifford algebra element $\not{\mathbf{v}} = \gamma(\mathbf{v})$ where γ is the map

$$\mathbf{v} \in \mathbf{R}^n \to \gamma(\mathbf{v}) = v_1\gamma_1 + v_2\gamma_2 + \cdots + v_n\gamma_n \in \text{Cliff}(n, \mathbf{R})$$

Using the Clifford algebra relations for the γ_j, given two vectors $\mathbf{v}$, $\mathbf{w}$ the product of their associated Clifford algebra elements satisfies

$$\begin{aligned} \not{\mathbf{v}}\not{\mathbf{w}} + \not{\mathbf{w}}\not{\mathbf{v}} &= [v_1\gamma_1 + v_2\gamma_2 + \cdots + v_n\gamma_n,\ w_1\gamma_1 + w_2\gamma_2 + \cdots + w_n\gamma_n]_+ \\ &= 2(v_1w_1 + v_2w_2 + \cdots + v_nw_n) \\ &= 2\langle \mathbf{v}, \mathbf{w} \rangle \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the symmetric bilinear form on $\mathbf{R}^n$ corresponding to the standard inner product of vectors. Note that taking $\mathbf{v} = \mathbf{w}$ one has

$$\not{\mathbf{v}}^2 = \langle \mathbf{v}, \mathbf{v} \rangle = ||\mathbf{v}||^2$$

The Clifford algebra Cliff$(n, \mathbf{R})$ contains $\mathbf{R}^n$ as the subspace of linear combinations of the generators γ_j, and one can think of it as a sort of enhancement of the vector space $\mathbf{R}^n$ that encodes information about the inner product. In this larger structure one can multiply as well as add vectors, with the multiplication determined by the inner product.

In general one can define a Clifford algebra whenever one has a vector space with a symmetric bilinear form:

Definition (Clifford algebra of a symmetric bilinear form)**.** *Given a vector space V with a symmetric bilinear form $\langle \cdot, \cdot \rangle$, the Clifford algebra Cliff$(V, \langle \cdot, \cdot \rangle)$ is the algebra generated by* 1 *and elements of V, with the relations*

$$\not{v}\not{w} + \not{w}\not{v} = 2\langle v, w \rangle$$

Note that different people use different conventions here, with

$$\not{v}\not{w} + \not{w}\not{v} = -2\langle v, w \rangle$$

another common choice. One also sees variants without the factor of 2.

For n dimensional vector spaces over $\mathbf{C}$, we have seen that for any non-degenerate symmetric bilinear form a basis can be found such that $\langle \cdot, \cdot \rangle$ has the standard form

$$\langle \mathbf{z}, \mathbf{w} \rangle = z_1 w_1 + z_2 w_2 + \cdots + z_n w_n$$

As a result, there is just one complex Clifford algebra in dimension n, the one we defined as Cliff$(n, \mathbf{C})$.

For n dimensional vector spaces over $\mathbf{R}$ with a non-degenerate symmetric bilinear forms of type r, s such that $r+s = n$, the corresponding Clifford algebras Cliff$(r, s, \mathbf{R})$ are the ones defined in terms of generators in the last chapter.

In special relativity, space-time is a real 4-dimensional vector space with an indefinite inner product corresponding to (depending on one's choice of convention) either the case $r = 1, s = 3$ or the case $s = 1, r = 3$. The group of linear transformations preserving this inner product is called the Lorentz group, and its orientation preserving component is written as $SO(3, 1)$ or $SO(1, 3)$ depending on the choice of convention. In later chapters we will consider what happens to quantum mechanics in the relativistic case, and there encounter the corresponding Clifford algebras Cliff$(3, 1, \mathbf{R})$ or Cliff$(1, 3, \mathbf{R})$. The generators γ_j of such a Clifford algebra are well-known in the subject as the "Dirac γ- matrices".

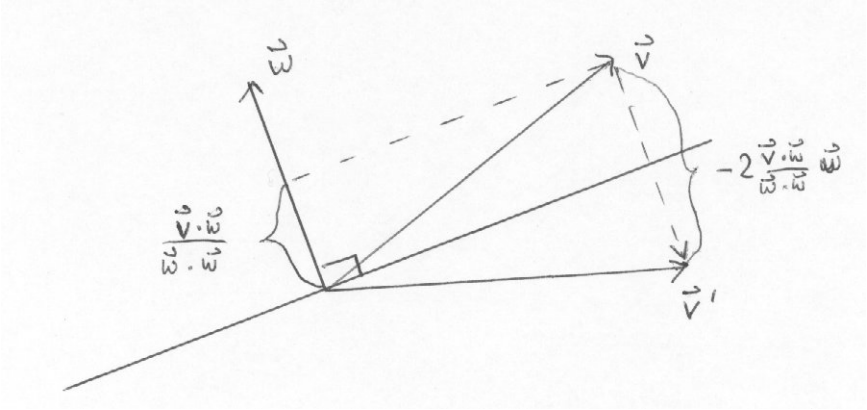
For now though, we will restrict attention to the positive definite case, so just will be considering Cliff$(n, \mathbf{R})$ and seeing how it is used to study the group $O(n)$ of n-dimensional rotations in $\mathbf{R}^n$.

26.2.1 Rotations as iterated orthogonal reflections

We'll consider two different ways of seeing the relationship between the Clifford algebra $\text{Cliff}(n, \mathbf{R})$ and the group $O(n)$ of rotations in $\mathbf{R}^n$. The first is based upon the geometrical fact (known as the Cartan-Dieudonné theorem) that one can get any rotation by doing multiple orthogonal reflections in different hyperplanes. Orthogonal reflection in the hyperplane perpendicular to a vector $\mathbf{w}$ takes a vector $\mathbf{v}$ to the vector

$$\mathbf{v}' = \mathbf{v} - 2\frac{\langle \mathbf{v}, \mathbf{w} \rangle}{\langle \mathbf{w}, \mathbf{w} \rangle}\mathbf{w}$$

something that can easily be seen from the following picture



From now on we identify vectors $\mathbf{v}, \mathbf{v}', \mathbf{w}$ with the corresponding Clifford algebra elements by the map γ. The linear transformation given by reflection in $\mathbf{w}$ is

$$\begin{aligned} \not{v} \to \not{v}' =& \not{v} - 2\frac{\langle \mathbf{v}, \mathbf{w} \rangle}{\langle \mathbf{w}, \mathbf{w} \rangle}\not{w} \\ =& \not{v} - (\not{v}\not{w} + \not{w}\not{v})\frac{\not{w}}{\langle \mathbf{w}, \mathbf{w} \rangle} \end{aligned}$$

Since

$$\not{w}\frac{\not{w}}{\langle \mathbf{w}, \mathbf{w} \rangle} = \frac{\langle \mathbf{w}, \mathbf{w} \rangle}{\langle \mathbf{w}, \mathbf{w} \rangle} = 1$$

we have (for non-zero vectors $\mathbf{w}$)

$$\not{w}^{-1} = \frac{\not{w}}{\langle \mathbf{w}, \mathbf{w} \rangle}$$

and the reflection transformation is just conjugation by $\not{w}$ times a minus sign

$$\not{v} \to \not{v}' = \not{v} - \not{v} - \not{w}\not{v}\not{w}^{-1} = -\not{w}\not{v}\not{w}^{-1}$$

So, thinking of vectors as lying in the Clifford algebra, the orthogonal transformation that is the result of one reflection is just a conjugation (with a minus

sign). These lie in the group $O(n)$, but not in the subgroup $SO(n)$, since they change orientation. The result of two reflections in hyperplanes orthogonal to $\mathbf{w}_1, \mathbf{w}_2$ will be a conjugation by $\not{\mathbf{w}}_2\not{\mathbf{w}}_1$

$$\not{\mathbf{v}} \to \not{\mathbf{v}}' = -\not{\mathbf{w}}_2(-\not{\mathbf{w}}_1\not{\mathbf{v}}\not{\mathbf{w}}_1^{-1})\not{\mathbf{w}}_2^{-1} = (\not{\mathbf{w}}_2\not{\mathbf{w}}_1)\not{\mathbf{v}}(\not{\mathbf{w}}_2\not{\mathbf{w}}_1)^{-1}$$

This will be a rotation preserving the orientation, so of determinant one and in the group $SO(n)$.

This construction not only gives an efficient way of representing rotations (as conjugations in the Clifford algebra), but it also provides a construction of the group $Spin(n)$ in arbitrary dimension n. One can define

Definition ($Spin(n)$)**.** *The group $Spin(n)$ is the set of invertible elements of the Clifford algebra $Cliff(n)$ of the form*

$$\not{\mathbf{w}}_1\not{\mathbf{w}}_2\cdots\not{\mathbf{w}}_k$$

where the vectors $\mathbf{w}_j$ for $j = 1, \cdots, k$ are vectors in $\mathbf{R}^n$ satisfying $|\mathbf{w}_j|^2 = 1$ and k is even. Group multiplication is just Clifford algebra multiplication.

The action of $Spin(n)$ on vectors $\mathbf{v} \in \mathbf{R}^n$ will be given by conjugation

$$\not{\mathbf{v}} \to (\not{\mathbf{w}}_1\not{\mathbf{w}}_2\cdots\not{\mathbf{w}}_k)\not{\mathbf{v}}(\not{\mathbf{w}}_1\not{\mathbf{w}}_2\cdots\not{\mathbf{w}}_k)^{-1}$$

and this will correspond to a rotation of the vector $\mathbf{v}$. This construction generalizes to arbitrary n the one we gave in chapter 6 of $Spin(3)$ in terms of unit length elements of the quaternion algebra $\mathbf{H}$. One can see here the characteristic fact that there are two elements of the $Spin(n)$ group giving the same rotation in $SO(n)$ by noticing that changing the sign of the Clifford algebra element $\not{\mathbf{w}}_1\not{\mathbf{w}}_2\cdots\not{\mathbf{w}}_k$ does not change the conjugation action, where signs cancel.

26.2.2 The Lie algebra of the rotation group and quadratic elements of the Clifford algebra

For a second approach to understanding rotations in arbitrary dimension, one can use the fact that these are generated by taking products of rotations in the coordinate planes. A rotation by an angle θ in the $j-k$ coordinate plane ($j < k$) will be given by

$$\mathbf{v} \to e^{\theta\epsilon_{jk}}\mathbf{v}$$

where ϵ_{jk} is an n by n matrix with only two non-zero entries: jk entry -1 and kj entry $+1$ (see equation 5.2.1). Restricting attention to the $j-k$ plane, $e^{\theta\epsilon_{jk}}$ acts as the standard rotation matrix in the plane

$$\begin{pmatrix} v_j \\ v_k \end{pmatrix} \to \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} v_j \\ v_k \end{pmatrix}$$

In the $SO(3)$ case we saw that there were three of these matrices

$$\epsilon_{23} = l_1, \quad \epsilon_{13} = -l_2, \quad \epsilon_{12} = l_3$$

providing a basis of the Lie algebra $\mathfrak{so}(3)$. In n dimensions there will be $\frac{1}{2}(n^2-n)$ of them, providing a basis of the Lie algebra $\mathfrak{so}(n)$.

Just as in the case of $SO(3)$ where unit length quaternions were used, we can use elements of the Clifford algebra to get these same rotation transformations, but as conjugations in the Clifford algebra. To see how this works, consider the quadratic Clifford algebra element $\gamma_j\gamma_k$ for $j \neq k$ and notice that

$$(\gamma_j\gamma_k)^2 = \gamma_j\gamma_k\gamma_j\gamma_k = -\gamma_j\gamma_j\gamma_k\gamma_k = -1$$

so one has

$$\begin{aligned} e^{\frac{\theta}{2}\gamma_j\gamma_k} =& (1 - \frac{(\theta/2)^2}{2!} + \cdots) + \gamma_j\gamma_k(\theta/2 - \frac{(\theta/2)^3}{3!} + \cdots) \\ =& \cos(\frac{\theta}{2}) + \gamma_j\gamma_k \sin(\frac{\theta}{2}) \end{aligned}$$

Conjugating a vector $v_j\gamma_j + v_k\gamma_k$ in the $j-k$ plane by this, one can show that

$$e^{-\frac{\theta}{2}\gamma_j\gamma_k}(v_j\gamma_j + v_k\gamma_k)e^{\frac{\theta}{2}\gamma_j\gamma_k} = (v_j\cos\theta - v_k\sin\theta)\gamma_j + (v_j\sin\theta + v_k\cos\theta)\gamma_k$$

which is just a rotation by θ in the $j-k$ plane. Such a conjugation will also leave invariant the γ_l for $l \neq j, k$. Thus one has

$$e^{-\frac{\theta}{2}\gamma_j\gamma_k}\gamma(\mathbf{v})e^{\frac{\theta}{2}\gamma_j\gamma_k} = \gamma(e^{\theta\epsilon_{jk}}\mathbf{v}) \tag{26.1}$$

and the infinitesimal version

$$[-\frac{1}{2}\gamma_j\gamma_k, \gamma(\mathbf{v})] = \gamma(\epsilon_{jk}\mathbf{v}) \tag{26.2}$$

Note that these relations are closely analogous to equations 18.7 and 18.6, which in the symplectic case show that a rotation in the Q, P plane is given by conjugation by the exponential of an operator quadratic in Q, P. We will examine this analogy in greater detail in chapter 28.

One can also see that, just as in our earlier calculations in three dimensions, one gets a double cover of the group of rotations, with here the elements $e^{\frac{\theta}{2}\gamma_j\gamma_k}$ of the Clifford algebra giving a double cover of the group of rotations in the $j-k$ plane (as θ goes from 0 to 2π). General elements of the spin group can be constructed by multiplying these for different angles in different coordinate planes. One sees that the Lie algebra $\mathfrak{spin}(n)$ can be identified with the Lie algebra $\mathfrak{so}(n)$ by

$$\epsilon_{jk} \leftrightarrow -\frac{1}{2}\gamma_j\gamma_k$$

Yet another way to see this would be to compute the commutators of the $-\frac{1}{2}\gamma_j\gamma_k$ for different values of j, k and show that they satisfy the same commutation relations as the corresponding matrices ϵ_{jk}.

Recall that in the bosonic case we found that quadratic combinations of the Q_j, P_k (or of the $a_{Bj}, a_{Bj}^\dagger$) gave operators satisfying the commutation relations

of the Lie algebra $\mathfrak{sp}(2n, \mathbf{R})$. This is the Lie algebra of the group $Sp(2n, \mathbf{R})$, the group preserving the non-degenerate antisymmetric bilinear form $\Omega(\cdot, \cdot)$ on the phase space $\mathbf{R}^{2n}$. The fermionic case is precisely analogous, with the role of the antisymmetric bilinear form $\Omega(\cdot, \cdot)$ replaced by the symmetric bilinear form $\langle \cdot, \cdot \rangle$ and the Lie algebra $\mathfrak{sp}(2n, \mathbf{R})$ replaced by $\mathfrak{so}(n) = \mathfrak{spin}(n)$.

In the bosonic case the linear functions of the Q_j, P_j satisfied the commutation relations of another Lie algebra, the Heisenberg algebra, but in the fermionic case this is not true for the γ_j. In chapter 27 we will see that one can define a notion of a "Lie superalgebra" that restores the parallelism.

26.3 For further reading

Some more detail about the relationship between geometry and Clifford algebras can be found in [38], and an exhaustive reference is [49].

Chapter 27

Anticommuting Variables and Pseudo-classical Mechanics

The analogy between the algebras of operators in the bosonic (Weyl algebra) and fermionic (Clifford algebra) cases can be extended by introducing a fermionic analog of phase space and the Poisson bracket. This gives a fermionic analog of classical mechanics, sometimes called "pseudo-classical mechanics", the quantization of which gives the Clifford algebra as operators, and spinors as state spaces. In this chapter we'll intoduce "anticommuting variables" ξ_j that will be the fermionic analogs of the variables q_j, p_j. These objects will become generators of the Clifford algebra under quantization, and will later be used in the construction of fermionic state spaces, by analogy with the Schrödinger and Bargmann-Fock constructions in the bosonic case.

27.1 The Grassmann algebra of polynomials on anticommuting generators

Given a phase space $V = \mathbf{R}^n$, one gets classical observables by taking polynomial functions on V. These are generated by the linear functions $q_j, p_j, j = 1, \ldots, d$ for $n = 2d$, which lie in the dual space V^*. It is also possible to start with the same space V^* of linear functions on V (with n not necessarily even), and pick a different notion of multiplication, one that is anticommutative on elements of V^*. Using such a multiplication, we can generate an analog of the algebra of polynomials on V, sometimes called the Grassmann algebra:

Definition (Grassmann algebra)**.** *The algebra over the real numbers generated by $\xi_j, j = 1, \ldots, n$, satisfying the relations*

$$\xi_j \xi_k + \xi_k \xi_j = 0$$

is called the Grassmann algebra, and denoted $\Lambda^*(\mathbf{R}^n)$.

Note that these relations imply that generators satisfy $\xi_j^2 = 0$. Also note that sometimes the product in the Grassmann algebra is called the "wedge product" and the product of ξ_j and ξ_k is denoted $\xi_j \wedge \xi_k$. We will not use a different symbol for the product in the Grassmann algebra, relying on the notation for generators to keep straight what is a generator of a conventional polynomial algebra (e.g. q_j or p_j) and what is a generator of a Grassman algebra (e.g. ξ_j).

Recall from section 9.5 that the algebra of polynomial functions on V could be thought of as $S^*(V^*)$, the symmetric part of the tensor algebra on V^*, with multiplication of two linear functions l_1, l_2 in V^* given by

$$l_1 l_2 = \frac{1}{2}(l_1 \otimes l_2 + l_2 \otimes l_1) \in S^2(V^*)$$

Similarly, the Grassman algebra on V is the antisymmetric part of the tensor algebra on V^*, with the wedge product of two linear functions l_1, l_2 in V^* given by

$$l_1 \wedge l_2 = \frac{1}{2}(l_1 \otimes l_2 - l_2 \otimes l_1) \in \Lambda^2(V^*)$$

The Grassmann algebra behaves in many ways like the polynomial algebra on $\mathbf{R}^n$, but it is finite dimensional, with basis

$$1, \quad \xi_j, \quad \xi_j\xi_k, \quad \xi_j\xi_k\xi_l, \quad \cdots, \quad \xi_1\xi_2\cdots\xi_n$$

for indices $j < k < l < \cdots$ taking values $1, 2, \ldots, n$. As with polynomials, monomials are characterized by a degree (number of generators in the product), which takes values from 0 to n. $\Lambda^k(\mathbf{R}^n)$ is the subspace of $\Lambda^*(\mathbf{R}^n)$ of linear combinations of monomials of degree k.

Digression (Differential forms)**.** *The Grassmann algebra is also known as the exterior algebra, and readers may have already seen it in the context of differential forms on* $\mathbf{R}^n$. *These are known to physicists as "antisymmetric tensor fields", and given by taking elements of the exterior algebra* $\Lambda^*(\mathbf{R}^n)$ *with coefficients not constants, but functions on* $\mathbf{R}^n$. *This construction is important in the theory of manifolds, where at a point* x *in a manifold* M*, one has a tangent space* T_xM *and its dual space* $(T_xM)^*$. *A set of local coordinates* x_j *on* M *gives basis elements of* $(T_xM)^*$ *denoted by* dx_j *and differential forms locally can be written as sums of terms of the form*

$$f(x_1, x_2, \cdots, x_n) dx_j \wedge \cdots \wedge dx_k \wedge \cdots \wedge dx_l$$

where the indices j, k, l *satisfy* $1 \leq j < k < l \leq n$.

A fundamental principle of mathematics is that a good way to understand a space is in terms of the functions on it. One can think of what we have done here as creating a new kind of space out of $\mathbf{R}^n$, where the algebra of functions on the space is $\Lambda^*(\mathbf{R}^n)$, generated by coordinate functions ξ_j with respect to a

basis of $\mathbf{R}^n$. The enlargement of conventional geometry to include new kinds of spaces such that this makes sense is known as "supergeometry", but we will not attempt to pursue this subject here. Spaces with this new kind of geometry have functions on them, but do not have conventional points: one can't ask what the value of an anticommuting function at a point is.

Remarkably, one can do calculus on such unconventional spaces, introducing analogs of the derivative and integral for anticommuting functions. For the case $n = 1$, an arbitrary function is

$$F(\xi) = c_0 + c_1\xi$$

and one can take

$$\frac{\partial}{\partial\xi}F = c_1$$

For larger values of n, an arbitrary function can be written as

$$F(\xi_1, \xi_2, \ldots, \xi_n) = F_A + \xi_j F_B$$

where F_A, F_B are functions that do not depend on the chosen ξ_j (one gets F_B by using the anticommutation relations to move ξ_j all the way to the left). Then one can define

$$\frac{\partial}{\partial\xi_j}F = F_B$$

This derivative operator has many of the same properties as the conventional derivative, although there are unconventional signs one must keep track of. An unusual property of this derivative that is easy to see is that one has

$$\frac{\partial}{\partial\xi_j}\frac{\partial}{\partial\xi_j} = 0$$

Taking the derivative of a product one finds this version of the Leibniz rule for monomials F and G

$$\frac{\partial}{\partial\xi_j}(FG) = (\frac{\partial}{\partial\xi_j}F)G + (-1)^{|F|}F(\frac{\partial}{\partial\xi_j}G)$$

where $|F|$ is the degree of the monomial F.

A notion of integration (often called the "Berezin integral") with many of the usual properties of an integral can also be defined. It has the peculiar feature of being the same operation as differentiation, defined in the $n = 1$ case by

$$\int (c_0 + c_1\xi)d\xi = c_1$$

and for larger n by

$$\int F(\xi_1, \xi_2, \cdots, \xi_n)d\xi_1 d\xi_2 \cdots d\xi_n = \frac{\partial}{\partial\xi_n}\frac{\partial}{\partial\xi_{n-1}}\cdots\frac{\partial}{\partial\xi_1}F = c_n$$

where c_n is the coefficient of the basis element $\xi_1\xi_2\cdots\xi_n$ in the expression of F in terms of basis elements.

This notion of integration is a linear operator on functions, and it satisfies an analog of integration by parts, since if one has

$$F = \frac{\partial}{\partial \xi_j} G$$

then

$$\int F d\xi_j = \frac{\partial}{\partial \xi_j} F = \frac{\partial}{\partial \xi_j}\frac{\partial}{\partial \xi_j} G = 0$$

using the fact that repeated derivatives give zero.

27.2 Pseudo-classical mechanics and the fermionic Poisson bracket

The basic structure of Hamiltonian classical mechanics depends on an even dimensional phase space $\mathbf{R}^{2d}$ with a Poisson bracket $\{\cdot,\cdot\}$ on functions on this space. Time evolution of a function f on phase space is determined by

$$\frac{d}{dt} f = \{f, h\}$$

for some Hamiltonian function h. This says that taking the derivative of any function in the direction of the velocity vector of a classical trajectory is the linear map

$$f \to \{f, h\}$$

on functions. As we saw in chapter 12, since this linear map is a derivative, the Poisson bracket will have the derivation property, satisfying the Leibniz rule

$$\{f_1, f_2 f_3\} = f_2\{f_1, f_3\} + \{f_1, f_2\} f_3$$

for arbitrary functions f_1, f_2, f_3 on phase space. Using the Leibniz rule and antisymmetry, one can calculate Poisson brackets for any polynomials, just from knowing the Poisson bracket on generators q_j, p_j (or, equivalently, the antisymmetric bilinear form $\Omega(\cdot,\cdot)$), which we chose to be

$$\{q_j, q_k\} = \{p_j, p_k\} = 0, \quad \{q_j, p_k\} = -\{p_k, q_j\} = \delta_{jk}$$

Notice that we have a symmetric multiplication on generators, while the Poisson bracket is antisymmetric.

To get pseudo-classical mechanics, we think of the Grassmann algebra $\Lambda^*(\mathbf{R}^n)$ as our algebra of classical observables, an algebra we can think of as functions on a "fermionic" phase space $\mathbf{R}^n$ (note that in the fermionic case, the phase space does not need to be even dimensional). We want to find an appropriate notion of fermionic Poisson bracket operation on this algebra, and it turns out

that this can be done. While the standard Poisson bracket is an antisymmetric bilinear form $\Omega(\cdot,\cdot)$ on linear functions, the fermionic Poisson bracket will be based on a choice of symmetric bilinear form on linear functions, equivalently, a notion of inner product $\langle\cdot,\cdot\rangle$.

Denoting the fermionic Poisson bracket by $\{\cdot,\cdot\}_+$, for a multiplication anti-commutative on generators one has to adjust signs in the Leibniz rule, and the derivation property analogous to the derivation property of the usual Poisson bracket is

$$\{F_1F_2,F_3\}_+ = F_1\{F_2,F_3\}_+ + (-1)^{|F_2||F_3|}\{F_1,F_3\}_+F_2$$

where $|F_2|$ and $|F_3|$ are the degrees of F_2 and F_3. It will also have the symmetry property

$$\{F_1,F_2\}_+ = -(-1)^{|F_1||F_2|}\{F_2,F_1\}_+$$

and one can use these properties to compute the fermionic Poisson bracket for arbitrary functions in terms of the relations for generators.

One can think of the ξ_j as the "anti-commuting coordinate functions" with respect to a basis $\mathbf{e}_i$ of $\mathbf{R}^n$. We have seen that the symmetric bilinear forms on $\mathbf{R}^n$ are classified by a choice of positive signs for some basis vectors, negative signs for the others. So, on generators ξ_j one can choose

$$\{\xi_j,\xi_k\}_+ = \pm\delta_{jk}$$

with a plus sign for $j=k=1,\cdots,r$ and a minus sign for $j=k=r+1,\cdots,n$, corresponding to the possible inequivalent choices of non-degenerate symmetric bilinear forms.

Taking the case of a positive-definite inner product for simplicity, one can calculate explicitly the fermionic Poisson brackets for linear and quadratic combinations of the generators. One finds

$$\{\xi_j\xi_k,\xi_l\}_+ = \xi_j\{\xi_k,\xi_l\}_+ - \{\xi_j,\xi_l\}_+\xi_k = \delta_{kl}\xi_j - \delta_{jl}\xi_k \tag{27.1}$$

and

$$\begin{aligned}\{\xi_j\xi_k,\xi_l\xi_m\}_+ =&\{\xi_j\xi_k,\xi_l\}_+\xi_m + \xi_l\{\xi_j\xi_k,\xi_m\}_+\\ =&\delta_{kl}\xi_j\xi_m - \delta_{jl}\xi_k\xi_m + \delta_{km}\xi_l\xi_j - \delta_{jm}\xi_l\xi_k\end{aligned} \tag{27.2}$$

The second of these equations shows that the quadratic combinations of the generators ξ_j satisfy the relations of the Lie algebra of the group of rotations in n dimensions ($\mathfrak{so}(n) = \mathfrak{spin}(n)$). The first shows that the $\xi_k\xi_l$ acts on the ξ_j as infinitesimal rotations in the $k-l$ plane.

In the case of the conventional Poisson bracket, the antisymmetry of the bracket and the fact that it satisfies the Jacobi identity implies that it is a Lie bracket determining a Lie algebra (the infinite dimensional Lie algebra of functions on a phase space $\mathbf{R}^{2d}$). The fermionic Poisson bracket provides an example of something called a Lie superalgebra. These can be defined for vector spaces with some usual and some fermionic coordinates:

Definition (Lie superalgebra)**.** *A Lie superalgebra structure on a real or complex vector space V is given by a Lie superbracket $[\cdot,\cdot]_\pm$. This is a bilinear map on V which on generators X, Y, Z (which may be usual coordinates or fermionic ones) satisfies*

$$[X,Y]_\pm = -(-1)^{|X||Y|}[Y,X]_\pm$$

and a super-Jacobi identity

$$[X,[Y,Z]_\pm]_\pm = [[X,Y]_\pm,Z]_\pm + (-1)^{|X||Y|}[Y,[X,Z]_\pm]_\pm$$

where $|X|$ takes value 0 for a usual generator, 1 for a fermionic generator.

Analogously to the bosonic case, on polynomials in generators with order of the poynomial less than or equal to two, the fermionic Poisson bracket $\{\cdot,\cdot\}_+$ is a Lie superbracket, giving a Lie superalgebra of dimension $1+n+\frac{1}{2}(n^2-n)$ (since there is one constant, n linear terms ξ_j and $\frac{1}{2}(n^2-n)$ quadratic terms $\xi_j\xi_k$). On functions of order two this Lie superalgebra is a Lie algebra, $\mathfrak{so}(n)$. We will see in chapter 28 that one can generalize the definition of a representation to Lie superalgebras, and quantization will give a distinguished representation of this Lie superalgebra, in a manner quite parallel to that of the Schrödinger or Bargmann-Fock constructions of a representation in the bosonic case.

The relation between between the quadratic and linear polynomials in the generators is parallel to what happens in the bosonic case. Here we have the fermionic analog of the bosonic theorem 14.1:

Theorem 27.1. *The Lie algebra $\mathfrak{so}(n,\mathbf{R})$ is isomorphic to the Lie algebra $\Lambda^2(M^*)$ (with Lie bracket $\{\cdot,\cdot\}_+$) of order two anticommuting polynmials on $M=\mathbf{R}^n$, by the isomorphism*

$$L \leftrightarrow \mu_L$$

where $L \in \mathfrak{so}(n,\mathbf{R})$ is an antisymmetric n by n real matrix, and

$$\mu_L = \frac{1}{2}\boldsymbol{\xi}\cdot L\boldsymbol{\xi} = \frac{1}{2}\sum_{j,k} L_{jk}\xi_j\xi_k$$

The $\mathfrak{so}(n,\mathbf{R})$ action on anticommuting coordinate functions is

$$\{\mu_L,\xi_k\}_+ = \sum_j L_{jk}\xi_j$$

or

$$\{\mu_L,\boldsymbol{\xi}\}_+ = L^T\boldsymbol{\xi}$$

Proof. The theorem follows from equations 27.1 and 27.2, or one can proceed by analogy with the proof of theorem 14.1 as follows. First prove the second part of the theorem by computing

$$\begin{aligned}\{\frac{1}{2}\sum_{j,k}\xi_j L_{jk}\xi_k, \xi_l\}_+ =& \frac{1}{2}\sum_{j,k} L_{jk}(\xi_j\{\xi_k,\xi_l\}_+ - \{\xi_j,\xi_l\}_+\xi_k)\\ =& \frac{1}{2}(\sum_j L_{jl}\xi_j - \sum_k L_{lk}\xi_k)\\ =& \sum_j L_{jl}\xi_j \quad (\text{since } L = -L^T)\end{aligned}$$

For the first part of the theorem, the map

$$L \to \mu_L$$

is a vector space isomorphism of the space of antisymmetric matrices and $\Lambda^2(\mathbf{R}^n)$. To show that it is a Lie algebra isomorphism, one can use an analogous argument to that of the proof of 14.1. Here one considers the action

$$\xi \to \{\mu_L, \xi\}$$

of $\mu_L \in \mathfrak{so}(n, \mathbf{R})$ on an arbitrary

$$\xi = \sum_j c_j \xi_j$$

and uses the super-Jacobi identity relating the fermionic Poisson brackets of $\mu_L, \mu_{L'}, \xi$. □

27.3 Examples of pseudo-classical mechanics

In pseudo-classical mechanics, the dynamics will be determined by choosing a Hamiltonian h in $\Lambda^*(\mathbf{R}^n)$. Observables will be other functions $F \in \Lambda^*(\mathbf{R}^n)$, and they will satisfy the analog of Hamilton's equations

$$\frac{d}{dt}F = \{F, h\}_+$$

We'll consider two of the simplest possible examples.

27.3.1 The classical spin degree of freedom

Using pseudo-classical mechanics, one can find a "classical" analog of something that is quintessentially quantum: the degree of freedom that appears in the qubit or spin 1/2 system that we have seen repeatedly in this course. Taking $\mathbf{R}^3$ with the standard inner product as fermionic phase space, we have three generators ξ_1, ξ_2, ξ_3 satisfying the relations

$$\{\xi_j, \xi_k\}_+ = \delta_{jk}$$

and an 8 dimensional space of functions with basis

$$1,\ \xi_1,\ \xi_2,\ \xi_3,\ \xi_1\xi_2,\ \xi_1\xi_3,\ \xi_2\xi_3,\ \xi_1\xi_2\xi_3$$

If we want the Hamiltonian function to be non-trivial and of even degree, it will have to be a linear combination

$$h = B_{12}\xi_1\xi_2 + B_{13}\xi_1\xi_3 + B_{23}\xi_2\xi_3$$

The equations of motion on generators will be

$$\frac{d}{dt}\xi_j(t) = \{\xi_j, h\}_+$$

but since h is a quadratic combination of the generators, by theorem 27.1 the right hand side is just an infinitesimal rotation. The solution to the classical equations of motion will be a time-dependent rotation of the ξ_j in the plane perpendicular to

$$\mathbf{B} = (B_{23}, -B_{13}, B_{12})$$

at a constant speed proportional to $|\mathbf{B}|$.

27.3.2 The classical fermionic oscillator

We have already studied the fermionic oscillator as a quantum system, and one can ask whether there is a corresponding pseudo-classical system. Such a system is given by taking an even dimensional fermionic phase space $\mathbf{R}^{2d}$, with a basis of coordinate functions $\xi_1, \cdots, \xi_{2d}$ that generate $\Lambda^*(\mathbf{R}^{2d})$. On generators the fermionic Poisson bracket relations come from the standard choice of positive definite symmetric bilinear form

$$\{\xi_j, \xi_k\}_+ = \delta_{jk}$$

As shown in theorem 27.1, quadratic products $\xi_j\xi_k$ act on the generators by infinitesimal rotations in the $j-k$ plane, and satisfy the commutation relations of $\mathfrak{so}(2d)$.

To get a pseudo-classical system corresponding to the fermionic oscillator one makes the choice

$$h = i\sum_{j=1}^{d} \xi_{2j-1}\xi_{2j}$$

As in the bosonic case, we can make the standard choice of complex structure $J = J_0$ on $\mathbf{R}^{2d}$ and get a decomposition

$$\mathbf{R}^{2d} \otimes \mathbf{C} = \mathbf{C}^d \oplus \mathbf{C}^d$$

into eigenspaces of J of eigenvalue $\pm i$. This is done by defining

$$\theta_j = \frac{1}{\sqrt{2}}(\xi_{2j-1} - i\xi_{2j}),\quad \overline{\theta}_j = \frac{1}{\sqrt{2}}(\xi_{2j-1} + i\xi_{2j})$$

for $j = 1, \ldots, d$. These satisfy the fermionic Poisson bracket relations

$$\{\theta_j, \theta_k\}_+ = \{\overline{\theta}_j, \overline{\theta}_k\}_+ = 0, \quad \{\theta_j, \overline{\theta}_k\}_+ = \delta_{jk}$$

In terms of the θ_j, the Hamiltonian is

$$h = \sum_{j=1}^{d} \theta_j \overline{\theta}_j$$

Using the derivation property of $\{\cdot, \cdot\}_+$ one finds

$$\{h, \theta_j\}_+ = \sum_{k=1}^{d} (\theta_k \{\overline{\theta}_k, \theta_j\}_+ - \{\theta_k, \theta_j\}_+ \overline{\theta}_k) = \theta_j$$

and, similarly,

$$\{h, \overline{\theta}_j\}_+ = -\overline{\theta}_j$$

so one sees that h is just the generator of $U(1) \subset U(d)$ phase rotations on the variables θ_j.

27.4 For further reading

For more details on pseudo-classical mechanics, a very readable original reference is [6], and there is a detailed discussion in the textbook [64], chapter 7.

Chapter 28

Fermionic Quantization and Spinors

In this chapter we'll begin by investigating the fermionic analog of the notion of quantization, which takes functions of anticommuting variables on a phase space with symmetric bilinear form $\langle \cdot, \cdot \rangle$ and gives an algebra of operators with generators satisfying the relations of the corresponding Clifford algebra. We will then consider analogs of the constructions used in the bosonic case which there gave us the Schrödinger and Bargmann-Fock representations of the Weyl algebra on a space of states.

We know that for a fermionic oscillator with d degrees of freedom, the algebra of operators will be Cliff$(2d, \mathbf{C})$, the algebra generated by annihilation and creation operators $a_{Fj}, a_{Fj}^\dagger$. These operators will act on $\mathcal{H}_F$, a complex vector space of dimension 2^d, and this will be our fermionic analog of the bosonic Γ'. Since the spin group consists of invertible elements of the Clifford algebra, it has a representation on $\mathcal{H}_F$. This is known as the "spinor representation", and it can be constructed by analogy with the construction of the metaplectic in the bosonic case. We'll also consider the analog in the fermionic case of the Schrödinger representation, which turns out to have a problem with unitarity, but finds a use in physics as "ghost" degrees of freedom.

28.1 Quantization of pseudo-classical systems

In the bosonic case, quantization was based on finding a representation of the Heisenberg Lie algebra of linear functions on phase space, or more explicitly, for basis elements q_j, p_j of this Lie algebra finding operators Q_j, P_j satisfying the Heisenberg commutation relations. In the fermionic case, the analog of the Heisenberg Lie algebra is not a Lie algebra, but a Lie superalgebra, with basis elements $1, \xi_j, j = 1, \ldots, n$ and a Lie superbracket given by the fermionic

Poisson bracket, which on basis elements is

$$\{\xi_j, \xi_k\}_+ = \pm\delta_{jk}, \quad \{\xi_j, 1\}_+ = 0, \ \{1, 1\}_+ = 0$$

Quantization is given by finding a representation of this Lie superalgebra. One can generalize the definition of a Lie algebra representation to that of a Lie superalgebra representation by

Definition (Representation of a Lie superalgebra)**.** *A representation of a Lie superalgebra is a homomorphism Φ preserving the superbracket*

$$[\Phi(X), \Phi(Y)]_\pm = \Phi([X, Y]_\pm)$$

and taking values in a Lie superalgebra of linear operators, with $|\Phi(X)| = |X|$ and

$$[\Phi(X), \Phi(Y)]_\pm = \Phi(X)\Phi(Y) - (-)^{|X||Y|}\Phi(Y)\Phi(X)$$

A representation of the pseudo-classical Lie superalgebra (and thus a quantization of the pseudo-classical system) will be given by finding a linear map Γ^+ that takes basis elements ξ_j to operators $\Gamma^+(\xi_j)$ satisfying the anticommutation relations

$$[\Gamma^+(\xi_j), \Gamma^+(\xi_k)]_+ = \pm\delta_{jk}\Gamma^+(1), \quad [\Gamma^+(\xi_j), \Gamma^+(1)] = [\Gamma^+(1), \Gamma^+(1)] = 0$$

One can satisfy these relations by taking

$$\Gamma^+(\xi_j) = \frac{1}{\sqrt{2}}\gamma_j, \quad \Gamma^+(1) = \mathbf{1}$$

since then

$$[\Gamma^+(\xi_j), \Gamma^+(\xi_k)]_+ = \frac{1}{2}[\gamma_j, \gamma_k]_+ = \pm\delta_{jk}$$

are exactly the Clifford algebra relations

As mentioned in chapter 25, it can be shown that the real Clifford algebras $\text{Cliff}(r, s, \mathbf{R})$ are isomorphic to either one or two copies of the matrix algebras $M(2^l, \mathbf{R}), M(2^l, \mathbf{C})$, or $M(2^l, \mathbf{H})$, with the power l depending on r, s. The irreducible representations of such a matrix algebra are just the column vectors of dimension 2^l, and there will be either one or two such irreducible representations for $\text{Cliff}(r, s, \mathbf{R})$ depending on the number of copies of the matrix algebra.

Note that here we are not introducing the factors of i into the definition of quantization that in the bosonic case were necessary to get a unitary representation of the Lie group corresponding to the real Heisenberg Lie algebra $\mathfrak{h}_{2d+1}$. In the bosonic case we worked with all complex linear combinations of powers of the Q_j, P_j (the complex Weyl algebra $\text{Weyl}(2d, \mathbf{C})$), and thus had to identify the specific complex linear combinations of these that gave unitary representations of the Lie algebra $h_{2d+1} \rtimes \mathfrak{sp}(2d, \mathbf{R})$. Here we are not complexifying for now, but working with the real Clifford algebra $\text{Cliff}(r, s, \mathbf{R})$, and it is the irreducible representations of this algebra that provide an analog of the unique interesting irreducible representation of $\mathfrak{h}_{2d+1}$. In the Clifford algebra case, the

representations of interest are not Lie algebra representations and may be on real vector spaces. There is no analog of the unitarity property of the $\mathfrak{h}_{2d+1}$ representation.

In the bosonic case we found that $Sp(2d, \mathbf{R})$ acted on the bosonic dual phase space, preserving the antisymmetric bilinear form Ω that determined the Lie algebra $\mathfrak{h}_{2d+1}$, so it acted on this Lie algebra by automorphisms. We saw (see chapter 18) that intertwining operators there gave us a representation of the double cover of $Sp(2d, \mathbf{R})$ (the metaplectic representation), with the Lie algebra representation given by the quantization of quadratic functions of the q_j, p_j phase space coordinates. There is a closely analogous story in the fermionic case, where $SO(r, s, \mathbf{R})$ acts on the fermionic phase space, preserving the symmetric bilinear form that determines the Clifford algebra relations. Here one can construct the spinor representation of the spin group $Spin(r, s, \mathbf{R})$ double covering $SO(r, s, \mathbf{R})$ using intertwining operators, with the Lie algebra representation given by quadratic combinations of the quantizations of the fermionic coordinates ξ_j.

The fermionic analog of 18.1 is

$$U_k \Gamma^+(\xi) U_k^{-1} = \Gamma^+(\phi_{k_0}(\xi)) \tag{28.1}$$

Here $k_0 \in SO(r, s, \mathbf{R})$, $\xi \in M^* = \mathbf{R}^n$ $(n = r + s)$, ϕ_{k_0} is the action of k_0 on M^*. The U_k for $k = \Phi^{-1}(k_0) \in Spin(r, s)$ (Φ_k is the 2-fold covering map) are the intertwining operators we are looking for (they will give the spinor representation). The fermionic analog of 18.5 is

$$[U'_L, \Gamma^+(\xi)] = \Gamma^+(L \cdot \xi)$$

where $L \in \mathfrak{so}(r, s, \mathbf{R})$ and L acts on M^* as an infinitesimal orthogonal transformation. In terms of basis vectors of M^*

$$\boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix}$$

this says

$$[U'_L, \Gamma^+(\boldsymbol{\xi})] = \Gamma^+(L^T \boldsymbol{\xi})$$

Just as in the bosonic case, the U'_L can be found by looking first at the pseudo-classical case, where one has theorem 27.1 which says

$$\{\mu_L, \boldsymbol{\xi}\}_+ = L^T \boldsymbol{\xi}$$

where

$$\mu_L = \frac{1}{2} \boldsymbol{\xi} \cdot L \boldsymbol{\xi} = \frac{1}{2} \sum_{j,k} L_{jk} \xi_j \xi_k$$

One can extend the representation Γ^+ to all functions of the ξ_j of order two or less by

Theorem. *A representation of the Lie superalgebra of anticommuting functions of coordinates ξ_j on $\mathbf{R}^d$ is given by*

$$\Gamma^+(1) = \mathbf{1}, \quad \Gamma^+(\xi_j) = \frac{1}{\sqrt{2}}\gamma_j, \quad \Gamma^+(\xi_j\xi_k) = \frac{1}{2}\gamma_j\gamma_k$$

Proof. We have already seen that this is a representation on polynomials of degee zero and one. For simplicity just considering the case $s = 0$, in degree two the fermionic Poisson bracket relations are given by equations 27.1 and 27.2. For 27.1, one can show that the products of Clifford algebra generators

$$\Gamma^+(\xi_j\xi_k) = \frac{1}{2}\gamma_j\gamma_k$$

satisfy

$$[\frac{1}{2}\gamma_j\gamma_k, \gamma_l] = \delta_{kl}\gamma_j - \delta_{jl}\gamma_k$$

by using the Clifford algebra relations, or by noting that this is the special case of equation 26.2 for $\mathbf{v} = \mathbf{e}_l$. That equation shows that commuting by $-\frac{1}{2}\gamma_j\gamma_k$ acts by the infinitesimal rotation ϵ_{jk} in the $j-k$ coordinate plane.

For 27.2, one can again just use the Clifford algebra relations to show

$$[\frac{1}{2}\gamma_j\gamma_k, \frac{1}{2}\gamma_l\gamma_m] = \delta_{kl}\frac{1}{2}\gamma_j\gamma_m - \delta_{jl}\frac{1}{2}\gamma_k\gamma_m + \delta_{km}\frac{1}{2}\gamma_l\gamma_j - \delta_{jm}\frac{1}{2}\gamma_l\gamma_k$$

One could also instead use the commutation relations for the $\mathfrak{so}(n)$ Lie algebra satisfied by the basis elements ϵ_{jk} corresponding to infinitesimal rotations. One must get identical commutation relations for the $-\frac{1}{2}\gamma_j\gamma_k$ and can show that these are the relations needed for commutators of $\Gamma^+(\xi_j\xi_k)$ and $\Gamma^+(\xi_l\xi_m)$. □

Returning to our construction of the representation for an arbitrary $L \in \mathfrak{so}(n)$ we have

$$U'_L = \Gamma^+(\mu_L) = \frac{1}{4}\sum_{j,k} L_{jk}\gamma_j\gamma_k$$

For the case of a rotation in the $j-k$ plane, with $L = \epsilon_{jk}$ we recover formulas 26.1 and 26.2 from chapter 26, with

$$[-\frac{1}{2}\gamma_j\gamma_k, \gamma(\mathbf{v})] = \gamma(\epsilon_{jk}\mathbf{v})$$

the infinitesimal action of a rotation on the γ matrices, and

$$\gamma(\mathbf{v}) \to e^{-\frac{\theta}{2}\gamma_j\gamma_k}\gamma(\mathbf{v})e^{\frac{\theta}{2}\gamma_j\gamma_k} = \gamma(e^{\theta\epsilon_{jk}}\mathbf{v})$$

the group version. Just as in the symplectic case, exponentiating the U'_L only gives a representation up to sign, and one needs to go to the double cover of $SO(n)$ to get a true representation. As in that case, the necessity of the double cover is best seen by use of a complex structure and an analog of the Bargmann-Fock construction.

Note that at this point, while we know that our Clifford algebras must be matrix algebras, and thus our U'_L will be represented on column vectors of a given dimension, we still lack what we had in the bosonic case: a coordinate-invariant construction of the state space of our representation. In the next sections we'll examine fermionic analogs of the constructions used in the bosonic case.

28.2 The Schrödinger representation for fermions: ghosts

We would like to construct representations of Cliff$(r, s, \mathbf{R})$ and thus fermionic state spaces by using analogous constructions to the Schrödinger and Bargmann-Fock ones in the bosonic case. The Schrödinger construction took the state space $\mathcal{H}$ to be a space of functions on a subspace of the classical phase space which had the property that the basis coordinate functions Poisson-commuted. Two examples of this are the position coordinates q_j, since $\{q_j, q_k\} = 0$, or the momentum coordinates p_j, since $\{p_j, p_k\} = 0$. Unfortunately, for symmetric bilinear forms $\langle \cdot, \cdot \rangle$ of definite sign, such as the positive definite case Cliff$(n, \mathbf{R})$, the only subspace the bilinear form is zero on is the zero subspace.

To get an analog of the bosonic situation, one needs to take the case of signature (d, d). The fermionic phase space will then be $2d$ dimensional, with d-dimensional subspaces on which $\langle \cdot, \cdot \rangle$ and thus the fermionic Poisson bracket is zero. Quantization will give the Clifford algebra

$$\text{Cliff}(d, d, \mathbf{R}) = M(2^d, \mathbf{R})$$

which has just one irreducible representation, $\mathbf{R}^{2^d}$. One can complexify this to get a complex state space

$$\mathcal{H}_F = \mathbf{C}^{2^d}$$

This state space will come with a representation of $Spin(d, d, \mathbf{R})$ from exponentiating quadratic combinations of the generators of Cliff$(d, d, \mathbf{R})$. However, this is a non-compact group, and one can show that on general grounds it cannot have unitary finite-dimensional representations, so there must be a problem with unitarity.

To see what happens explicitly, consider the simplest case $d = 1$ of one degree of freedom. In the bosonic case the classical phase space is $\mathbf{R}^2$, and quantization gives operators Q, P which in the Schrödinger representation act on functions of q, with $Q = q$ and $P = -i\frac{\partial}{\partial q}$. In the fermionic case with signature $(1, 1)$, basis coordinate functions on phase space are ξ_1, ξ_2, with

$$\{\xi_1, \xi_1\}_+ = 1, \quad \{\xi_2, \xi_2\}_+ = -1, \quad \{\xi_1, \xi_2\}_+ = 0$$

Defining

$$\eta = \frac{1}{\sqrt{2}}(\xi_1 + \xi_2), \quad \pi = \frac{1}{\sqrt{2}}(\xi_1 - \xi_2)$$

we get objects with fermionic Poisson bracket analogous to those of q and p

$$\{\eta, \eta\}_+ = \{\pi, \pi\}_+ = 0, \quad \{\eta, \pi\}_+ = 1$$

Quantizing, we get analogs of the Q, P operators

$$\hat{\eta} = \Gamma^+(\eta) = \frac{1}{\sqrt{2}}(\Gamma^+(\xi_1) + \Gamma^+(\xi_2)), \quad \hat{\pi} = \Gamma^+(\pi) = \frac{1}{\sqrt{2}}(\Gamma^+(\xi_1) - \Gamma^+(\xi_2))$$

which satisfy anticommutation relations

$$\hat{\eta}^2 = \hat{\pi}^2 = 0, \quad \hat{\eta}\hat{\pi} + \hat{\pi}\hat{\eta} = 1$$

and can be realized as operators on the space of functions of one fermionic variable η as

$$\hat{\eta} = \text{multiplication by } \eta, \quad \hat{\pi} = \frac{\partial}{\partial \eta}$$

This state space is two complex dimensional, with an arbitrary state

$$f(\eta) = c_1 1 + c_2 \eta$$

with c_j complex numbers. The inner product on this space is given by the fermionic integral

$$(f_1(\eta), f_2(\eta)) = \int f_1^*(\eta) f_2(\eta) d\eta$$

with

$$f^*(\xi) = \overline{c_1} 1 + \overline{c_2} \eta$$

With respect to this inner product, one has

$$(1, 1) = (\eta, \eta) = 0, \quad (1, \eta) = (\eta, 1) = 1$$

This inner product is indefinite and can take on negative values, since

$$(1 - \eta, 1 - \eta) = -2$$

Having such negative-norm states ruins any standard interpretation of this as a physical system, since this negative number is supposed to the probability of finding the system in this state. Such quantum systems are called "ghosts", and do have applications in the description of various quantum systems, but only when a mechanism exists for the negative-norm states to cancel or otherwise be removed from the physical state space of the theory.

28.3 Spinors and the Bargmann-Fock construction

While the fermionic analog of the Schrödinger construction does not give a unitary representation of the spin group, it turns out that the fermionic analog of

the Bargmann-Fock construction does, on the fermionic oscillator state space discussed in chapter 24. This will work for the case of a positive definite symmetric bilinear form $\langle \cdot, \cdot \rangle$. Note though that n must be even since this will require choosing a complex structure on the fermionic phase space $\mathbf{R}^n$.

The corresponding pseudo-classical system will be the classical fermionic oscillator studied in section 27.3.2. Recall that this uses a choice of complex structure J on the fermionic phase space $\mathbf{R}^{2d}$, with the standard choice $J = J_0$ giving the relations

$$\theta_j = \frac{1}{\sqrt{2}}(\xi_{2j-1} - i\xi_{2j}), \quad \overline{\theta}_j = \frac{1}{\sqrt{2}}(\xi_{2j-1} + i\xi_{2j})$$

for $j = 1, \ldots, d$ between real and complex coordinates. Here $\langle \cdot, \cdot \rangle$ is positive-definite, and the ξ_j are coordinates with respect to an orthonormal basis, so we have the standard relation $\{\xi_j, \xi_k\}_+ = \delta_{jk}$ and the $\theta_j, \overline{\theta}_j$ satisfy

$$\{\theta_j, \theta_k\}_+ = \{\overline{\theta}_j, \overline{\theta}_k\}_+ = 0, \quad \{\theta_j, \overline{\theta}_k\}_+ = \delta_{jk}$$

To quantize this system we need to find operators $\Gamma^+(\theta_j)$ and $\Gamma^+(\overline{\theta}_j)$ that satisfy

$$[\Gamma^+(\theta_j), \Gamma^+(\theta_k)]_+ = [\Gamma^+(\overline{\theta}_j), \Gamma^+(\overline{\theta}_k)]_+ = 0$$
$$[\Gamma^+(\theta_j), \Gamma^+(\overline{\theta}_k)]_+ = \delta_{jk}\mathbf{1}$$

but these are just the CAR satisfied by fermionic annihilation and creation operators. We can choose

$$\Gamma^+(\theta_j) = {a_F}_j^\dagger, \quad \Gamma^+(\overline{\theta}_j) = a_{Fj}$$

and realize these operators as

$$a_{Fj} = \frac{\partial}{\partial \chi_j}, \quad {a_F}_j^\dagger = \text{multiplication by } \chi_j$$

on the state space $\Lambda^* \mathbf{C}^d$ of polynomials in the anticommuting variables χ_j. This is a complex vector space of dimension 2^d, isomorphic with the state space $\mathcal{H}_F$ of the fermionic oscillator in d degrees of freedom, with the isomorphism given by

$$1 \leftrightarrow |0\rangle_F$$
$$\chi_j \leftrightarrow {a_F}_j^\dagger |0\rangle_F$$
$$\chi_j \chi_k \leftrightarrow {a_F}_j^\dagger {a_F}_k^\dagger |0\rangle$$
$$\cdots$$
$$\chi_1 \cdots \chi_d \leftrightarrow {a_F}_1^\dagger {a_F}_2^\dagger \cdots {a_F}_d^\dagger |0\rangle_F$$

where the indices $j, k, \ldots$ take values $1, 2, \ldots, d$ and satisfy $j < k < \cdots$.

If one defines a Hermitian inner product $(\cdot, \cdot)$ on $\mathcal{H}_F$ by taking these basis elements to be orthonormal, the operators a_{Fj} and ${a_F}_j^\dagger$ will be adjoints with

respect to this inner product. This same inner product can also be defined using fermionic integration by analogy with the Bargmann-Fock definition in the bosonic case as

$$(f_1(\chi_1, \cdots, \chi_d), f_2(\chi_1, \cdots, \chi_d)) = \int e^{-\sum_{j=1}^{d} \overline{\chi}_j \chi_j} \overline{f_1} f_2 d\chi_1 d\overline{\chi}_1 \cdots d\chi_d d\overline{\chi}_d$$

where f_1 and f_2 are complex linear combinations of the powers of the anticommuting variables χ_j. For the details of the construction of this inner product, see chapter 7.2 of [64] or chapters 7.5 and 7.6 of [79].

The quantization using fermionic annihilation and creation operators given here provides an explicit realization of a representation of the Clifford algebra Cliff$(2d, \mathbf{R})$ on the complex vector space $\mathcal{H}_F$ since we know that the $\sqrt{2}\Gamma^+(\xi_j)$ will satisfy the Clifford algebra relations, and we have

$$\xi_{2j-1} = \frac{1}{\sqrt{2}}(\theta_j + \overline{\theta}_j), \quad \xi_{2j} = \frac{i}{\sqrt{2}}(\theta_j - \overline{\theta}_j)$$

As a result, the following linear combinations of annihilation and creation operators

$$a_{F\,j} + {a_F}_j^\dagger, \quad i(a_{F\,j} - {a_F}_j^\dagger)$$

will satisfy the same Clifford algebra relations as $\gamma_{2j-1}, \gamma_{2j}$ and taking quadratic combinations of these operators on $\mathcal{H}_F$ provides a representation of the Lie algebra $\mathfrak{spin}(2d)$.

This representation exponentiates to a representation up to sign of the group $SO(2d)$, and a true representation of its double-cover $Spin(2d)$. The representation that we have constructed here on the fermionic oscillator state space $\mathcal{H}_F$ is called the spinor representation of $Spin(2d)$, and we will sometimes denote $\mathcal{H}_F$ with this group action as S.

In the bosonic case, $\mathcal{H} = \mathcal{F}_d$ is an irreducible representation of the Heisenberg group, but as a representation of $Mp(2d, \mathbf{R})$, it has two irreducible components, corresponding to even and odd polynomials. The fermionic analog is that $\mathcal{H}_F$ is irreducible under the action of the Clifford algebra Cliff$(2d, \mathbf{C})$. To show this, note that Cliff$(2d, \mathbf{C})$ is isomorphic to the matrix algebra $M(2^d, \mathbf{C})$ and its action on $\mathcal{H}_F = \mathbf{C}^{2^d}$ is isomorphic to the action of matrices on column vectors.

While $\mathcal{H}_F$ is irreducible as a representation of the Clifford algebra, it is the sum of two irreducible representations of $Spin(2d)$, the so-called "half-spinor" representations. $Spin(2d)$ is generated by quadratic combinations of the Clifford algebra generators, so these will preserve the subspaces

$$S_+ = \text{span}\{|0\rangle_F, \quad {a_F}_j^\dagger {a_F}_k^\dagger |0\rangle_F, \cdots\} \subset S = \mathcal{H}_F$$

and

$$S_- = \text{span}\{{a_F}_j^\dagger |0\rangle_F, \quad {a_F}_j^\dagger {a_F}_k^\dagger {a_F}_l^\dagger |0\rangle_F, \cdots\} \subset S = \mathcal{H}_F$$

corresponding to the action of an even or odd number of creation operators on $|0\rangle_F$. This is because quadratic combinations of the $a_{F\,j}, {a_F}_j^\dagger$ preserve the parity of the number of creation operators used to get an element of S by action on $|0\rangle_F$.

28.4 Dependence on the choice of complex structure

The construction of the spinor representation here has involved making a specific choice of relation between the Clifford algebra generators and the fermionic annihilation and creation operators. This corresponds to a standard choice of complex structure J_0, which appears in a manner closely parallel to that of the Bargmann-Fock case of section 21.1. The difference here is that for the analogous construction of spinors a complex structure J must be chosen to preserve not an antisymmetric bilinear form Ω, but the inner product, so one has

$$\langle J(\cdot), J(\cdot)\rangle = \langle \cdot, \cdot\rangle$$

We will here restrict to the case of $\langle \cdot, \cdot\rangle$ positive definite, and unlike in the bosonic case, no additional positivity condition on J will be required.

J splits the complexification of the real dual phase space $M^* = \mathcal{M} = \mathbf{R}^{2d}$ with its coordinates ξ_j into a d-dimensional complex vector space and a conjugate complex vector space. As in the bosonic case one has

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$$

and quantization of vectors in $\mathcal{M}_J^+$ gives linear combinations of creation operators, while vectors in $\mathcal{M}_J^-$ are taken to linear combinations of annihilation operators. The choice of J is reflected in the existence of a distinguished direction $|0\rangle_F$ in the spinor space $S = \mathcal{H}_F$ which is determined (up to phase) by the condition that it is annihilated by all linear combinations of annihilation operators.

The choice of J also picks out a subgroup $U(d) \subset SO(2d)$ of those orthogonal transformations that commute with J. Just as in the bosonic case, two different representations of the Lie algebra $\mathfrak{u}(d)$ of $U(d)$ are used:

- The restriction of $\mathfrak{u}(d) \subset \mathfrak{so}(2d)$ of the spinor representation described above. This exponentiates to give a representation not of $U(d)$, but of a double cover of $U(d)$ that is a subgroup of $Spin(2d)$.

- By normal-ordering operators, one shifts the spinor representation of $\mathfrak{u}(d)$ by a constant and gets a representation that exponentiates to a true representation of $U(d)$. This representation is reducible, with irreducible components the $\Lambda^k(\mathbf{C}^d)$ for $k = 0, 1, \ldots, d$.

In both cases the representation of $\mathfrak{u}(d)$ is constructed using quadratic combinations of annihilation and creation operators involving one annihilation operator and one creation operator. Non-zero pairs of two annihilation or two creation operators will give "Bogoliubov transformations", changing $|0\rangle_F$.

Given any group element

$$g_0 = e^A \subset U(d)$$

acting on the fermionic dual phase space preserving J and the inner product, we can use exactly the same method as in theorems 23.1 and 23.2 to construct its action on the fermionic state space by the second of the above representations. For A a skew-adjoint matrix we have a fermionic moment map

$$A \in \mathfrak{u}(d) \to \mu_A = \sum_{j,k} \theta_j A_{jk} \overline{\theta}_k$$

satisfying

$$\{\mu_A, \mu_{A'}\}_+ = \mu_{[A,A']}$$

and

$$\{\mu_A, \boldsymbol{\theta}\}_+ = A^T \boldsymbol{\theta}, \quad \{\mu_A, \overline{\boldsymbol{\theta}}\}_+ = \overline{A^T}\overline{\boldsymbol{\theta}}$$

The Lie algebra representation operators are the

$$U'_A = \sum_{j,k} a^\dagger_{Fj} A_{jk} a_{Fk}$$

which satisfy (see theorem 24.1)

$$[U'_A, U'_{A'}] = U_{[A,A']}$$

and

$$[U'_A, \mathbf{a}^\dagger_F] = A^T \mathbf{a}^\dagger_F, \quad [U'_A, \mathbf{a}_F] = \overline{A^T}\mathbf{a}_F$$

Exponentiating these gives the intertwining operators, which act on the annihilation and creation operators as

$$U_{e^A} \mathbf{a}^\dagger_F (U_{e^A})^{-1} = e^{A^T} \mathbf{a}^\dagger_F, \quad U_{e^A} \mathbf{a}_F (U_{e^A})^{-1} = e^{\overline{A^T}} \mathbf{a}_F$$

For the simplest example, consider the $U(1) \subset U(d) \subset SO(2d)$ that acts by

$$\theta_j \to e^{-i\phi}\theta_j, \quad \overline{\theta}_j \to e^{i\phi}\overline{\theta}_j$$

corresponding to $A = -i\phi\mathbf{1}$. The moment map will be

$$\mu_A = -i\phi h$$

where

$$h = \sum_{j=1}^{d} \overline{\theta}_j \theta_j$$

is the Hamiltonian for the classical fermionic oscillator. Quantizing h by taking the Hamiltonian operator

$$H = \frac{1}{2}\sum_{j=1}^{d} (a_F{}^\dagger_j a_{Fj} - a_{Fj} a_F{}^\dagger_j) = \sum_{j=1}^{d} (a_F{}^\dagger_j a_{Fj} - \frac{1}{2})$$

will give a Lie algebra representation with half-integral eigenvalues ($\pm\frac{1}{2}$). Exponentiation will give a representation of a double cover of $U(d)$ (and of $Spin(d)$).

Quantizing h instead using normal-ordering

$$:H: = \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}$$

will give a true representation of $U(d)$ and

$$U'_A = -i\phi \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}$$

satisfying

$$[U'_A, \mathbf{a}_F^\dagger] = -i\phi \mathbf{a}_F^\dagger, \quad [U'_A, \mathbf{a}_F] = i\phi \mathbf{a}_F$$

Exponentiating, the action on annihilation and creation operators is

$$e^{-i\phi \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}} \mathbf{a}_F^\dagger e^{i\phi \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}} = e^{-i\phi} \mathbf{a}_F^\dagger$$

$$e^{-i\phi \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}} \mathbf{a}_F e^{i\phi \sum_{j=1}^{d} {a_F}_j^\dagger a_{Fj}} = e^{i\phi} \mathbf{a}_F$$

28.5 An example: spinors for $SO(4)$

Work out in detail the spin representation of $SO(4)$ in terms of fermionic creation and annihilation operators. Also give the standard matrix representation of the Clifford algebra.

28.6 For further reading

For more about pseudo-classical mechanics and quantization, see [64] Chapter 7. The fermionic quantization map, Clifford algebras, and the spinor representation are discussed in detail in [42]. For another discussion of the spinor representation from a similar point of view to the one here, see chapter 12 of [66]. Chapter 12 of [47] contains an extensive discussion of the role of different complex structures in the construction of the spinor representation.

Chapter 29

A Summary: Parallels Between Bosonic and Fermionic Quantization

To summarize much of the material we have covered, it may be useful to consider the following table, which explicitly gives the correspondence between the parallel constructions we have studied in the bosonic and fermionic cases.

Bosonic	**Fermionic**
Dual phase space $\mathcal{M} = \mathbf{R}^{2d}$	Dual phase space $\mathcal{M} = \mathbf{R}^{2d}$
Non-degenerate antisymmetric bilinear form $\Omega(\cdot, \cdot)$ on $\mathcal{M}$	Non-degenerate symmetric bilinear form $\langle \cdot, \cdot \rangle$ on $\mathcal{M}$
Poisson bracket $\{\cdot, \cdot\}$ on functions on $\mathcal{M} = \mathbf{R}^{2d}$	Poisson bracket $\{\cdot, \cdot\}_+$ on anticommuting functions on $\mathbf{R}^{2d}$
Lie algebra of polynomials of degree $0, 1, 2$	Lie superalgebra of anticommuting polynomials of degree $0, 1, 2$
Coordinates q_j, p_j, basis of $\mathcal{M}$	Coordinates ξ_j, basis of $\mathcal{M}$
Quadratics in q_j, p_j, basis for $\mathfrak{sp}(2d, \mathbf{R})$	Quadratics in ξ_j, basis for $\mathfrak{so}(2d)$
Weyl algebra Weyl$(2d, \mathbf{C})$	Clifford algebra Cliff$(2d, \mathbf{C})$
Momentum, position operators P_j, Q_j	Clifford algebra generators γ_j
$\mathcal{H} = \mathcal{F}_d^{fin} = \mathbf{C}[w_1, \ldots, w_d] = S^*(\mathbf{C}^d)$	$\mathcal{H} = \mathcal{H}_F = \Lambda^*(\mathbf{C}^d)$
$Sp(2d, \mathbf{R})$ preserves $\Omega(\cdot, \cdot)$	$SO(2d, \mathbf{R})$ preserves $\langle \cdot, \cdot \rangle$
Quadratics in P_j, Q_j provide representation of $\mathfrak{sp}(2d, \mathbf{R})$	Quadratics in γ_j provide representation of $\mathfrak{so}(2d)$

$J : J^2 = -\mathbf{1}$, $\Omega(Ju, Jv) = \Omega(u, v)$	$J : J^2 = -\mathbf{1}$, $\langle Ju, Jv\rangle = \langle u, v\rangle$
$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$	$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$
$U(d) \subset Sp(2d, \mathbf{R})$ commutes with J	$U(d) \subset SO(2d, \mathbf{R})$ commutes with J
Compatible $J \in Sp(2d, \mathbf{R})/U(d)$	Compatible $J \in O(2d)/U(d)$
$Mp(2d, \mathbf{R})$ double-cover of $Sp(2d, \mathbf{R})$	$Spin(2d)$ double-cover of $SO(2d)$
Metaplectic representation	Spinor representation
$a_j, a_j^\dagger$ satisfying CCR	$a_{j\,F}, a_{j\,F}^\dagger$ satisfying CAR
$a_j\|0\rangle = 0$, $\|0\rangle$ depends on J	$a_{j\,F}\|0\rangle = 0$, $\|0\rangle$ depends on J

Chapter 30

Supersymmetry, Some Simple Examples

If one considers fermionic and bosonic quantum system that each separately have operators coming from Lie algebra or superalgebra representations on their state spaces, when one combines the systems by taking the tensor product, these operators will continue to act on the combined system. In certain special cases new operators with remarkable properties will appear that mix the fermionic and bosonic systems. These are generically known as "supersymmetries". In such supersymmetrical systems, important conventional mathematical objects often appear in a new light. This has been one of the most fruitful areas of interaction between mathematics and physics in recent decades, beginning with Edward Witten's highly influential 1982 paper *Supersymmetry and Morse theory* [74]. A huge array of different supersymmetric quantum field theories have been studied over the years, although the goal of using these to develop a successful unified theory remains still out of reach. In this chapter we'll examine in detail some of the simplest such quantum systems, examples of "superymmetric quantum mechanics". These have the characteristic feature that the Hamiltonian operator is a square.

30.1 The supersymmetric oscillator

In the previous chapters we discussed in detail

- The bosonic harmonic oscillator in N degrees of freedom, with state space $\mathcal{H}_B$ generated by applying N creation operators a_{Bj} to a lowest energy state $|0\rangle_B$. The Hamiltonian is

$$H = \frac{1}{2}\hbar\omega\sum_{j=1}^{N}({a_B}_j^\dagger a_{Bj} + a_{Bj}{a_B}_j^\dagger) = \sum_{j=1}^{N}(N_{Bj} + \frac{1}{2})\hbar\omega$$

where N_{Bj} is the number operator for the j'th degree of freedom, with eigenvalues $n_{Bj} = 0, 1, 2, \cdots$.

- The fermionic harmonic oscillator in N degrees of freedom, with state space $\mathcal{H}_F$ generated by applying N creation operators a_{Fj} to a lowest energy state $|0\rangle_F$. The Hamiltonian is

$$H = \frac{1}{2}\hbar\omega \sum_{j=1}^{N} (a_F{}_j^\dagger a_{Fj} - a_{Fj} a_F{}_j^\dagger) = \sum_{j=1}^{N} (N_{Fj} - \frac{1}{2})\hbar\omega$$

where N_{Fj} is the number operator for the j'th degree of freedom, with eigenvalues $n_{Fj} = 0, 1$.

Putting these two systems together we get a new quantum system with state space

$$\mathcal{H} = \mathcal{H}_B \otimes \mathcal{H}_F$$

and Hamiltonian

$$H = \sum_{j=1}^{N} (N_{Bj} + N_{Fj})\hbar\omega$$

Notice that the lowest energy state $|0\rangle$ for the combined system has energy 0, due to cancellation between the bosonic and fermionic degrees of freedom.

For now, taking for simplicity the case $N = 1$ of one degree of freedom, the Hamiltonian is

$$H = (N_B + N_F)\hbar\omega$$

with eigenvectors $|n_B, n_F\rangle$ satisfying

$$H|n_B, n_F\rangle = (n_B + n_F)\hbar\omega$$

Notice that while there is a unique lowest energy state $|0, 0\rangle$ of zero energy, all non-zero energy states come in pairs, with two states

$$|n, 0\rangle \quad \text{and} \quad |n-1, 1\rangle$$

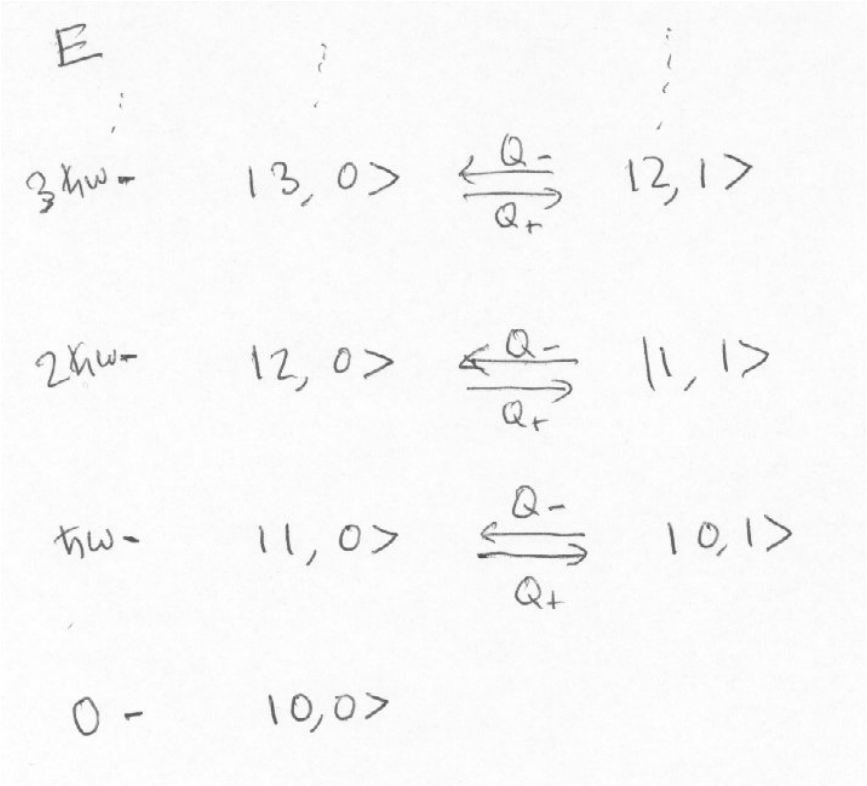
both having energy $n\hbar\omega$.

This kind of degeneracy of energy eigenvalues usually indicates the existence of some new symmetry operators commuting with the Hamiltonian operator. We are looking for operators that will take $|n, 0\rangle$ to $|n-1, 1\rangle$ and vice-versa, and the obvious choice is the two operators

$$Q_+ = a_B a_F^\dagger, \quad Q_- = a_B^\dagger a_F$$

which are not self adjoint, but are each other's adjoints ($(Q_-)^\dagger = Q_+$).

The pattern of energy eigenstates looks like



Computing anticommutators using the CCR and CAR for the bosonic and fermionic operators (and the fact that the bosonic operators commute with the fermionic ones since they act on different factors of the tensor product), one finds that

$$Q_+^2 = Q_-^2 = 0$$

and

$$(Q_+ + Q_-)^2 = [Q_+, Q_-]_+ = H$$

One could instead work with self-adjoint combinations

$$Q_1 = Q_+ + Q_-, \quad Q_2 = \frac{1}{i}(Q_+ - Q_-)$$

which satisfy

$$[Q_1, Q_2]_+ = 0, \quad Q_1^2 = Q_2^2 = H$$

Notice that the Hamiltonian H is a square of the self-adjoint operator $Q_+ + Q_-$, and this fact alone tells us that the energy eigenvalues will be non-negative. It also tells us that energy eigenstates of non-zero energy will come in pairs

$$|\psi\rangle, \quad (Q_+ + Q_-)|\psi\rangle$$

with the same energy. To find states of zero energy, instead of trying to solve the equation $H|0\rangle = 0$ for $|0\rangle$, one can look for solutions to

$$Q_1|0\rangle = 0 \quad \text{or} \quad Q_2|0\rangle = 0$$

These operators don't correspond to a Lie algebra representation as H does, but do come from a Lie superalgebra representation, so are described as generators of a "supersymmetry" transformation. In more general theories with operators like this with the same relation to the Hamiltonian, one may or may not have solutions to

$$Q_1|0\rangle = 0 \quad \text{or} \quad Q_2|0\rangle = 0$$

If such solutions exist, the lowest energy state has zero energy and is described as invariant under the supersymmetry. If no such solutions exist, the lowest energy state will have a non-zero, positive energy, and satisfy

$$Q_1|0\rangle \neq 0 \quad \text{or} \quad Q_2|0\rangle \neq 0$$

In this case one says that the supersymmetry is "spontaneously broken", since the lowest energy state is not invariant under supersymmetry.

There is an example of a physical quantum mechanical system that has exactly the behavior of this supersymmetric oscillator. A charged particle confined to a plane, coupled to a magnetic field perpendicular to the plane, can be described by a Hamiltonian that can be put in the bosonic oscillator form (to show this, we need to know how to couple quantum systems to electromagnetic fields, which we will come to later in the course). The equally spaced energy levels are known as "Landau levels". If the particle has spin one-half, there will be an additional term in the Hamiltonian coupling the spin and the magnetic field, exactly the one we have seen in our study of the two-state system. This additional term is precisely the Hamiltonian of a fermionic oscillator. For the case of gyromagnetic ratio $g = 2$, the coefficients match up so that we have exactly the supersymmetric oscillator described above, with exactly the pattern of energy levels seen there.

30.2 Supersymmetric quantum mechanics with a superpotential

The supersymmetric oscillator system can be generalized to a much wider class of potentials, while still preserving the supersymmetry of the system. In this section we'll introduce a so-called "superpotential" $W(q)$, with the harmonic oscillator the special case

$$W(q) = \frac{q^2}{2}$$

For simplicity, we will here choose constants $\hbar = \omega = 1$

Recall that our bosonic annihilation and creation operators were defined by

$$a_B = \frac{1}{\sqrt{2}}(Q + iP), \quad a_B^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$

Introducing an arbitrary superpotential $W(q)$ with derivative $W'(q)$ we can define new annihilation and creation operators:

$$a_B = \frac{1}{\sqrt{2}}(W'(Q) + iP), \quad a_B^\dagger = \frac{1}{\sqrt{2}}(W'(Q) - iP)$$

Here $W'(Q)$ is the multiplication operator $W'(q)$ in the Schrödinger representation on functions of q, defined by conjugation with a unitary operator in other unitarily equivalent representations. We keep our definition of the operators

$$Q_+ = a_B a_F^\dagger, \quad Q_- = a_B^\dagger a_F$$

These satisfy

$$Q_+^2 = Q_-^2 = 0$$

for the same reason as in the oscillator case: repeated factors of a_F or $a_F^\dagger$ vanish. Taking as the Hamiltonian the same square as before, we find

$$\begin{aligned} H =& (Q_+ + Q_-)^2 \\ =& \frac{1}{2}(W'(Q) + iP)(W'(Q) - iP)a_F^\dagger a_F + \frac{1}{2}(W'(Q) - iP)(W'(Q) + iP)a_F a_F^\dagger \\ =& \frac{1}{2}(W'(Q)^2 + P^2)(a_F^\dagger a_F + a_F a_F^\dagger) + \frac{1}{2}(i[P, W'(Q)])(a_F^\dagger a_F - a_F a_F^\dagger) \\ =& \frac{1}{2}(W'(Q)^2 + P^2) + \frac{1}{2}(i[P, W'(Q)])\sigma_3 \end{aligned}$$

But iP is the operator corresponding to infinitesimal translations in Q, so we have

$$i[P, W'(Q)] = W''(Q)$$

and

$$H = \frac{1}{2}(W'(Q)^2 + P^2) + \frac{1}{2}W''(Q)\sigma_3$$

which gives a large class of quantum systems, all with state space

$$\mathcal{H} = \mathcal{H}_B \otimes \mathcal{H}_F = L^2(\mathbf{R}) \otimes \mathbf{C}^2$$

(using the Schrödinger representation for the bosonic factor).

The energy eigenvalues will be non-negative, and energy eigenvectors with positive energy will occur in pairs

$$|\psi\rangle, \quad (Q_+ + Q_-)|\psi\rangle$$

.

There may or may not be a state with zero energy, depending on whether or not one can find a solution to the equation

$$(Q_+ + Q_-)|0\rangle = Q_1|0\rangle = 0$$

If such a solution does exist, thinking in terms of super Lie algebras, one calls Q_1 the generator of the action of a supersymmetry on the state space, and describes the ground state $|0\rangle$ as invariant under supersymmetry. If no such solution exists, one has a theory with a Hamiltonian that is invariant under supersymmetry, but with a ground state that isn't. In this situation one describes the supersymmetry as "spontaneously broken". The question of whether a given supersymmetric theory has its supersymmetry spontaneously broken or not is one that has become of great interest in the case of much more sophisticated supersymmetric quantum field theories. There, hopes (so far unrealized) of making contact with the real world rely on finding theories where the supersymmetry is spontaneously broken.

In this simple quantum mechanical system, one can try and explicitly solve the equation $Q_1|\psi\rangle = 0$. States can be written as two-component complex functions

$$|\psi\rangle = \begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix}$$

and the equation to be solved is

$$\begin{aligned}
(Q_+ + Q_-)|\psi\rangle &= \frac{1}{\sqrt{2}}((W'(Q) + iP)a_F^\dagger + (W'(Q) - iP)a_F) \begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix} \\
&= \frac{1}{\sqrt{2}}((W'(Q) + \frac{d}{dq}) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + (W'(Q) - \frac{d}{dq}) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}) \begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix} \\
&= \frac{1}{\sqrt{2}}(W'(Q) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{d}{dq} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}) \begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (\frac{d}{dq} - W'(Q)\sigma_3) \begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix} = 0
\end{aligned}$$

which has general solution

$$\begin{pmatrix} \psi_+(q) \\ \psi_-(q) \end{pmatrix} = e^{W(q)\sigma_3} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} c_+ e^{W(q)} \\ c_- e^{-W(q} \end{pmatrix}$$

for complex constants c_+, c_-. Such solutions will only be normalizable if

$$c_+ = 0, \ \lim_{q \to \pm\infty} W(q) = +\infty$$

or

$$c_- = 0, \ \lim_{q \to \pm\infty} W(q) = -\infty$$

If, for example, $W(q)$ is an odd polynomial, one will not be able to satisfy either of these conditions, so there will be no solution, and the supersymmetry will be spontaneously broken.

30.3 Supersymmetric quantum mechanics and differential forms

If one considers supersymmetric quantum mechanics in the case of d degrees of freedom and in the Schrödinger representation, one has

$$\mathcal{H} = L^2(\mathbf{R}^d) \otimes \Lambda^*(\mathbf{R}^d)$$

the tensor product of complex-valued functions on $\mathbf{R}^d$ (acted on by the Weyl algebra Weyl$(2d, \mathbf{C})$) and anticommuting functions on $\mathbf{R}^d$ (acted on by the Clifford algebra Cliff$(2d, \mathbf{C})$). There are two operators Q_+ and Q_-, adjoints of each other and of square zero. If one has studied differential forms, this should look familiar. This space $\mathcal{H}$ is well-known to mathematicians, as the complex valued differential forms on $\mathbf{R}^d$, often written $\Omega^*(\mathbf{R}^d)$, where here the * denotes an index taking values from 0 (the 0-forms, or functions) to d (the d-forms). In the theory of differential forms, it is well known that one has an operator d on $\Omega^*(\mathbf{R}^d)$ with square zero, called the de Rham differential. Using the inner product on $\mathbf{R}^d$, one can put a Hermitian inner product on $\Omega^*(\mathbf{R}^d)$ by integration, and then d has an adjoint δ, also of square zero. The Laplacian operator on differential forms is

$$\Box = (d + \delta)^2$$

The supersymmetric quantum system we have been considering corresponds precisely to this, once one conjugates d, δ as follows

$$Q_+ = e^{-V(q)} d e^{V(q)}, \quad Q_- = e^{V(q)} \delta e^{-V(q)}$$

In mathematics, the interest in differential forms mainly comes from the fact that one can construct them not just on $\mathbf{R}^d$, but on a general differentiable manifold M, with a corresponding construction of $d, \delta, \Box$ operators. In Hodge theory, one studies solutions of

$$\Box \psi = 0$$

(these are called "harmonic forms") and finds that the dimension of the space of such solutions can be used to get topological invariants of the manifold M. Witten's famous 1982 paper on supersymmetry and Morse theory [74] first exposed these connections, using them both to give new ways of thinking about the mathematics involved, as well as applications of topology to the question of deciding whether supersymmetry was spontaneously broken in various supersymmetric models.

30.4 For further reading

For a reference at the level of these notes, see [22]. For more details about supersymmetric quantum mechanics and its relationship to the Dirac operator and the index theorem, see the graduate level textbook of Tahktajan [64], and

lectures by Orlando Alvarez [1]. These last two sources also describe the formalism one can get by putting together the standard Hamiltonian mechanics and its fermionic analog, consistently describing a "classical" system with both commuting and anticommuting variables and its quantization to get the quantum systems described in this chapter.

Chapter 31

The Dirac Operator

In chapter 30 we considered supersymmetric quantum mechanical systems where both the bosonic and fermionic variables that get quantized take values in an even dimensional phase space $\mathbf{R}^{2d}$. There are then two supersymmetry operators Q_1 and Q_2, so this is sometimes called $N = 2$ supersymmetry (in an alternate normalization, counting complex variables, it is called $N = 1$). It turns out however that there are very interesting quantum mechanics systems that one can get by quantizing bosonic variables in $\mathbf{R}^{2d}$, but fermionic variables in $\mathbf{R}^d$. The operators appearing in such a theory will be given by the tensor product of the Weyl algebra in $2d$ variables and the Clifford algebra in d variables.

In such a theory the operator $-|\mathbf{P}|^2$ will have a square root, the Dirac operator $\not{\partial}$. This existence of a square root of the Casimir operator provides a new way to construct irreducible representations of the group of spatial symmetries, using a new sort of quantum free particle, one carrying an internal "spin" degree of freedom. Remarkably, fundamental matter particles are well-described in exactly this way.

31.1 The Dirac operator

Recall from chapter 26 that associated to $\mathbf{R}^d$ with a standard inner product, but of a general signature (r, s) (where $r + s = d$, r is the number of $+$ signs, s the number of $-$ signs) we have a Clifford algebra $\text{Cliff}(r, s)$ with generators γ_j satisfying

$$\gamma_j \gamma_k = -\gamma_k \gamma_j, \quad j \neq k$$
$$\gamma_j^2 = +1 \text{ for} j = 1, \cdots, r \quad \gamma_j^2 = -1, \text{ for} j = r+1, \cdots, d$$

To any vector $\mathbf{v} \in \mathbf{R}^d$ with components v_j recall that we can associate a corresponding element $\not{\mathbf{v}}$ in the Clifford algebra by

$$\mathbf{v} \in \mathbf{R}^d \to \not{\mathbf{v}} = \sum_{j=1}^{d} \gamma_j v_j \in \text{Cliff}(r, s)$$

Multiplying this Clifford algebra element by itself and using the relations above, we get a scalar, the length-squared of the vector

$$\not{\mathbf{v}}^2 = v_1^2 + v_2^2 \cdots + v_r^2 - v_{r+1}^2 - \cdots - v_d^2 = |\mathbf{v}|^2$$

This shows that by introducing a Clifford algebra, we can find an interesting new sort of square-root for expressions like $|\mathbf{v}|^2$. We can define

Definition (Dirac operator)**.** *The Dirac operator is the operator*

$$\not{\partial} = \sum_{j=1}^{d} \gamma_j \frac{\partial}{\partial q_j}$$

This will be a first-order differential operator with the property that its square is the Laplacian

$$\not{\partial}^2 = \frac{\partial^2}{\partial q_1^2} + \cdots + \frac{\partial^2}{\partial q_r^2} - \frac{\partial^2}{\partial q_{r+1}^2} - \cdots - \frac{\partial^2}{\partial q_d^2}$$

The Dirac operator $\not{\partial}$ acts not on functions but on functions taking values in the spinor vector space S that the Clifford algebra acts on. Picking a matrix representation of the γ_j, the Dirac operator will be a constant coefficient first order differential operator acting on wavefunctions with dim S components. In chapter 44 we will study in detail what happens for the case of $r = 3, s = 1$ and see how the Dirac operator there provides an appropriate wave-equation with the symmetries of special relativistic space-time.

31.2 The Pauli operator and free spin $\frac{1}{2}$ particles in $d = 3$

In dimension $d = 3$ ($r = 3, s = 0$), one can choose as generators of the Clifford algebra the three Pauli matrices σ_j. The Dirac operator can then be written as

$$\not{\partial} = \sigma_1 \frac{\partial}{\partial q_1} + \sigma_2 \frac{\partial}{\partial q_2} + \sigma_3 \frac{\partial}{\partial q_3} = \sigma \cdot \boldsymbol{\nabla}$$

and it operates on two-component wavefunctions

$$\begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix}$$

Using the Dirac operator (often called in this context the "Pauli operator") we can write a two-component version of the Schrödinger equation (often called the "Pauli equation" or "Schrödinger-Pauli equation")

$$i\frac{\partial}{\partial t}\begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix} = \frac{-1}{2m}(\sigma_1 \frac{\partial}{\partial q_1} + \sigma_2 \frac{\partial}{\partial q_2} + \sigma_3 \frac{\partial}{\partial q_3})^2 \begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix} \tag{31.1}$$

This free-particle version of the equation is just two copies of the standard free-particle Schrödinger equation, so physically just corresponds to two independent quantum free particles. It becomes much more non-trivial when a coupling to an electromagnetic field is introduced, as will be seen in chapter 42.

The introduction of a two-component wavefunction does allow us to find more interesting irreducible representations of the group $E(3)$. These have eigenvalue $\pm\frac{1}{2}p$ (where p^2 is the eigenvalue of the first Casimir operator $|\mathbf{P}|^2$) for the second Casimir operator $\mathbf{J}\cdot\mathbf{P}$ as opposed to the zero eigenvalue case of single wavefunctions studied in chapter 17.

These representations will as before be on the space of solutions of the time-independent equation, and irreducible for fixed choice of the energy E. Using the momentum operator this equation will be

$$\frac{1}{2m}(\sigma\cdot\mathbf{P})^2\begin{pmatrix}\psi_1(\mathbf{q})\\ \psi_2(\mathbf{q})\end{pmatrix}=E\begin{pmatrix}\psi_1(\mathbf{q})\\ \psi_2(\mathbf{q})\end{pmatrix}$$

In terms of the inverse Fourier transform

$$\psi_{1,2}(\mathbf{q})=\frac{1}{(2\pi)^{\frac{3}{2}}}\iiint e^{i\mathbf{p}\cdot\mathbf{q}}\widetilde{\psi}_{1,2}(\mathbf{p})d^3\mathbf{p}$$

this equation becomes

$$((\sigma\cdot\mathbf{p})^2-2mE)\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}=(|\mathbf{p}|^2-2mE)\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}=0 \tag{31.2}$$

and as in chapter 17 our solution space is given by functions $\widetilde{\psi}_{E,1,2}(\mathbf{p})$ on the sphere of radius $\sqrt{2mE}=|\mathbf{p}|$ in momentum space (although now, two such functions).

Another way to find solutions to this equation is to look for solutions to the pair of first-order equations involving the three-dimensional Dirac operator. Solutions to

$$\sigma\cdot\mathbf{p}\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}=\pm\sqrt{2mE}\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}$$

will give solutions to 31.2, for either sign. One can rewrite this as

$$\frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|}\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}=\pm\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix}$$

and we will write solutions to this equation with the $+$ sign as $\widetilde{\psi}_{E,+}(\mathbf{p})$, those for the $-$ sign as $\widetilde{\psi}_{E,-}(\mathbf{p})$. Note that $\widetilde{\psi}_{E,+}(\mathbf{p})$ and $\widetilde{\psi}_{E,+}(\mathbf{p})$ are each two-component complex functions of the momentum, supported on the sphere $\sqrt{2mE}=|\mathbf{p}|$.

In chapter 16 we saw that $R\in SO(3)$ acts on single-component momentum space solutions of the Schrödinger equation by

$$\widetilde{\psi}_E(\mathbf{p})\to\widetilde{u}(0,R)\widetilde{\psi}_E(\mathbf{p})\equiv\widetilde{\psi}_E(R^{-1}\mathbf{p})$$

This takes solutions to solutions since the operator $\widetilde{u}(0,R)$ commutes with the Casimir operator $|\mathbf{P}|^2$

$$\widetilde{u}(0,R)|\mathbf{P}|^2 = |\mathbf{P}|^2\widetilde{u}(0,R) \iff \widetilde{u}(0,R)|\mathbf{P}|^2\widetilde{u}(0,R)^{-1} = |\mathbf{P}|^2$$

This is true since

$$\begin{aligned}\widetilde{u}(0,R)|\mathbf{P}|^2\widetilde{u}(0,R)^{-1}\widetilde{\psi}(\mathbf{p}) =&\widetilde{u}(0,R)|\mathbf{P}|^2\widetilde{\psi}(R\mathbf{p})\\ =&|R^{-1}\mathbf{P}|^2\widetilde{\psi}(R^{-1}R\mathbf{p}) = |\mathbf{P}|^2\widetilde{\psi}(\mathbf{p})\end{aligned}$$

For two-component wavefunctions, we could try to just take the representation to be

$$\widetilde{u}(0,R)\begin{pmatrix}\widetilde{\psi}_1(\mathbf{p})\\ \widetilde{\psi}_2(\mathbf{p})\end{pmatrix} = \begin{pmatrix}\widetilde{\psi}_1(R^{-1}\mathbf{p})\\ \widetilde{\psi}_2(R^{-1}\mathbf{p})\end{pmatrix}$$

(or, equivalently, thinking of two component wavefunctions as the tensor product of the space of single component wavefunctionwith $\mathbf{C}^2$, just acting on the first factor). If we do this, the operator $\sigma\cdot\mathbf{P}$ does not commute with the representation $\widetilde{u}(0,R)$ because

$$\widetilde{u}(0,R)(\sigma\cdot\mathbf{P})\widetilde{u}(0,R)^{-1} = (\sigma\cdot R^{-1}\mathbf{P})) \neq \sigma\cdot\mathbf{P}$$

Then rotations do not act separately on the spaces $\widetilde{\psi}_{E,+}(\mathbf{p})$ and $\widetilde{\psi}_{E,-}(\mathbf{p})$.

If we want rotations to act separately on these spaces, we need to change the action of rotations to

$$\widetilde{\psi}_{E,\pm}(\mathbf{p}) \to \widetilde{u}_S(0,R)\widetilde{\psi}_{E,\pm}(\mathbf{p}) = \Omega\widetilde{\psi}_{E,\pm}(R^{-1}\mathbf{p})$$

where Ω is one of the two elements of $SU(2)$ corresponding to $R\in SO(3)$ (or, in terms of tensor products, action by $SU(2)$ on the $\mathbf{C}^2$ factor). Such an Ω can be constructed using equation 6.3

$$\Omega = \Omega(\phi,\mathbf{w}) = e^{-i\frac{\phi}{2}\mathbf{w}\cdot\sigma}$$

Equation 6.5 shows that Ω is the $SU(2)$ matrix corresponding to a rotation R by an angle ϕ about the axis given by a unit vector $\mathbf{w}$.

With this action on solutions we have

$$\begin{aligned}\widetilde{u}_S(0,R)(\sigma\cdot\mathbf{P})\widetilde{u}_S(0,R)^{-1}\widetilde{\psi}_{E,\pm}(\mathbf{p}) =&\widetilde{u}_S(0,R)(\sigma\cdot\mathbf{P})\Omega^{-1}\widetilde{\psi}_{E,\pm}(R\mathbf{p})\\ =&\Omega(\sigma\cdot R^{-1}\mathbf{P})\Omega^{-1}\widetilde{\psi}_{E,\pm}(R^{-1}R\mathbf{p})\\ =&(\sigma\cdot\mathbf{P})\widetilde{\psi}_{E,\pm}(\mathbf{p})\end{aligned}$$

where we have used equation 6.5 to show

$$\Omega(\sigma\cdot R^{-1}\mathbf{P})\Omega^{-1} = (\sigma\cdot RR^{-1}\mathbf{P}) = (\sigma\cdot\mathbf{P})$$

Note that the two representations we get this way are representations not of the rotation group $SO(3)$ but of its double cover $Spin(3) = SU(2)$ (because

otherwise there is a sign ambiguity since we don't know whether to choose Ω or $-\Omega$). The translation part of the spatial symmetry group is easily seen to commute with $\sigma \cdot \mathbf{P}$, so we have constructed representations of $E(3)$, or rather, of its double cover

$$\widetilde{E(3)} = \mathbf{R}^3 \rtimes SU(2)$$

on the two spaces of solutions $\widetilde{\psi}_{E,\pm}(\mathbf{p})$. We will see that these two representations are the $E(3)$ representations described in section 17.3, the ones labeled by the helicity $\pm\frac{1}{2}$ representations of the stabilizer group $SO(2)$.

The translation part of the group acts as in the one-component case, by the multiplication operator

$$\widetilde{u}_S(\mathbf{a}, \mathbf{1})\widetilde{\psi}_{E,\pm}(\mathbf{p}) = e^{-i(\mathbf{a}\cdot\mathbf{p})}\widetilde{\psi}_{E,\pm}(\mathbf{p})$$

and

$$\widetilde{u}_S(\mathbf{a}, \mathbf{1}) = e^{-i\mathbf{a}\cdot\mathbf{P}}$$

so the Lie algebra representation is given by the usual $\mathbf{P}$ operator. The $SU(2)$ part of the group acts by a commuting product of two different actions

1. The same action on the momentum coordinates as in the one-component case, just using $R = \Phi(\Omega)$, the $SO(3)$ rotation corresponding to the $SU(2)$ group element Ω. For example, for a rotation about the x-axis by angle ϕ we have

   $$\widetilde{\psi}_{E,\pm}(\mathbf{p}) \to \widetilde{\psi}_{E,\pm}(R(\phi, \mathbf{e}_1)^{-1}\mathbf{p})$$

   Recall that the operator that does this is $e^{-i\phi L_1}$ where

   $$-iL_1 = -i(Q_2P_3 - Q_3P_2) = -(q_2\frac{\partial}{\partial q_3} - q_3\frac{\partial}{\partial q_2})$$

   and in general we have operators

   $$-i\mathbf{L} = -i\mathbf{Q} \times \mathbf{P}$$

   that provide the Lie algebra version of the representation (recall that at the Lie algebra level, $SO(3)$ and $Spin(3)$ are isomorphic).

2. The action of the matrix $\Omega \in SU(2)$ on the two-component wavefunction by

   $$\widetilde{\psi}_{E,\pm}(\mathbf{p}) \to \Omega\widetilde{\psi}_{E,\pm}(\mathbf{p})$$

   For a rotation by angle ϕ about the x-axis we have

   $$\Omega = e^{-i\phi\frac{\sigma_1}{2}}$$

   and the operators that provide the Lie algebra version of the representation are the

   $$-i\mathbf{S} = -i\frac{1}{2}\sigma$$

The Lie algebra representation corresponding to the action of both of these transformations is given by the operator

$$-i\mathbf{J} = -i(\mathbf{L} + \mathbf{S})$$

and the standard terminology is to call $\mathbf{L}$ the "orbital" angular momentum, $\mathbf{S}$ the "spin" angular momentum, and $\mathbf{J}$ the "total" angular momentum.

The second Casimir operator for this case is

$$\mathbf{J} \cdot \mathbf{P}$$

and as in the one-component case the $\mathbf{L} \cdot \mathbf{P}$ part of this acts trivially on our solutions $\widetilde{\psi}_{E,\pm}(\mathbf{p})$. The spin component acts non-trivially and we have

$$(\mathbf{J} \cdot \mathbf{P})\widetilde{\psi}_{E,\pm}(\mathbf{p}) = (\frac{1}{2}\sigma \cdot \mathbf{p})\widetilde{\psi}_{E,\pm}(\mathbf{p}) = \pm\frac{1}{2}|\mathbf{p}|\widetilde{\psi}_{E,\pm}(\mathbf{p})$$

so we see that our solutions have helicity (eigenvalue of $\mathbf{J} \cdot \mathbf{P}$ divided by the square root of the eigenvalue of $|\mathbf{P}|^2$) values $\pm\frac{1}{2}$, as opposed to the integral helicity values discussed in chapter 17, where $E(3)$ appeared and not its double cover.

31.3 For further reading

The point of view here in terms of representations of $\widetilde{E(3)}$ is not very conventional, but the material here about spin and the Pauli equation can be found in any quantum mechanics book, see for example chapter 14 of [57].

Chapter 32

Lagrangian Methods and the Path Integral

In this chapter we'll give a rapid survey of a different starting point for developing quantum mechanics, based on the Lagrangian rather than Hamiltonian classical formalism. Lagrangian methods have quite different strengths and weaknesses than those of the Hamiltonian formalism, and we'll try and point these out, while referring to standard physics texts for more detail about these methods.

The Lagrangian formalism leads naturally to an apparently very different notion of quantization, one based upon formulating quantum theory in terms of infinite-dimensional integrals known as path integrals. A serious investigation of these would require another and very different volume, so again we'll have to restrict ourselves to outlining how path integrals work, describing their strengths and weaknesses, and giving references to standard texts for the details.

32.1 Lagrangian mechanics

In the Lagrangian formalism, instead of a phase space $\mathbf{R}^{2d}$ of positions q_j and momenta p_j, one considers just the position space $\mathbf{R}^d$. Instead of a Hamiltonian function $h(\mathbf{q}, \mathbf{p})$, one has

Definition (Lagrangian)**.** *The Lagrangian L for a classical mechanical system with configuration space $\mathbf{R}^d$ is a function*

$$L : (\mathbf{q}, \mathbf{v}) \in \mathbf{R}^d \times \mathbf{R}^d \to L(\mathbf{q}, \mathbf{v}) \in \mathbf{R}$$

Given differentiable paths in the configuration space defined by functions

$$\gamma : t \in [t_1, t_2] \to \mathbf{R}^d$$

which we will write in terms of their position and velocity vectors as

$$\gamma(t) = (\mathbf{q}(t), \dot{\mathbf{q}}(t))$$

one can define a functional on the space of such paths

Definition. *Action*

The action S for a path γ is

$$S[\gamma] = \int_{t_1}^{t_2} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))dt$$

The fundamental principle of classical mechanics in the Lagrangian formalism is that classical trajectories are given by critical points of the action functional. These may correspond to minima of the action (so this is sometimes called the "principle of least action"), but one gets classical trajectories also for critical points that are not minima of the action. One can define the appropriate notion of critical point as follows

Definition. *Critical point for S*

A path γ is a critical point of the functional $S[\gamma]$ if

$$\delta S(\gamma) \equiv \frac{d}{ds} S(\gamma_s)_{|s=0} = 0$$

when

$$\gamma_s : [t_1, t_2] \to \mathbf{R}^d$$

is a smooth family of paths parametrized by an interval $s \in (-\epsilon, \epsilon)$, with $\gamma_0 = \gamma$.

We'll now ignore analytical details and adopt the physicist's interpretation of this as the first-order change in S due to an infinitesimal change $\delta\gamma = (\delta\mathbf{q}(t), \delta\dot{\mathbf{q}}(t))$ in the path.

When $(\mathbf{q}(t), \dot{\mathbf{q}}(t))$ satisfy a certain differential equation, the path γ will be a critical point and thus a classical trajectory:

Theorem. *Euler-Lagrange equations*

One has

$$\delta S[\gamma] = 0$$

for all variations of γ with endpoints $\gamma(t_1)$ and $\gamma(t_2)$ fixed if

$$\frac{\partial L}{\partial q_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t)) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}(t), \dot{\mathbf{q}}(t))\right) = 0$$

for $j = 1, \cdots, d$. These are called the Euler-Lagrange equations.

Proof. Ignoring analytical details, the Euler-Lagrange equations follow from the following calculations, which we'll just do for $d = 1$, with the generalization to higher d straightfoward. We are calculating the first-order change in S due to an infinitesimal change $\delta\gamma = (\delta q(t), \delta\dot{q}(t))$

$$\begin{aligned}
\delta S[\gamma] &= \int_{t_1}^{t_2} \delta L(q(t), \dot{q}(t))dt \\
&= \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q}(q(t), \dot{q}(t))\delta q(t) + \frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t))\delta\dot{q}(t)\right)dt
\end{aligned}$$

But

$$\delta\dot{q}(t) = \frac{d}{dt}\delta q(t)$$

and, using integration by parts

$$\frac{\partial L}{\partial \dot{q}}\delta\dot{q}(t) = \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}\delta q) - (\frac{d}{dt}\frac{\partial L}{\partial \dot{q}})\delta q$$

so

$$\begin{aligned}\delta S[\gamma] &= \int_{t_1}^{t_2}((\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}})\delta q - \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}\delta q))dt \\ &= \int_{t_1}^{t_2}(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}})\delta q dt - (\frac{\partial L}{\partial \dot{q}}\delta q)(t_2) + (\frac{\partial L}{\partial \dot{q}}\delta q)(t_1)\end{aligned}$$

If we keep the endpoints fixed so $\delta q(t_1) = \delta q(t_2) = 0$, then for solutions to

$$\frac{\partial L}{\partial q}(q(t), \dot{q}(t)) - \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t))) = 0$$

the integral will be zero for arbitrary variations δq. □

As an example, a particle moving in a potential $V(\mathbf{q})$ will be described by a Lagrangian

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}m\sum_{j=1}^{d}\dot{q}_j^2 - V(\mathbf{q})$$

for which the Euler-Lagrange equations will be

$$-\frac{\partial V}{\partial q_j} = \frac{d}{dt}(m\dot{q}_j)$$

This is just Newton's second law which says that the force coming from the potential is equal to the mass times the acceleration of the particle.

The derivation of the Euler-Lagrange equations can also be used to study the implications of Lie group symmetries of a Lagrangian system. When a Lie group G acts on the space of paths, preserving the action S, it will take classical trajectories to classical trajectories, so we have a Lie group action on the space of solutions to the equations of motion (the Euler-Lagrange equations). In good cases, this space of solutions is just the phase space of the Hamiltonian formalism. On this space of solutions, we have, from the calculation above

$$\delta S[\gamma] = (\frac{\partial L}{\partial \dot{q}}\delta q(X))(t_1) - (\frac{\partial L}{\partial \dot{q}}\delta q(X))(t_2)$$

where now $\delta q(X)$ is the infinitesimal change in a classical trajectory coming from the infinitesimal group action by an element X in the Lie algebra of G. From invariance of the action S under G we must have δS=0, so

$$(\frac{\partial L}{\partial \dot{q}}\delta q(X))(t_2) = (\frac{\partial L}{\partial \dot{q}}\delta q(X))(t_1)$$

This is an example of a more general result known as "Noether's theorem". It says that given a Lie group action on a Lagrangian system that leaves the action invariant, for each element X of the Lie algebra we will have a conserved quantity

$$\frac{\partial L}{\partial \dot{q}} \delta q(X)$$

which is independent of time along the trajectory. A basic example is when the Lagrangian is independent of the position variables q_j, depending only on the velocities $\dot{q}_j$, for example in the case of a free particle, when $V(\mathbf{q}) = 0$. In such a case one has invariance under the Lie group $\mathbf{R}^d$ of space-translations. An infinitesimal transformation in the j-direction is given by

$$\delta q_j(t) = \epsilon$$

and the conserved quantity is

$$\frac{\partial L}{\partial \dot{q}_j}$$

For the case of the free particle, this will be

$$\frac{\partial L}{\partial \dot{q}_j} = m\dot{q}_j$$

and the conservation law is conservation of momentum.

Given a Lagrangian classical mechanical system, one would like to be able to find a corresponding Hamiltonian system that will give the same equations of motion. To do this, we proceed by defining the momenta p_j as above, as the conserved quantities corresponding to space-translations, so

$$p_j = \frac{\partial L}{\partial \dot{q}_j}$$

Then, instead of working with trajectories characterized at time t by

$$(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \in \mathbf{R}^{2d}$$

we would like to instead use

$$(\mathbf{q}(t), \mathbf{p}(t)) \in \mathbf{R}^{2d}$$

where $p_j = \frac{\partial L}{\partial \dot{q}_j}$ and this $\mathbf{R}^{2d}$ is the Hamiltonian phase space with the conventional Poisson bracket.

This transformation between position-velocity and phase space is known as the Legendre transform, and in good cases (for instance when L is quadratic in all the velocities) it is an isomorphism. In general though, this is not an isomorphism, with the Legendre transform often taking position-velocity space to a lower-dimensional subspace of phase space. Such cases require a much more elaborate version of Hamiltonian formalism, known as "constrained Hamiltonian

dynamics" and are not unusual: one example we will see later is that of the equations of motion of a free electromagnetic field (Maxwell's equations).

Besides a phase space, for a Hamiltonian system one needs a Hamiltonian function. Choosing

$$h = \sum_{j=1}^{d} p_j \dot{q}_j - L(\mathbf{q}, \dot{\mathbf{q}})$$

will work, provided one can use the relation

$$p_j = \frac{\partial L}{\partial \dot{q}_j}$$

to solve for the velocities $\dot{q}_j$ and express them in terms of the momentum variables. In that case, computing the differential of h one finds (for $d = 1$, the generalization to higher d is straightforward)

$$\begin{aligned} dh =& p d\dot{q} + \dot{q} dp - \frac{\partial L}{\partial q} dq - \frac{\partial L}{\partial \dot{q}} d\dot{q} \\ =& \dot{q} dp - \frac{\partial L}{\partial q} dq \end{aligned}$$

So one has

$$\frac{\partial h}{\partial p} = \dot{q}, \quad \frac{\partial h}{\partial q} = -\frac{\partial L}{\partial q}$$

but these are precisely Hamilton's equations since the Euler-Lagrange equations imply

$$\frac{\partial L}{\partial q} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = \dot{p}$$

The Lagrangian formalism has the advantage of depending concisely just on the choice of action functional, which does not distinguish time in the same way that the Hamiltonian formalism does by its dependence on a choice of Hamiltonian function h. This makes the Lagrangian formalism quite useful in the case of relativistic quantum field theories, where one would like to exploit the full set of space-time symmetries, which can mix space and time directions. On the other hand, one loses the infinite dimensional group of symmetries of phase space for which the Poisson bracket is the Lie bracket (the so-called "canonical transformations"). In the Hamiltonian formalism we saw that the harmonic oscillator could be best understood using such symmetries, in particular the $U(1)$ symmetry generated by the Hamiltonian function. The harmonic oscillator is a more difficult problem in the Lagrangian formalism, where this symmetry is not manifest.

32.2 Path integrals

After the Legendre transform of a Lagrangian classical system to phase space and thus to Hamiltonian form, one can then apply the method of quantization

we have discussed extensively earlier (known to physicists as "canonical quantization"). There is however a very different approach to quantization, which completely bypasses the Hamiltonian formalism. This is the path integral formalism, which is based upon a method for calculating matrix elements of the time-evolution operator

$$\langle q_T | e^{-\frac{i}{\hbar}HT} | q_0 \rangle$$

in the position eigenstate basis in terms of an integral over the space of paths that go from q_0 to q_1 in time T. Here $|q_0\rangle$ is an eigenstate of Q with eigenvalue q_0 (a delta-function at q_0 in the position space representation), and $|q_T\rangle$ has Q eigenvalue q_T (as in many cases, we'll stick to $d = 1$ for this discussion). This matrix element has a physical interpretation as the amplitude for a particle starting at q_0 at $t = 0$ to have position q_T at time T, with its norm-squared giving the probability density for observing the particle at position q_T.

To try and derive a path-integral expression for this, one breaks up the interval $[0, T]$ into N equal-sized sub-intervals and calculates

$$\langle q_T | (e^{-\frac{i}{N\hbar}HT})^N | q_0 \rangle$$

If the Hamiltonian breaks up as $H = K + V$, the Trotter product formula shows that

$$\langle q_T | e^{-\frac{i}{\hbar}HT} | q_0 \rangle = \lim_{N\to\infty} \langle q_T | (e^{-\frac{i}{N\hbar}KT} e^{-\frac{i}{N\hbar}VT})^N | q_0 \rangle$$

If $K(P)$ can be chosen to depend only on the momentum operator P and $V(Q)$ depends only on the operator Q then one can insert alternate copies of the identity operator in the forms

$$\int_{-\infty}^{\infty} |q\rangle\langle q| dq = \mathbf{1}, \quad \int_{-\infty}^{\infty} |p\rangle\langle p| dp = \mathbf{1}$$

This gives a product of terms that looks like

$$\langle q_j | e^{-\frac{i}{N\hbar}K(P)T} | p_j \rangle \langle p_j | e^{-\frac{i}{N\hbar}V(Q)T} | q_{j-1} \rangle$$

where the index j goes from 1 to N and the p_j, q_j variable will be integrated over. Such a term can be evaluated as

$$\begin{aligned} &\langle q_j | p_j \rangle \langle p_j | q_{j-1} \rangle e^{-\frac{i}{N\hbar}K(p_j)T} e^{-\frac{i}{N\hbar}V(q_{j-1})T} \\ &= \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}q_j p_j} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}q_{j-1} j p_j} e^{-\frac{i}{N\hbar}K(p_j)T} e^{-\frac{i}{N\hbar}V(q_{j-1})T} \\ &= \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar}p_j(q_j - q_{j-1})} e^{-\frac{i}{N\hbar}(K(p_j)+V(q_{j-1}))T} \end{aligned}$$

The N factors of this kind give an overall factor of $(\frac{1}{2\pi\hbar})^N$ times something which is a discretized approximation to

$$e^{\frac{i}{\hbar}\int_0^T (p\dot{q} - h(q(t),p(t)))dt}$$

where the phase in the exponential is just the action. Taking into account the integrations over q_j and p_j one should have something like

$$\langle q_T|e^{-\frac{i}{\hbar}HT}|q_0\rangle = \lim_{N\to\infty}(\frac{1}{2\pi\hbar})^N \prod_{j=1}^{N}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dp_j dq_j e^{\frac{i}{\hbar}\int_0^T (p\dot{q}-h(q(t),p(t)))dt}$$

although one should not do the first and last integrals over q but fix the first value of q to q_0 and the last one to q_T. One can try and interpret this sort of integration in the limit as an integral over the space of paths in phase space, thus a "phase space path integral".

This is an extremely simple and seductive expression, apparently saying that, once the action S is specified, a quantum system is defined just by considering integrals

$$\int D\gamma\ e^{\frac{i}{\hbar}S[\gamma]}$$

over paths γ in phase space, where $D\gamma$ is some sort of measure on this space of paths. Since the integration just involves factors of $dpdq$ and the exponential just pdq and h, this formalism seems to share the same sort of invariance under the infinite-dimensional group of canonical transformations (transformations of the phase space preserving the Poisson bracket) as the classical Hamiltonian formalism. It also appears to solve our problem with operator ordering ambiguities, since introducing products of Ps and Q's at various times will just give a phase space path integral with the corresponding p and q factors in the integrand, but these commute.

Unfortunately, we know from the Groenewold-van Hove theorem that this is too good to be true. This expression cannot give a unitary representation of the full group of canonical transformations, at least not one that is irreducible and restricts to what we want on transformations generated by linear functions q and p. Another way to see the problem is that a simple argument shows that by canonical transformations one can transform any Hamiltonian into a free-particle Hamiltonian, so all quantum systems would just be free particles in some choice of variables. For the details of these arguments and a careful examination of what goes wrong, see chapter 31 of [54]. One aspect of the problem is that, as a measure on the discrete sets of points q_j, p_j, points in phase space for successive values of j are not likely to be close together, so thinking of the integral as an integral over paths is not justified.

When the Hamiltonian h is quadratic in the momentum p, the p_j integrals will be Gaussian integrals that can be performed exactly. Equivalently, the kinetic energy part K of the Hamiltonian operator will have a kernel in position space that can be computed exactly. Using one of these, the p_j integrals can be eliminated, leaving just integrals over the q_j that one might hope to interpret as a path integral over paths not in phase space, but in position space. One finds, if $K = \frac{P^2}{2m}$

$$\langle q_T|e^{-\frac{i}{\hbar}HT}|q_0\rangle =$$

$$\lim_{N\to\infty}(\frac{i2\pi\hbar T}{Nm})^{\frac{N}{2}}\sqrt{\frac{m}{i2\pi\hbar T}}\prod_{j=1}^{N}\int_{-\infty}^{\infty}dq_j e^{\frac{i}{\hbar}\sum_{j=1}^{N}(\frac{m(q_j-q_{j-1})^2}{2T/N}-V(q_j)\frac{T}{N})}$$

In the limit $N\to\infty$ the phase of the exponential becomes

$$S(\gamma)=\int_0^T dt(\frac{1}{2}m(\dot{q}^2)-V(q(t)))$$

One can try and properly normalize things so that this limit becomes an integral

$$\int D\gamma\ e^{\frac{i}{\hbar}S[\gamma]}$$

where now the paths $\gamma(t)$ are paths in the position space.

An especially attractive aspect of this expression is that it provides a simple understanding of how classical behavior emerges in the classical limit as $\hbar\to 0$. The stationary phase approximation method for oscillatory integrals says that, for a function f with a single critical point at $x=x_c$ (i.e. $f'(x_c)=0$) and for a small parameter ϵ, one has

$$\frac{1}{\sqrt{i2\pi\epsilon}}\int_{-\infty}^{+\infty}dx\ e^{if/\epsilon}=\frac{1}{\sqrt{f''(c)}}e^{if(x_c)/\epsilon}(1+O(\epsilon))$$

Using the same principle for the infinite-dimensional path integral, with $f=S$ the action functional on paths, and $\epsilon=\hbar$, one finds that for $\hbar\to 0$ the path integral will simplify to something that just depends on the classical trajectory, since by the principle of least action, this is the critical point of S.

Such position-space path integrals do not have the problems of principle of phase space path integrals coming from the Groenewold-van Hove theorem, but they still have serious analytical problems since they involve an attempt to integrate a wildly oscillating phase over an infinite-dimensional space. One does not naturally get a unitary result for the time evolution operator, and it is not clear that whatever results one gets will be independent of the details of how one takes the limit to define the infinite-dimensional integral.

Such path integrals though are closely related to integrals that are known to make sense, ones that occur in the theory of random walks. There, a well-defined measure on paths does exist, Wiener measure. In some sense Wiener measure is what one gets in the case of the path integral for a free particle, but taking the time variable t to be complex and analytically continuing

$$t\to it$$

So, one can use Wiener measure techniques to define the path integral, getting results that need to be analytically continued back to the physical time variable.

In summary, the path integral method has the following advantages:

- Study of the classical limit and "semi-classical" effects (quantum effects at small $\hbar$) is straightforward.

- Calculations for free particles and for series expansions about the free particle limit can be done just using Gaussian integrals, and these are relatively easy to evaluate and make sense of, despite the infinite-dimensionality of the space of paths.

- After analytical continuation, path integrals can be rigorously defined using Wiener measure techniques, and often evaluated numerically even in cases where no exact solution is known.

On the other hand, there are disadvantages:

- Some path integrals such as phase space path integrals do not at all have the properties one might expect, so great care is required in any use of them.

- How to get unitary results can be quite unclear. The analytic continuation necessary to make path integrals well-defined can make their physical interpretation obscure.

- Symmetries with their origin in symmetries of phase space that aren't just symmetries of configuration space are difficult to see using the configuration space path integral, with the harmonic oscillator providing a good example. One can see such symmetries using the phase-space path integral, but this is not reliable.

Path integrals for anticommuting variables can also be defined by analogy with the bosonic case, using the notion of fermionic integration discussed earlier.

32.3 For further reading

For much more about Lagrangian mechanics and its relation to the Hamiltonian formalism, see [2]. More along the lines of the discussion here can be found in most quantum mechanics and quantum field theory textbooks. For the path integral, Feynman's original paper [14] or his book [15] are quite readable. A typical textbook discussion is the one in chapter 8 of Shankar [57]. The book by Schulman [54] has quite a bit more detail, both about applications and about the problems of phase-space path integrals. Yet another fairly comprehensive treatment, including the fermionic case, is the book by Zinn-Justin [79].

Chapter 33

Quantization of Infinite-dimensional Phase Spaces

Up until this point we have been dealing with finite-dimensional phase spaces and their quantization in terms of Weyl and Clifford algebras. We will now turn to the study of quantum systems (both bosonic and fermionic) corresponding to infinite-dimensional phase spaces. The phase spaces of interest are spaces of solutions of some partial differential equation, so these solutions are classical fields. The corresponding quantum theory is thus called a "quantum field theory". In this chapter we'll just make some general comments about the new phenomena that appear when one deals with such infinite-dimensional examples, without going into any detail at all. Formulating quantum field theories in a mathematically rigorous way is a major and ongoing project in mathematical physics research, one far beyond the scope of this text. We will treat this subject at a physicist's level of rigor, while trying to give some hint of how one might proceed with precise mathematical constructions when they exist. We will also try and indicate where there are issues that require much deeper or even still unknown ideas, as opposed to those where the needed mathematical techniques are of a conventional nature.

While finite-dimensional Lie groups and their representations are rather well-understood mathematical objects, this is not at all true for infinite-dimensional Lie groups, where mathematical results are rather fragmentary. For the case of infinite-dimensional phase spaces, bosonic or fermionic, the symplectic or orthogonal groups acting on these spaces will be infinite-dimensional. One would like to find infinite-dimensional analogs of the role these groups and their representations play in quantum theory in the finite-dimensional case.

33.1 Inequivalent irreducible representations

In our discussion of the Weyl and Clifford algebras in finite dimensions, an important part of this story was the Stone-von Neumann theorem and its fermionic analog, which say that these algebras each have only one interesting irreducible representation (the Schrödinger representation in the bosonic case, the spinor representation in the fermionic case). Once we go to infinite dimensions, this is no longer true: there will be an infinite number of inequivalent irreducible representations, with no known complete classification of the possibilities. Before one can even begin to compute things like expectation values of observables, one needs to find an appropriate choice of representation, adding a new layer of difficulty to the problem that goes beyond that of just increasing the number of degrees of freedom.

To get some idea of how the Stone-von Neumann theorem can fail, one can consider the Bargmann-Fock quantization of the harmonic oscillator with d degrees of freedom, and note that it necessarily depends upon making a choice of an appropriate complex structure J (see chapter 22), with the conventional choice denoted J_0. Changing from J_0 to a different J corresponds to changing the definition of annihilation and creation operators (but in a manner that preserves their commutation relations). Physically, this entails a change in the Hamiltonian and a change in the lowest-energy or vacuum state:

$$|0\rangle_{J_0} \to |0\rangle_J$$

But $|0\rangle_J$ is still an element of the same state space $\mathcal{H}$ as $|0\rangle_{J_0}$, and one gets the same $\mathcal{H}$ by acting with annihilation and creation operators on $|0\rangle_{J_0}$ or on $|0\rangle_J$. The two constructions of the same $\mathcal{H}$ correspond to unitarily equivalent representations of the Heisenberg group H_{2d+1}.

For a phase space with $d = \infty$, what can happen is that there can be choices of J such that acting with annihilation and creation operators on $|0\rangle_{J_0}$ and $|0\rangle_J$ gives two different state spaces $\mathcal{H}_{J_0}$ and $\mathcal{H}_J$, providing two inequivalent representations of the Heisenberg group. For quantum systems with an infinite number of degrees of freedom, one can thus have the same algebra of operators, but a different choice of Hamiltonian can give both a different vacuum state and a different state space $\mathcal{H}$ on which the operators act. This same phenomenon occurs both in the bosonic and fermionic cases, as one goe to infinite dimensional Weyl or Clifford algebras.

It turns out though that if one restricts the class of complex structures J to ones not that different from J_0, then one can recover a version of the Stone-von Neumann theorem and have much the same behavior as in the finite-dimensional case. Note that for invertible linear map g on phase space, g acts on the complex structure, taking

$$J_0 \to J_g = g \cdot J_0$$

One can define subgroups of the infinite-dimensional symplectic or orthogonal groups as follows:

Definition (Restricted symplectic and orthogonal groups)**.** *The group of linear transformations g of an infinite-dimensional symplectic vector space preserving the symplectic structure and also satisfying the condition*

$$tr(A^\dagger A) < \infty$$

on the operator

$$A = [J_g, J_0]$$

is called the restricted symplectic group and denoted Sp_{res}. The group of linear transformations g of an infinite-dimensional inner-product space preserving the inner-product and satisfying the same condition as above on $[J_g, J_0]$ is called the restricted orthogonal group and denoted O_{res}.

An operator A satisfying $tr(A^\dagger A) < \infty$ is said to be a Hilbert-Schmidt operator.

One then has the following replacement for the Stone-von Neumann theorem:

Theorem. *Given two complex structures J_1, J_2 on a Hilbert space such that $[J_1, J_2]$ is Hilbert-Schmidt, acting on the states*

$$|0\rangle_{J_1}, \quad |0\rangle_{J_2}$$

by annihilation and creation operators will give unitarily equivalent representations of the Weyl algebra (in the bosonic case), or the Clifford algebra (in the fermionic case).

The standard reference for the proof of this statement is the original papers of Shale [55] and Shale-Stinespring [56]. A detailed discussion of the theorem can be found in [44].

When $g \in Sp_{res}$ one can construct an action of this group by automorphisms on the algebra generated by annihilation and creation operators, by much the same method as in the finite-dimensional case (see section 23.2). Elements of the Lie algebra of the group are represented as quadratic combinations of annihilation and creation operators, with the Hilbert-Schmidt condition ensuring that these quadratic operators have well-defined commutation relations. This also holds true for O_{res} and the fermionic annihilation and creation operators.

Add to this section a calculation of an example giving an explicit free field theory example of a family of J. See for instance the example on page 100 of Pressley-Segal.

33.2 The anomaly and the Schwinger term

The groups Sp_{res} and O_{res} each have a subgroup of elements that commute with J_0 exactly, not just up to a Hilbert-Schmidt operator. One can construct a unitary representation of this group (which we'll call $U(\infty)$) using quadratic combinations of annihilation and creation operators to get a representation of the Lie algebra, in much the same manner as in the finite-dimensional case of

section 23.2. The group $U(\infty)$ will act trivially on the vacuum state $|0\rangle_{J_0}$, and the finite-dimensional groups of symmetries of quantum field theories (coming from, for example, the action of the rotation group on physical space) will be subgroups of this group. For these, the problem to be discussed in this section will not occur.

Recall though that knowing the action of the symplectic group as automorphisms the Weyl algebra only determines its representation on the state space up to a phase factor. In the finite-dimensional case it turned out that this phase factor could be chosen to be just a sign, giving a representation (the metaplectic representation) that was a representation up to sign (and a true representation of a double cover of the symplectic group). In the infinite dimensional case of Sp_{res}, it turns out that the phase factors cannot be reduced to signs, and the analog of the metaplectic representation is a representation of Sp_{res} only up to a phase. To get a true representation, one needs to extend Sp_{res} to a larger group $\widetilde{Sp_{res}}$ that is not just a cover, but has an extra dimension.

In terms of Lie algebras one has

$$\widetilde{\mathfrak{sp}_{res}} = \mathfrak{sp}_{res} \oplus \mathbf{R}$$

with elements non-zero only in the $\mathbf{R}$ direction commuting with everything else. For all commutation relations, there are now possible scalar terms to keep track of. In the finite dimensional case we saw that such terms would occur when we used normal-ordered operators (an example is the the shift by the scalar $\frac{1}{2}$ in the Hamiltonian operator for a harmonic oscillator with one degree of freedom), but without normal-ordering no such terms were needed. In the infinite-dimensional case normal-ordering is needed to avoid having a representation that acts on states like $|0\rangle_{J_0}$ by an infinite phase change, and one can not eliminate the effect of normal-ordering by making a well-defined finite phase change on the way the operators act.

Commuting two elements of the Lie sub-algebra $\mathfrak{u}(\infty)$ will not give a scalar factor, but such factors can occur when one commutes the action of elements of $\mathfrak{sp}_{res}$ not in $\mathfrak{u}(\infty)$, in which case they are known as "Schwinger terms". Already in finite dimensions, we saw that commuting the action a^2 with that of $(a^\dagger)^2$ gave a scalar factor with respect to the normal ordered $a^\dagger a$ operator (see section 22.3), and in infinite dimensions, it is this that cannot be redefined away.

This phenomenon of new scalar terms in the commutation relations of the operators in a quantum theory coming from a Lie algebra representation is known as an "anomaly", and while we have described it for the bosonic case, much the same thing happens in the fermionic case for the Lie algebra $\mathfrak{o}_{res}$. This is normally considered to be something that happens due to quantization, with the "anomaly" the extra scalar terms in commutation relations not there in the corresponding classical Poisson bracket relations. From another point of view this is a phenomenon coming not from quantization, but from infinite-dimensionality, already visible in Poisson brackets when one makes a choice of complex structure on the phase space. It is the occurrence for infinite-dimensional phase spaces of certain inherently different ways of choosing the

complex structure that is relevant. We will see in later chapters that in quantum field theories one often wants to choose a complex structure on an infinite dimensional space of solutions of a classical field equation by taking positive energy complexified solutions to be eigenvectors of the complex structure with eigenvalue $+i$, those with negative energy to have eigenvalue $-i$, and it is this choice of complex structure that introduces the anomaly phenomenon.

33.3 Higher order operators and renormalization

We have generally restricted ourselves to considering only products of the fundamental position and momentum operators of degree less than or equal to two, since it is these that have an interpretation as the operators of a Lie algebra representation. By the Groenewold-van Hove theorem, higher-order products of position and momentum variables have no unique quantization (the operator-ordering problem). In the finite dimensional case one can of course consider higher-order products of operators, for instance systems with Hamiltonian operators of higher order than quadratic. Unlike the quadratic case, typically no exact solution for eigenvectors and eigenvalues will exist, but various approximation methods may be available. In particular, for Hamiltonians that are quadratic plus a term with a small parameter, perturbation theory methods can be used to compute a power-series approximation in the small parameter. This is an important topic in physics, covered in detail in the standard textbooks.

The standard approach to quantization of infinite-dimensional systems is to begin with "regularization", somehow modifying the system to only have a finite-dimensional phase space. One quantizes this theory, taking advantage of the uniqueness of its representation, then tries to take a limit that recovers the infinite-dimensional system. Such a limit will generally be quite singular, leading to an infinite result, and the process of manipulating these potential infinities is called "renormalization". Techniques for taking limits of this kind in a manner that leads to a consistent and physically sensible result typically take up a large part of standard quantum field theory textbooks. For many theories, no appropriate such techniques are known, and conjecturally none are possible. For others there is good evidence that such a limit can be successfully taken, but the details of how to do this remain unknown (with for instance a $1 million Millenium Prize offered for showing rigorously this is possible in the case of Yang-Mills gauge theory).

In succeeding chapters we will go on to study a range of quantum field theories, but due to the great complexity of the issues involved, will not address what happens for non-quadratic Hamiltonians. Physically this means that we will just be able to study theories of free particles, although with methods that generalize to particles moving in non-trivial background classical fields. For a treatment of the subject that includes interacting quantized multi-particle systems, one of the conventional textbooks will be needed to supplement what

is here.

33.4 For further reading

Berezin's *The Method of Second Quantization* [5] develops in detail the infinite-dimensional version of the Bargmann-Fock construction, both in the bosonic and fermionic cases. Infinite-dimensional versions of the metaplectic and spinor representations are given there in terms of operators defined by integral kernels. For a discussion of the infinite-dimensional Weyl and Clifford algebras, together with a realization of their automorphism groups Sp_{res} and O_{res} (and the corresponding Lie algebras) in terms of annihilation and creation operators acting on the infinite-dimensional metaplectic and spinor representations, see [44]. The book [47] contains an extensive discussion of the groups Sp_{res} and O_{res} and the infinite-dimensional version of their metaplectic and spinor representations. It emphasizes the origin of novel infinite-dimensional phenomena here in the nature of the complex structures of interest in infinite dimensional examples.

Chapter 34

Multi-particle Systems and Non-relativistic Quantum Fields

The quantum mechanical systems we have studied so far describe a finite number of degrees of freedom, which may be of a bosonic or fermionic nature. In particular we have seen how to describe a quantized free particle moving in three-dimensional space. By use of the notion of tensor product, we can then describe any particular fixed number of such particles. We would, however, like a formalism capable of conveniently describing an arbitrary number of particles. From very early on in the history of quantum mechanics, it was clear that at least certain kinds of particles, photons, were most naturally described not one by one, but by thinking of them as quantized excitations of a classical system with an infinite number of degrees of freedom: the electromagnetic field. In our modern understanding of fundamental physics not just photons, but all elementary particles are best described in this way.

Conventional textbooks on quantum field theory often begin with relativistic systems, but we'll start instead with the non-relativistic case. We'll study a simple quantum field theory that extends the conventional single-particle quantum systems we have dealt with so far to deal with multi-particle systems. This version of quantum field theory is what gets used in condensed matter physics, and is in many ways simpler than the relativistic case, which we'll take up in a later chapter.

Quantum field theory is a large and complicated subject, suitable for a full-year course at an advanced level. We'll be giving only a very basic introduction, mostly just considering free fields, which correspond to systems of non-interacting particles. Most of the complexity of the subject only appears when one tries to construct quantum field theories of interacting particles. A remarkable aspect of the theory of free quantum fields is that in many ways it is little more than something we have already discussed in great detail, the quantum

harmonic oscillator problem. However, the classical harmonic oscillator phase space that is getting quantized in this case is an infinite dimensional one, the space of solutions to the free particle Schrödinger equation. To describe multiple non-interacting fermions, we just need to use fermionic oscillators.

For simplicity we'll set $\hbar = 1$ and start with the case of a single spatial dimension. We'll also begin using x to denote a spatial variable instead of the q conventional when this is the coordinate variable in a finite-dimensional phase space.

34.1 Multi-particle quantum systems as quanta of a harmonic oscillator

It turns out that quantum systems of identical particles are best understood by thinking of such particles as quanta of a harmonic oscillator system. We will begin with the bosonic case, then later consider the fermionic case, which uses the fermionic oscillator system.

34.1.1 Bosons and the quantum harmonic oscillator

A fundamental postulate of quantum mechanics is that given a space of states $\mathcal{H}_1$ describing a bosonic single particle, a collection of N particles is described by

$$(\underbrace{\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}_{N-times})^S$$

where the superscript S means we take elements of the tensor product invariant under the action of the group S_N by permutation of the factors. We want to consider state spaces containing an arbitrary number of particles, so we define

Definition (Bosonic Fock space, the symmetric algebra)**.** *Given a complex vector space V, the symmetric Fock space is defined as*

$$\mathcal{F}^S(V) = \mathbf{C} \oplus V \oplus (V \otimes V)^S \oplus (V \otimes V \otimes V)^S \oplus \cdots$$

This is known to mathematicians as the "symmetric algebra" $S^*(V)$, with

$$S^N(V) = (\underbrace{V \otimes \cdots \otimes V}_{N-times})^S$$

(recall chapter 9)

A quantum harmonic oscillator with d degrees of freedom has a state space consisting of linear combinations of states with N "quanta" (i.e. states one gets by applying N creation operators to the lowest energy state), for $N = 0, 1, 2, \ldots$. We have seen in our discussion of the quantization of the harmonic oscillator that in the Bargmann-Fock representation, the state space is just $\mathbf{C}[z_1, z_2, \ldots, z_d]$, the space of polynomials in d complex variables.

The part of the state space with N quanta has dimension

$$\binom{N+d-1}{N}$$

which grows with N. This is just the binomial coefficient giving the number of d-variable monomials of degree N. The quanta of a harmonic oscillator are indistinguishable, which corresponds to the fact that the space of states with N quanta can be identified with the symmetric part of the tensor product of N copies of $\mathbf{C}^d$.

More precisely, what one has is

Theorem. *Given a vector space V, there is an isomorphism of algebras between the symmetric algebra $S^*(V^*)$ (where V^* is the dual vector space to V) and the algebra $\mathbf{C}[V]$ of polynomial functions on V.*

We won't try and give a detailed proof of this here, but one can exhibit the isomorphism explicitly on generators. If $z_j \in V^*$ are the coordinate functions with respect to a basis $\mathbf{e}_j$ of V (i.e. $z_j(\mathbf{e}_k) = \delta_{jk}$), they give a basis of V^* which is also a basis of the linear polynomial functions on V. For higher degrees, one makes the identification

$$\underbrace{z_j \otimes \cdots \otimes z_j}_{N-times} \in S^N(V^*) \leftrightarrow z_j^N$$

between N-fold symmetric tensor products and monomials in the polynomial algebra.

Besides describing states of multiple identical quantum systems as polynomials or as symmetric parts of tensor products, a third description is useful. This is the so-called "occupation number representation", where states are labeled by d non-negative integers $n_j = 0, 1, 2, \cdots$, with an identification with the polynomial description as follows:

$$|n_1, n_2, \ldots, n_j, \ldots, n_d\rangle \leftrightarrow z_1^{n_1} z_2^{n_2} \cdots z_j^{n_j} \cdots z_d^{n_d}$$

So, starting with a single particle state space $\mathcal{H}_1$, we have three equivalent descriptions of the Fock space describing multi-particle bosonic states

- As a symmetric algebra $S^*(\mathcal{H}_1^*)$ defined in terms of tensor products of the $\mathcal{H}_1^*$, the dual vector space to $\mathcal{H}_1$.
- As polynomial functions on $\mathcal{H}_1$.
- As linear combinations of states labeled by occupation numbers $n_j = 0, 1, 2, \ldots$.

For each of these descriptions, one can define d annihilation or creation operators $a_j, a_j^\dagger$, satisfying the canonical commutation relations, and these will generate an algebra of operators on the Fock space.

34.1.2 Fermions and the fermionic oscillator

For the case of fermionic particles, there's an analogous Fock space construction using tensor products:

Definition (Fermionic Fock space, exterior algebra)**.** *Given a complex vector space V, the fermionic Fock space is*

$$\mathcal{F}^A(V) = \mathbf{C} \oplus V \oplus (V \otimes V)^A \oplus (V \otimes V \otimes V)^A \oplus \cdots$$

where the superscript A means the subspace of the tensor product that just changes sign under interchange of two factors. This is known to mathematicians as the "exterior algebra" $\Lambda^*(V)$, with

$$\Lambda^N(V) = (\underbrace{V \otimes \cdots \otimes V}_{N-times})^A$$

As in the bosonic case, one can interpret $\Lambda^*(V^*)$ as polynomials on V, but now polynomials in anticommuting variables.

For the case of fermionic particles with single particle state space $\mathcal{H}_1$, one can again define the multi-particle state space in three equivalent ways:

- Using tensor products and antisymmetry, as the exterior algebra $\Lambda^*(\mathcal{H}_1^*)$.
- As polynomial functions in anticommuting coordinates on $\mathcal{H}_1$. One can also think of such polynomials as antisymmetric multilinear functions on the product of copies of $\mathcal{H}_1$.
- In terms of occupation numbers n_j, where now the only possibilities are $n_j = 0, 1$.

For each of these descriptions, one can define d annihilation or creation operators $a_j, a_j^\dagger$ satisfying the canonical anticommutation relations, and these will generate an algebra of operators on the Fock space.

34.2 Solutions to the free particle Schrödinger equation

To describe multi-particle quantum systems we will take as our single-particle state space $\mathcal{H}_1$ the space of solutions of the free-particle Schrödinger equation, as already studied in chapter 10. As we saw in that chapter, one can use a "finite box" normalization, which gives a discrete, countable basis for this space and then try and take the limit of infinite box size. To fully exploit the symmetries of phase space though, we will need the "continuum normalization", which requires considering not just functions but distributions.

34.2.1 Box normalization

Recall that for a free particle in one dimension the state space $\mathcal{H}$ consists of complex-valued functions on $\mathbf{R}$, with observables the self-adjoint operators for momentum

$$P = -i\frac{d}{dx}$$

and energy (the Hamiltonian)

$$H = \frac{P^2}{2m} = -\frac{1}{2m}\frac{d^2}{dx^2}$$

Eigenfunctions for both P and H are the functions of the form

$$\psi_p(x) \propto e^{ipx}$$

for $p \in \mathbf{R}$, with eigenvalues p for P and $\frac{p^2}{2m}$ for H.

Note that these eigenfunctions are not normalizable, and thus not in the conventional choice of state space as $L^2(\mathbf{R})$. One way to deal with this issue is to do what physicists sometimes refer to as "putting the system in a box", by imposing periodic boundary conditions

$$\psi(x + L) = \psi(x)$$

for some number L, effectively restricting the relevant values of x to be considered to those on an interval of length L. For our eigenfunctions, this condition is

$$e^{ip(x+L)} = e^{ipx}$$

so we must have

$$e^{ipL} = 1$$

which implies that

$$p = \frac{2\pi}{L}l$$

for l an integer. Then p will take on a countable number of discrete values corresponding to the $l \in \mathbf{Z}$, and

$$|l\rangle = \psi_l(x) = \frac{1}{\sqrt{L}}e^{ipx} = \frac{1}{\sqrt{L}}e^{i\frac{2\pi l}{L}x}$$

will be orthornormal eigenfunctions satisfying

$$\langle l'|l\rangle = \delta_{ll'}$$

This "box" normalization is one form of what physicists call an "infrared cutoff", a way of removing degrees of freedom that correspond to arbitrarily large sizes, in order to make a problem well-defined. To get a well-defined problem one starts with a fixed value of L, then one studies the limit $L \to \infty$.

The number of degrees of freedom is now countable, but still infinite. In order to get a completely well-defined problem, one typically needs to first make the number of degrees of freedom finite. This can be done with an additional cutoff, an "ultraviolet cutoff", which means restricting attention to $|p| \leq \Lambda$ for some finite Λ, or equivalently $|l| < \frac{\Lambda L}{2\pi}$. This makes the state space finite dimensional and one then studies the $\Lambda \to \infty$ limit.

For finite L and Λ our single-particle state space $\mathcal{H}_1$ is finite dimensional, with orthonormal basis elements $\psi_l(x)$. An arbitrary solution to the Schrödinger equation is then given by

$$\psi(x,t) = \sum_{l=-\frac{\Lambda L}{2\pi}}^{+\frac{\Lambda L}{2\pi}} \alpha_l e^{i\frac{2\pi l}{L}x} e^{-i\frac{4\pi^2 l^2}{2mL^2}t}$$

for arbitrary complex coefficients α_l and can be completely characterized by its initial value at $t = 0$

$$\psi(x,0) = \sum_{l=-\frac{\Lambda L}{2\pi}}^{+\frac{\Lambda L}{2\pi}} \alpha(l) e^{i\frac{2\pi l}{L}x}$$

Vectors in $\mathcal{H}_1$ have coordinates $\alpha_l \in \mathbf{C}$ with respect to our chosen basis, and these coordinates are in the dual space $\mathcal{H}_1^*$.

Multi-particle states are now described by the Fock spaces $\mathcal{F}^S(\mathcal{H}_1^*)$ or $\mathcal{F}^A(\mathcal{H}_1^*)$, depending on whether the particles are bosons or fermions. In the occupation number representation of the Fock space, orthonormal basis elements are

$$|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle$$

where the subscript j indexes the possible values of the momentum p (which are discretized in units of $\frac{2\pi}{L}$, and in the interval $[-\Lambda, \Lambda]$). The occupation number n_{p_j} is the number of particles in the state with momentum p_j. In the bosonic case it takes values $0, 1, 2, \cdots, \infty$, in the fermionic case it takes values 0 or 1. The state with all occupation numbers equal to zero is denoted

$$|\cdots, 0, 0, 0, \cdots\rangle = |0\rangle$$

and called the "vacuum" state.

For each p_j we can define annihilation and creation operators a_{p_j} and $a_{p_j}^\dagger$. These satisfy the commutation relations

$$[a_{p_j}, a_{p_k}^\dagger] = \delta_{jk}$$

and act on states in the occupation number representation as

$$a_{p_j}|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle = \sqrt{n_{p_j}}|\cdots, n_{p_{j-1}}, n_{p_j} - 1, n_{p_{j+1}}, \cdots\rangle$$

$$a_{p_j}^\dagger|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle = \sqrt{n_{p_j} + 1}|\cdots, n_{p_{j-1}}, n_{p_j} + 1, n_{p_{j+1}}, \cdots\rangle$$

Observables one can build out of these operators include

- The number operator

$$\widehat{N} = \sum_k a^\dagger_{p_k} a_{p_k}$$

  which will have as eigenvalues the total number of particles

$$\widehat{N}|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle = (\sum_k n_{p_k})|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle$$

- The momentum operator

$$\widehat{P} = \sum_k p_k a^\dagger_{p_k} a_{p_k}$$

  with eigenvalues the total momentum of the multiparticle system.

$$\widehat{P}|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle = (\sum_k n_k p_k)|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}\rangle$$

- The Hamiltonian

$$\widehat{H} = \sum_k \frac{p_k^2}{2m} a^\dagger_{p_k} a_{p_k}$$

  which has eigenvalues the total energy

$$\widehat{H}|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle = (\sum_k n_k \frac{p_k^2}{2m})|\cdots, n_{p_{j-1}}, n_{p_j}, n_{p_{j+1}}, \cdots\rangle$$

With ultraviolet and infrared cutoffs in place, the possible values of p_j are finite in number, $\mathcal{H}_1$ is finite dimensional and this is nothing but the standard quantized harmonic oscillator (with a Hamiltonian that has different frequencies

$$\omega(p_j) = \frac{p_j^2}{2m}$$

for different values of j). In the limit as one or both cutoffs are removed, $\mathcal{H}_1$ becomes infinite dimensional, the Stone-von Neumann theorem no longer applies, and we are in the situation discussed in chapter 33. State spaces with different choices of vacuum state $|0\rangle$ can be unitarily inequivalent, with not just the dynamics of states in the state space dependent on the Hamiltonian, but the state space itself depending on the Hamiltonian (through the characterization of $|0\rangle$ as lowest energy state). Even for the free particle, we have here defined the Hamiltonian as the normal-ordered version, which for finite dimensional $\mathcal{H}_1$ differs from the non-normal-ordered one just by a constant, but as cut-offs are removed this constant becomes infinite, requiring careful treatment of the limit.

34.2.2 Continuum normalization

A significant problem introduced by using cutoffs such as the box normalization is that these ruin some of the space-time symmetries of the system. The one-particle space with an infrared cutoff is a space of functions on a discrete set of points, and this set of points will not have the same symmetries as the usual continuous momentum space (for instance in three dimensions it will not carry an action of the rotation group $SO(3)$). In our study of quantum field theory we would like to exploit the action of space-time symmetry groups on the state space of the theory, so need a formalism that preserves such symmetries.

In our earlier discussion of the free particle, we saw that physicists often work with a "continuum normalization" such that

$$|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{ipx}, \quad \langle p'|p\rangle = \delta(p-p')$$

where formulas such as the second one need to be interpreted in terms of distributions. In quantum field theory we want to be able to think of each value of p as corresponding to a classical degree of freedom that gets quantized, and this "continuum" normalization will then correspond to an uncountable number of degrees of freedom, requiring great care when working in such a formalism. This will however allow us to readily see the action of space-time symmetries on the states of the quantum field theory and to exploit the duality between position and momentum space embodied in the Fourier transform.

In the continuum normalization, an arbitrary solution to the free-particle Schrödinger equation is given by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \alpha(p) e^{ipx} e^{-i\frac{p^2}{2m}t} dp$$

for some function complex-valued function $\alpha(p)$ on momentum space. Such solutions are in one-to-one correspondence with initial data

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \alpha(p) e^{ipx} dp$$

This is exactly the Fourier inversion formula, expressing a function $\psi(x,0)$ in terms of its Fourier transform $\widetilde{\psi(x,0)}(p) = \alpha(p)$. Note that we want to consider not just square integrable functions $\alpha(p)$, but non-integrable functions like $\alpha(p) = 1$ (which corresponds to $\psi(x,0) = \delta(x)$), and distributions such as $\alpha(p) = \delta(p)$, which corresponds to $\psi(x,0) = 1$.

We will generally work with this continuum normalization, taking as our single-particle space $\mathcal{H}_1$ the space of complex valued functions $\psi(x,0)$ on $\mathbf{R}$. One can think of the $|p\rangle$ as an orthornomal basis of $\mathcal{H}_1$, with $\alpha(p)$ the coordinate function for the $|p\rangle$ basis vector. $\alpha(p)$ is then an element of $\mathcal{H}_1^*$, the linear function on $\mathcal{H}_1$ given by taking the coefficient of the $|p\rangle$ basis vector.

Quantization should take $\alpha(p) \in \mathcal{H}_1^*$ to corresponding annihilation and creation operators $a(p), a^\dagger(p)$. Such operators though need to be thought of as

operator-valued distributions: what is really a well-defined operator is not $a(p)$, but

$$\int_{-\infty}^{+\infty} f(p)a(p)dp$$

for sufficiently well-behaved functions $f(p)$. From the point of view of quantization of $\mathcal{H}_1^*$, it is vectors in $\mathcal{H}_1^*$ that one can write in the form

$$\alpha(f) = \int_{-\infty}^{+\infty} f(p)\alpha(p)dp$$

that have well-defined quantizations as operators.

Typically though we will follow the the standard physicist's practice of writing formulas which are straight-forward generalizations of the finite-dimensional case, with sums becoming integrals. Some examples are

$$\widehat{N} = \int_{-\infty}^{+\infty} a(p)^\dagger a(p)dp$$

for the number operator,

$$\widehat{P} = \int_{-\infty}^{+\infty} pa(p)^\dagger a(p)dp$$

for the momentum operator, and

$$\widehat{H} = \int_{-\infty}^{+\infty} \frac{p^2}{2m} a(p)^\dagger a(p)dp$$

for the Hamiltonian operator.

To properly manipulate these formulas one must be aware that they should be interpreted as formulas for distributions, and that in particular products of distributions need to be treated with care. Expressions like $a(p)^\dagger a(p)$ will only give sensible operators when integrated against well-behaved functions. What we really have is for instance an operator $\widehat{N}(f)$ which we will write formally as

$$\widehat{N}(f) = \int_{-\infty}^{+\infty} a(p)^\dagger a(p)dp$$

but which is only defined for some particularly well-behaved f (and in particular is not defined for the non-integrable choice of $f = 1$).

34.3 Quantum field operators

The formalism developed so far works well to describe states of multiple free particles, but does so purely in terms of states with well-defined momenta, with no information at all about their position. To get operators that know about position, one can Fourier transform the annihilation and creation operators for momentum eigenstates as follows (we'll begin with the box normalization):

Definition (Quantum field operator)**.** *The quantum field operators for the free particle system are*

$$\widehat{\psi}(x) = \sum_p \psi_p(x) a_p = \sum_p \frac{1}{\sqrt{L}} e^{ipx} a_p$$

and its adjoint

$$\widehat{\psi}^\dagger(x) = \sum_p \psi_p^*(x) a_k^\dagger = \sum_k \frac{1}{\sqrt{L}} e^{-ikx} a_k^\dagger$$

(where k takes the discrete values $k_j = \frac{2\pi j}{L}$).

Note that these are not self-adjoint operators, and thus not themselves observables. To get some idea of their behavior, one can calculate what they do to the vacuum state. One has

$$\widehat{\psi}(x)|0\rangle = 0$$

$$\widehat{\psi}^\dagger(x)|0\rangle = \frac{1}{\sqrt{L}} \sum_p e^{-ipx} |\cdots, 0, n_p = 1, 0, \cdots\rangle$$

While this sum makes sense as long as it is finite, when cutoffs are removed it is clear that $\hat{\psi}^\dagger(x)$ will have a rather singular limit as an infinite sum of operators. It can be in some vague sense thought of as the (ill-defined) operator that creates a particle localized precisely at x.

The field operators allow one to recover conventional wavefunctions, for single and multiple-particle states. One sees by orthonormality of the occupation number basis states that

$$\langle \cdots, 0, n_p = 1, 0, \cdots | \widehat{\psi}^\dagger(x)|0\rangle = \frac{1}{\sqrt{L}} e^{-ipx} = \overline{\psi}_p(x)$$

the complex conjugate wavefunction of the single-particle state of momentum p. An arbitrary one particle state $|\Psi_1\rangle$ with wavefunction $\psi(x)$ is a linear combination of such states, and taking complex conjugates one finds

$$\langle 0|\widehat{\psi}(x)|\Psi_1\rangle = \psi(x)$$

Similarly, for a two-particle state of identical particles with momenta p_{j_1} and p_{j_2} one finds

$$\langle 0|\widehat{\psi}(x_1)\widehat{\psi}(x_2)|\cdots, 0, n_{p_{j_1}} = 1, 0, \cdots, 0, n_{p_{j_2}} = 1, 0, \cdots\rangle = \psi_{p_{j_1}, p_{j_2}}(x_1, x_2)$$

where

$$\psi_{p_{j_1}, p_{j_2}}(x_1, x_2)$$

is the wavefunction (symmetric under interchange of x_1 and x_2 for bosons) for this two particle state. For a general two-particle state $|\Psi_2\rangle$ with wavefunction $\psi(x_1, x_2)$ one has

$$\langle 0|\widehat{\psi}(x_1)\widehat{\psi}(x_2)|\Psi_2\rangle = \psi(x_1, x_2)$$

and one can easily generalize this to see how field operators are related to wavefunctions for an arbitrary number of particles.

Cutoffs ruin translational invariance and calculations with them quickly become difficult. We'll now adopt the physicist's convention of working directly in the continuous case with no cutoff, at the price of having formulas that only make sense as distributions. One needs to be aware that the correct interpretation of such formulas may require going back to the cutoff version.

In the continuum normalization we take as normalized eigenfunctions for the free particle

$$|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{ipx}$$

with

$$\langle p'|p\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(p-p')x}dx = \delta(p-p')$$

The annihilation and creation operators satisfy

$$[a(p), a^\dagger(p')] = \delta(p-p')$$

The field operators are then

$$\widehat{\psi}(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ipx}a(p)dx$$

$$\widehat{\psi}^\dagger(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ipx}a^\dagger(p)dx$$

and one can compute the commutators

$$[\widehat{\psi}(x), \widehat{\psi}(x')] = [\widehat{\psi}^\dagger(x), \widehat{\psi}^\dagger(x')] = 0$$

$$\begin{aligned}
[\widehat{\psi}(x), \widehat{\psi}^\dagger(x')] =& \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ipx}e^{-ip'x'}[a(p), a^\dagger(p')]dpdp' \\
=& \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ipx}e^{-ip'x'}\delta(p-p')dpdp' \\
=& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ip(x-x')}dp \\
=& \delta(x-x')
\end{aligned}$$

One should really think of such continuum-normalized field operators as operator-valued distributions, with the distributions defined on some appropriately chosen function space, for instance the Schwartz space of functions such that the function and its derivatives fall off faster than any power at $\pm\infty$. Given such functions f, g, one gets operators

$$\widehat{\psi}(f) = \int_{-\infty}^{\infty} f(x)\widehat{\psi}(x)dx, \quad \widehat{\psi}^\dagger(g) = \int_{-\infty}^{\infty} g(x)\widehat{\psi}^\dagger(x)dx$$

and the commutator relation above means

$$[\widehat{\psi}(f), \widehat{\psi}^\dagger(g)] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x)g(x')\delta(x-x')dxdx' = \int_{-\infty}^{\infty} f(x)g(x)dx$$

A major source of difficulties when manipulating quantum fields is that powers of distributions are not necessarily defined, so one has trouble making sense of rather innocuous looking expressions like

$$(\widehat{\psi}(x))^4$$

There are observables that one can define simply using field operators. These include:

- The number operator $\hat{N}$. One can define a number density operator

  $$\widehat{n}(x) = \widehat{\psi}^\dagger(x)\widehat{\psi}(x)$$

  and integrate it to get an operator with eigenvalues the total number of particles in a state

  $$\begin{aligned}\widehat{N} &= \int_{-\infty}^{\infty} \widehat{n}(x)dx \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-ip'x} a^\dagger(p') \frac{1}{\sqrt{2\pi}} e^{ipx} a(p) dpdp'dx \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(p-p')a^\dagger(p')a(p)dpdp' \\ &= \int_{-\infty}^{\infty} a^\dagger(p)a(p)dp\end{aligned}$$

- The total momentum operator $\widehat{P}$. This can be defined in terms of field operators as

  $$\begin{aligned}\widehat{P} &= \int_{-\infty}^{\infty} \widehat{\psi}^\dagger(x)(-i\frac{d}{dx})\widehat{\psi}(x)dx \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-ip'x} a^\dagger(p')(-i)(ip) \frac{1}{\sqrt{2\pi}} e^{ipx} a(p) dpdp'dx \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(p-p')pa^\dagger(p')a(p)dpdp' \\ &= \int_{-\infty}^{\infty} pa^\dagger(p)a(p)dp\end{aligned}$$

- The Hamiltonian $\widehat{H}$. This can be defined much like the momentum, just changing

  $$-i\frac{d}{dx} \to -\frac{1}{2m}\frac{d^2}{dx^2}$$

to find

$$\widehat{H} = \int_{-\infty}^{\infty} \widehat{\psi}^\dagger(x)(-\frac{1}{2m}\frac{d^2}{dx^2})\widehat{\psi}(x)dx = \int_{-\infty}^{\infty} \frac{p^2}{2m} a^\dagger(p)a(p)dp$$

All of these formulas really need to be interpreted as operator valued distributions: what really makes sense is not $\widehat{N}$, but $\widehat{N}(f)$ for some class of functions f, which can formally be written as

$$\widehat{N}(f) = \int_{-\infty}^{\infty} f(x)\widehat{\psi}^\dagger(x)\widehat{\psi}(x)dx$$

We will see that one can more generally use quadratic expressions in field operators to define an observable $\widehat{\mathcal{O}}$ corresponding to a one-particle quantum mechanical observable $\mathcal{O}$ by

$$\widehat{\mathcal{O}} = \int_{-\infty}^{\infty} \widehat{\psi}^\dagger(x)\mathcal{O}\widehat{\psi}(x)dx$$

In particular, to describe an arbitrary number of particles moving in an external potential $V(x)$, one takes the Hamiltonian to be

$$\widehat{H} = \int_{-\infty}^{\infty} \widehat{\psi}^\dagger(x)(-\frac{1}{2m}\frac{d^2}{dx^2} + V(x))\widehat{\psi}(x)dx$$

If one can solve the one-particle Schrödinger equation for a complete set of orthonormal wavefunctions $\psi_n(x)$, one can describe this quantum system using the same techniques as for the free particle. A creation-annihilation operator pair $a_n, a_n^\dagger$ is associated to each eigenfunction, and quantum fields are defined by

$$\widehat{\psi}(x) = \sum_n \psi_n(x)a_n, \quad \widehat{\psi}^\dagger(x) = \sum_n \overline{\psi}_n(x)a_n^\dagger$$

For Hamiltonians just quadratic in the quantum fields, quantum field theories are quite tractable objects. They are in some sense just free quantum oscillator systems, with all of their symmetry structure intact, but taking the number of degrees of freedom to infinity. Higher order terms though make quantum field theory a difficult and complicated subject, one that requires a year-long graduate level course to master basic computational techniques, and one that to this day resists mathematician's attempts to prove that many examples of such theories have even the basic expected properties. In the theory of charged particles interacting with an electromagnetic field, when the electromagnetic field is treated classically one still has a Hamiltonian quadratic in the field operators for the particles. But if the electromagnetic field is treated as a quantum system, it acquires its own field operators, and the Hamiltonian is no longer quadratic in the fields, a vastly more complicated situation described as an"interacting quantum field theory".

Even if one restricts attention to the quantum fields describing one kind of particles, there may be interactions between particles that add terms to the

Hamiltonian, and these will be higher order than quadratic. For instance, if there is an interaction between such particles described by an interaction energy $v(y-x)$, this can be described by adding the following quartic term to the Hamiltonian

$$\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\widehat{\psi}^{\dagger}(x)\widehat{\psi}^{\dagger}(y)v(y-x)\widehat{\psi}(y)\widehat{\psi}(x)dxdy$$

The study of "many-body" quantum systems with interactions of this kind is a major topic in condensed matter physics.

One can easily extend the above to three spatial dimensions, getting field operators $\widehat{\psi}(\mathbf{x})$ and $\widehat{\psi}^{\dagger}(\mathbf{x})$, defined by integrals over three-dimensional momentum space. For instance, in the continuum normalization

$$\widehat{\psi}(\mathbf{x}) = (\frac{1}{2\pi})^{\frac{3}{2}}\int_{\mathbf{R}^3} e^{i\mathbf{p}\cdot\mathbf{x}}a(\mathbf{p})d^3\mathbf{p}$$

and the Hamiltonian for the free field is

$$\widehat{H} = \int_{\mathbf{R}^3}\widehat{\psi}^{\dagger}(\mathbf{x})(-\frac{1}{2m}\nabla^2)\widehat{\psi}(\mathbf{x})d^3\mathbf{x}$$

More remarkably, one can also very easily write down theories of quantum systems with an arbitrary number of fermionic particles, just by changing commutators to anticommutators for the creation-annihilation operators and using fermionic instead of bosonic oscillators. One gets fermionic fields that satisfy anticommutation relations

$$[\widehat{\psi}(x),\widehat{\psi}^{\dagger}(x')]_+ = \delta(x-x')$$

and states that in the occupation number representation have $n_k = 0, 1$.

34.4 For further reading

This material is discussed in essentially any quantum field theory textbook. Many do not explicitly discuss the non-relativistic case, two that do are [23] and [32]. Two books aimed at mathematicians that cover the subject much more carefully than those for physicists are [20] and [11].

A good source for learning about quantum field theory from the point of view of non-relativistic many-body theory is Feynman's lecture notes on statistical mechanics [18].

Chapter 35

Field Quantization and Dynamics for Non-relativistic Quantum Fields

In finite dimensions, we saw that we could think of phase space M as the space parametrizing solutions to the equations of motion of a classical system, that linear functions on this space carried the structure of a Lie algebra (the Heisenberg Lie algebra), and that quantization was given by finding an irreducible unitary representation of this Lie algebra.

Instead of motivating the definition of quantum fields by starting with annihilation and creation operators for a free particle of fixed momentum, one can more simply just define them as what one gets by taking the space $\mathcal{H}_1$ of solutions of the free single particle Schrödinger equation as a classical phase space, and quantizing to get a unitary representation (of a Heisenberg algebra that is now infinite-dimensional). This procedure is sometimes called "second quantization", with "first quantization" what was done when one started with the classical phase space for a single particle and quantized to get the space $\mathcal{H}_1$ of wavefunctions.

In this chapter we'll consider the properties of quantum fields from this point of view, including seeing how quantization of classical Hamiltonian dynamics gives the dynamics of quantum fields.

35.1 Quantization of classical fields

The Schrödinger equation is first-order in time, so solutions are determined by the initial values $\psi(x) = \psi(x, 0)$ of the wavefunction at $t = 0$ and elements of the space $\mathcal{H}_1$ of solutions can be identified with their initial-value data, the

wavefunction at $t = 0$. Note that this is unlike typical finite-dimensional classical mechanical systems, where the equation of motion is second-order in time, with solutions determined by two pieces of initial-value data, the coordinates and momenta (since one needs initial velocities as well as positions). Taking $M = \mathcal{H}_1$ as a classical phase space, it has the property that there is no natural splitting of coordinates into position-like variables and momentum-like variables, and thus no natural way of setting up an infinite-dimensional Schrödinger representation where states would be functionals of position-like variables.

On the other hand, since wavefunctions are complex valued, $\mathcal{H}_1$ is already a complex vector space, and we can quantize by the Bargmann-Fock method using this complex structure. This is quite unlike our previous examples of quantization, where we started with a real phase space and needed to choose a complex structure (to get annihilation and creation operators).

Using Fourier transforms we can think of $\mathcal{H}_1$ either as a space of functions ψ of position x, or as a space of functions $\widetilde{\psi}$ of momentum p. This corresponds to two possible choices of orthonormal bases of the function space $\mathcal{H}_1$: the $|p\rangle$ (plane waves of momentum p) or the $|x\rangle$ (delta-functions at position x). In the finite dimensional case it is the coordinate functions q_j, p_j on phase space, which lie in the dual phase space $\mathcal{M} = M^*$, that get mapped to operators Q_j, P_j under quantization. Here what corresponds to the q_j, p_j is either the $\alpha(p)$ (coordinates with respect to the $|p\rangle$ basis) which quantize to annihilation operators $a(p)$, or the $\psi(x)$ (field value at x, coordinates with respect to the $|x\rangle$ basis) which quantize to field operators $\widehat{\psi}(x)$.

As described in chapter 34 though, what is really well-defined is not the quantization of $\psi(x)$, but of $\psi(f)$ for some class of functions f. $\psi(x)$ is the linear function on the space of solutions $\mathcal{H}_1$ given by

$$\psi(x) : \psi \in \mathcal{H}_1 \to \psi(x, 0)$$

but to get a well-defined operator, one wants the quantization not of this, but of elements of $\mathcal{H}_1^*$ of the form

$$\psi(f) : \psi \in \mathcal{H}_1 \to \int_{-\infty}^{\infty} f(x)\psi(x, 0)dx$$

To get all elements of $\mathcal{H}_1^*$ we will also need the $\overline{\psi}(x)$ and

$$\overline{\psi}(g) : \psi \in \mathcal{H}_1 \to \int_{-\infty}^{\infty} g(x)\overline{\psi}(x, 0)dx$$

Despite the potential for confusion, we will write $\psi(x)$ for the distribution given by evaluation at x, which corresponds to taking f to be the delta-function $\delta(x - x')$. This convenient notational choice means that one needs to be aware that $\psi(x)$ may be a complex number, or may be the "evaluation at x" linear function on $\mathcal{H}_1$.

So quantum fields should be "operator-valued distributions" and the proper mathematical treatment of this situation becomes quite challenging, with one

class of problems coming from the theory of distributions. What class of functions should appear in the space $\mathcal{H}_1$? What class of linear functionals on this space should be used? What properties should the operators $\widehat{\psi}(f)$ satisfy? These issues are far beyond what we can discuss here, and they are not purely mathematical, with the fact that the product of two distributions does not have an unambiguous sense one indication of the difficulties of quantum field theory.

To understand the Poisson bracket structure on functions on $\mathcal{H}_1$, one should recall that in the Bargmann-Fock quantization we found that, choosing a complex structure and complex coordinates z_j on phase space, the non-zero Poisson bracket relations were

$$\{z_j, i\overline{z}_l\} = \delta_{jl}$$

If we use the $|p\rangle$ basis for $\mathcal{H}_1$, our complex coordinates will be $\alpha(p), \overline{\alpha}(p)$ with Poisson bracket

$$\{\alpha(p), \alpha(p')\} = \{\overline{\alpha}(p), \overline{\alpha}(p')\} = 0, \quad \{\alpha(p), i\overline{\alpha}(p')\} = \delta(p - p')$$

and under quantization we have

$$\alpha(p) \to a(p), \quad \overline{\alpha}(p) \to a^\dagger(p), \quad 1 \to \mathbf{1}$$

Multiplying these operators by $-i$ gives a Heisenberg Lie algebra representation Γ' (unitary on the real and imaginary parts of $\alpha(p)$) with

$$\Gamma'(\alpha(p)) = -ia(p), \quad \Gamma'(\overline{\alpha}(p)) = -ia^\dagger(p)$$

and the commutator relations

$$[a(p), a(p')] = [a^\dagger(p), a^\dagger(p')] = 0, \quad [a(p), a^\dagger(p')] = \delta(p - p')\mathbf{1}$$

Using instead the $|x\rangle$ basis for $\mathcal{H}_1$, our complex coordinates will be $\psi(x), \overline{\psi}(x)$ with Poisson brackets

$$\{\psi(x), \psi(x')\} = \{\overline{\psi}(x), \overline{\psi}(x')\} = 0, \quad \{\psi(x), i\overline{\psi}(x')\} = \delta(x - x')$$

and quantization takes

$$\psi(x) \to -i\widehat{\psi}(x), \quad \overline{\psi}(x) \to -i\widehat{\psi}^\dagger(x), \quad 1 \to -i\mathbf{1}$$

This gives a Heisenberg Lie algebra representation Γ' (unitary on the real and imaginary parts of $\psi(x)$) with commutator relations

$$[\widehat{\psi}(x), \widehat{\psi}(x')] = [\widehat{\psi}^\dagger(x), \widehat{\psi}^\dagger(x')] = 0 \quad [\widehat{\psi}(x), \widehat{\psi}^\dagger(x')] = \delta(x - x')\mathbf{1}$$

To get well-defined operators, these formulas need to be interpreted in terms of distributions. What we should really consider is, for functions f, g in some properly chosen class, elements

$$\psi(f) + \overline{\psi}(g) = \int_{-\infty}^{\infty} (f(x)\psi(x) + g(x)\overline{\psi}(x))dx$$

of $\mathcal{H}_1^*$ with Poisson bracket relations

$$\{\psi(f_1) + \overline{\psi}(g_1), \psi(f_2) + \overline{\psi}(g_2)\} = -i\int_{-\infty}^{\infty}(f_1(x)g_2(x) - f_2(x)g_1(x))dx$$

Here the right-hand size of the equation is the symplectic form Ω for the dual phase space $\mathcal{M} = \mathcal{H}_1^*$, and this should be thought of as an infinite-dimensional version of formula **??**. This is the Lie bracket relation for an infinite-dimensional Heisenberg Lie algebra, with quantization giving a representation of the Lie algebra, with commutation relations for field operators

$$[\widehat{\psi}(f_1) + \widehat{\psi}^\dagger(g_1), \widehat{\psi}(f_2) + \widehat{\psi}^\dagger(g_2)] = \int_{-\infty}^{\infty}(f_1(x)g_2(x) - f_2(x)g_1(x))dx \cdot \mathbf{1}$$

Pretty much exactly the same formalism works to describe fermions, with the same $\mathcal{H}_1$ and the same choice of bases. The only difference is that the coordinate functions are now taken to be anticommuting, satisfying the fermionic Poisson bracket relations of a super Lie algebra rather than a Lie algebra. After quantization, the fields $\widehat{\psi}(x), \widehat{\psi}^\dagger(x)$ or the annihilation and creation operators $a(p), a^\dagger(p)$ satisfy anticommutation relations and generate an infinite-dimensional Clifford algebra, rather than the Weyl algebra of the bosonic case.

35.2 Dynamics of the free quantum field

In classical Hamiltonian mechanics, the Hamiltonian function h determines how an observable f evolves in time by the differential equation

$$\frac{d}{dt}f = \{f, h\}$$

Quantization takes f to an operator $\widehat{f}$, and h to a self-adjoint operator H. Multiplying this by $-i$ gives a skew-adjoint operator that exponentiates (we'll assume here H time-independent) to the unitary operator

$$U(t) = e^{-iHt}$$

that determines how states (in the Schrödinger picture) evolve under time translation. In the Heisenberg picture states stay the same and operators evolve, with their time evolution given by

$$\widehat{f}(t) = e^{iHt}\widehat{f}(0)e^{-iHt}$$

Such operators satisfy

$$\frac{d}{dt}\widehat{f} = [\widehat{f}, -iH]$$

which is the quantization of the classical dynamical equation.

To describe the time evolution of a quantum field theory system, it is generally easier to work with the Heisenberg picture (in which the time dependence

is in the quantum field operators) than the Schrödinger picture (in which the time dependence is in the states). This is especially true in relativistic systems where one wants to as much as possible treat space and time on the same footing. It is however also true in non-relativistic cases due to the complexity of the description of the states (inherent since one is trying to describe arbitrary numbers of particles) versus the description of the operators, which are built simply out of the quantum fields.

The classical phase space to be quantized is the space $\mathcal{H}_1$ of solutions of the free particle Schrödinger equation, parametrized by the initial data of a complex-valued wavefunction $\psi(x,0) \equiv \psi(x)$, with Poisson bracket

$$\{\psi(x), i\overline{\psi}(x')\} = \delta(x-x')$$

Time translation on this space is given by the Schrödinger equation, which says that wavefunctions will evolve with time dependence given by

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{i}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

If we take our Hamiltonian function on $\mathcal{H}_1$ to be

$$h = \int_{-\infty}^{+\infty} \overline{\psi}(x)\frac{-1}{2m}\frac{\partial^2}{\partial x^2}\psi(x)dx$$

then we will get the single-particle Schrödinger equation from the Hamiltonian dynamics, since

$$\begin{aligned}
\frac{\partial}{\partial t}\psi(x,t) =& \{\psi(x,t), h\} \\
=& \{\psi(x,t), \int_{-\infty}^{+\infty} \overline{\psi}(x',t)\frac{-1}{2m}\frac{\partial^2}{\partial x'^2}\psi(x',t)dx'\} \\
=& \frac{-1}{2m}\int_{-\infty}^{+\infty} (\{\psi(x,t), \overline{\psi}(x',t)\}\frac{\partial^2}{\partial x'^2}\psi(x',t) + \\
& \qquad \overline{\psi}(x',t)\{\psi(x,t), \frac{\partial^2}{\partial x'^2}\psi(x',t)\})dx') \\
=& \frac{-1}{2m}\int_{-\infty}^{+\infty} (-i\delta(x-x')\frac{\partial^2}{\partial x'^2}\psi(x',t) + \overline{\psi}(x',t)\frac{\partial^2}{\partial x'^2}\{\psi(x,t), \psi(x',t)\})dx') \\
=& \frac{i}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)
\end{aligned}$$

Here we have used the derivation property of the Poisson bracket and the linearity of the operator $\frac{\partial^2}{\partial x'^2}$.

Note that there are other forms of the same Hamiltonian function, related to the one we chose by integration by parts. One has

$$\begin{aligned}
\overline{\psi}(x)\frac{d^2}{dx^2}\psi(x) =& \frac{d}{dx}(\overline{\psi}(x)\frac{d}{dx}\psi(x)) - |\frac{d}{dx}\psi(x)|^2 \\
=& \frac{d}{dx}(\overline{\psi}(x)\frac{d}{dx}\psi(x) - (\frac{d}{dx}\overline{\psi}(x))\psi(x)) + (\frac{d^2}{dx^2}\overline{\psi}(x))\psi(x)
\end{aligned}$$

so neglecting integrals of derivatives (assuming boundary terms go to zero at infinity), one could have used

$$h = \frac{1}{2m}\int_{-\infty}^{+\infty} |\frac{d}{dx}\psi(x)|^2 dx \text{ or } h = \frac{-1}{2m}\int_{-\infty}^{+\infty} (\frac{d^2}{dx^2}\overline{\psi}(x))\psi(x)dx$$

Instead of working with position space fields $\psi(x,t)$ we could work with their momentum space components. Recall that we can write solutions to the Schrödinger equation as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \alpha(p,t)e^{ipx}dp$$

where

$$\alpha(p,t) = \alpha(p)e^{-i\frac{p^2}{2m}t}$$

Using these as our coordinates on the $\mathcal{H}_1$, dynamics is given by

$$\frac{\partial}{\partial t}\alpha(p,t) = \{\alpha(p,t), h\} = -i\frac{p^2}{2m}\alpha(p,t)$$

and one can easily see that one can choose

$$h = \int_{-\infty}^{\infty} \frac{p^2}{2m}|\alpha(p)|^2 dp$$

as Hamiltonian function in momentum space coordinates. This is the same expression one would get by substituting the expression for ψ in terms of α and calculating h from its formula as a quadratic polynomial in the fields.

In momentum space, quantization is simply given by

$$\alpha(p) \to a(p), \quad h \to \widehat{H} = \int_{-\infty}^{\infty} \frac{p^2}{2m}a^\dagger(p)a(p)dp$$

where we have normal-ordered $\widehat{H}$ so that the vacuum energy is zero.

In position space the expression for the Hamiltonian operator (again normal-ordered) will be:

$$\widehat{H} = \int_{-\infty}^{+\infty} \widehat{\psi}^\dagger(x)\frac{-1}{2m}\frac{\partial^2}{\partial x^2}\widehat{\psi}(x)dx$$

Using this quantized form, essentially the same calculation as before (now with operators and commutators instead of functions and Poisson brackets) shows that the quantum field dynamical equation

$$\frac{d}{dt}\widehat{\psi}(x,t) = -i[\widehat{\psi}(x,t), \widehat{H}]$$

becomes

$$\frac{\partial}{\partial t}\widehat{\psi}(x,t) = \frac{i}{2m}\frac{\partial^2}{\partial x^2}\widehat{\psi}(x,t)$$

The field operator $\widehat{\psi}(x,t)$ satisfies the Schrödinger equation which now appears as a differential equation for operators rather than for wavefunctions. One can explicitly solve such a differential equation just as for wavefunctions, by Fourier transforming and turning differentiation into multiplication. If the operator $\widehat{\psi}(x,t)$ is related to the operator $a(p,t)$ by

$$\widehat{\psi}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ipx} a(p,t) dp$$

then the Schrödinger equation for the $a(p,t)$ will be

$$\frac{\partial}{\partial t} a(p,t) = \frac{-ip^2}{2m} a(p,t)$$

with solution

$$a(p,t) = e^{-i\frac{p^2}{2m}t} a(p,0)$$

The solution for the field will then be

$$\widehat{\psi}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ipx} e^{-i\frac{p^2}{2m}t} a(p) dp$$

where the operators $a(p) \equiv a(p,0)$ are the initial values.

We will not enter into the important topic of how to compute observables in quantum field theory that can be connected to experimentally important quantities such as scattering cross-sections. A crucial role in such calculations is played by the following observables:

Definition (Green's function or propagator)**.** *The Green's function or propagator for a quantum field theory is the amplitude, for $t > t'$*

$$G(x,t,x',t') = \langle 0 | \widehat{\psi}(x,t) \widehat{\psi}^{\dagger}(x',t') | 0 \rangle$$

The physical interpretation of these functions is that they describe the amplitude for a process in which a one-particle state localized at x is created at time t', propagates for a time $t - t'$, and then its wavefunction is compared to that of a one-particle state localized at x. Using the solution for the time-dependent field operator given earlier we find

$$\begin{aligned} G(x,t,x',t') =& \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \langle 0 | e^{ipx} e^{-i\frac{p^2}{2m}t} a(p) e^{-ip'x} e^{i\frac{p'^2}{2m}t'} a^{\dagger}(p') | 0 \rangle dp dp' \\ =& \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{ipx} e^{-i\frac{p^2}{2m}t} e^{-ip'x'} e^{i\frac{p'^2}{2m}t'} \delta(p - p') dp dp' \\ =& \int_{-\infty}^{+\infty} e^{ip(x-x')} e^{-i\frac{p^2}{2m}(t-t')} dp \end{aligned}$$

One can evaluate this integral, finding

$$G(x',t',x,t) = \left(\frac{-im}{2\pi(t'-t)}\right)^{\frac{3}{2}} e^{\frac{-im}{2\pi(t'-t)}(x'-x)^2}$$

and that

$$\lim_{t \to t'} G(x', t', x, t) = \delta(x' - x)$$

While we have worked purely in the Hamiltonian formalism, one could instead start with a Lagrangian for this system. A Lagrangian that will give the Schrödinger equation as an Euler-Lagrange equation is

$$L = i\overline{\psi}\frac{\partial}{\partial t}\psi - h = i\overline{\psi}\frac{\partial}{\partial t}\psi + \overline{\psi}\frac{1}{2m}\frac{\partial^2}{\partial x^2}\psi$$

or, using integration by parts to get an alternate form of h mentioned earlier

$$L = i\overline{\psi}\frac{\partial}{\partial t}\psi - \frac{1}{2m}|\frac{\partial}{\partial x}\psi|^2$$

If one tries to define a canonical momentum for ψ as $\frac{\partial L}{\partial \dot{\psi}}$ one just gets $i\overline{\psi}$. This justifies the Poisson bracket relation

$$\{\psi(x), i\overline{\psi}(x')\} = \delta(x - x')$$

but, as expected for a case where the equation of motion is first-order in time, such a canonical momentum is not independent of ψ and the space of the wavefunctions ψ is already a phase space. One could try and quantize this system by path integral methods, for instance computing the propagator by doing the integral

$$\int D\gamma \; e^{\frac{i}{\hbar}S[\gamma]}$$

over paths γ from (x, t) to (x', t'). However one needs to keep in mind the warnings given earlier about path integrals over phase space, since that is what one has here.

35.3 For further reading

As with the last chapter, the material here is discussed in essentially any quantum field theory textbook, with two that explicitly discuss the non-relativistic case [23] and [32]. For a serious mathematical treatment of quantum fields as distribution-valued operators, a standard reference is [62].

Chapter 36

Symmetries and Non-relativistic Quantum Fields

In our study of the harmonic oscillator (chapter 22) we found that the symmetries of the system could be studied using quadratic functions on the phase space. Classically these gave a Lie algebra under the Poisson bracket, and quantization provided a unitary representation Γ' of the Lie algebra, with quadratic functions becoming quadratic operators. In the case of fields, the same pattern holds, with the phase space now an infinite dimensional space, the single particle Hilbert space $\mathcal{H}_1$. Certain specific quadratic functions of the fields will provide a Lie algebra under the Poisson bracket, with quantization then providing a unitary representation of the Lie algebra in terms of quadratic field operators.

In chapter 35 we saw how this works for time translation symmetry, which determines the dynamics of the theory. For the case of a free particle, the field theory Hamiltonian is a quadratic function of the fields, providing a basic example of how such functions generate a unitary representation on the states of the quantum theory by use of a quadratic combination of the quantum field operators. In this chapter we will see how other group actions on the space $\mathcal{H}_1$ also lead to quadratic operators and unitary transformations on the full quantum field theory. We would like to find a formula to these, something that will be simplest to do in the case that the group acts on phase space as unitary transformations, preserving the complex structure used in Bargmann-Fock quantization.

36.1 Internal symmetries

Since the phase space $\mathcal{H}_1$ is a space of complex functions, there is a group that acts unitarily on this space is the group $U(1)$ of phase transformations of the

complex values of the function. Such a group action that acts trivially on the spatial coordinates but non-trivially on the values of $\psi(x)$ is called an "internal symmetry". If the fields ψ have multiple components, taking values in $\mathbf{C}^m$, there will be a unitary action of the larger group $U(m)$.

36.1.1 $U(1)$ symmetry

In chapter 2 we saw that the fact that irreducible representations of $U(1)$ are labeled by integers is what is responsible for the term "quantization": since quantum states are representations of this group, they break up into states characterized by integers, with these integers counting the number of "quanta". In the non-relativistic quantum field theory, the integer will just be the total particle number. Such a theory can be thought of as an harmonic oscillator with an infinite number of degrees of freedom, and the total particle number is just the total occupation number, summed over all degrees of freedom.

The $U(1)$ action on the fields $\psi(x)$ which provide coordinates on $\mathcal{H}_1$ is given by

$$\psi(x) \to e^{i\theta}\psi(x), \quad \overline{\psi}(x) \to e^{-i\theta}\overline{\psi}(x)$$

(recall that the fields are in the dual space to $\mathcal{H}_1$, so the action is the inverse to the action of $U(1)$ on $\mathcal{H}_1$ itself by multiplication by $e^{-i\theta}$).

To understand the infinitesimal generator of this symmetry, first recall the simple case of a harmonic oscillator in one variable, identifying the phase space $\mathbf{R}^2$ with $\mathbf{C}$ so the coordinates are $z, \overline{z}$, with a $U(1)$ action

$$z \to e^{i\theta}z, \quad \overline{z} \to e^{-i\theta}\overline{z}$$

The Poisson bracket is

$$\{z, \overline{z}\} = -i$$

which implies

$$\{z\overline{z}, z\} = iz, \quad \{z\overline{z}, \overline{z}\} = -i\overline{z}$$

Quantizing takes $z \to a, \overline{z} \to a^\dagger$ and we saw in chapter 22 that we have a choice to make for the unitary operator that will be the quantization of $z\overline{z}$:

- $$z\overline{z} \to -\frac{i}{2}(a^\dagger a + aa^\dagger)$$

  This will have eigenvalues $-i(n + \frac{1}{2})$, $n = 0, 1, 2 \dots$.

- $$z\overline{z} \to -ia^\dagger a$$

  This is the normal-ordered form, with eigenvalues $-in$.

With either choice, we get a number operator

$$N = \frac{1}{2}(a^\dagger a + aa^\dagger), \quad \text{or} \quad N = \frac{1}{2} : (a^\dagger a + aa^\dagger) := a^\dagger a$$

In both cases we have

$$[N, a] = -a, \quad [N, a^\dagger] = a^\dagger$$

so

$$e^{-i\theta N} a e^{i\theta N} = e^{i\theta} a, \quad e^{-i\theta N} a^\dagger e^{i\theta N} = e^{-i\theta} a^\dagger$$

Either choice of N will give the same action on operators. Hoever, on states only the normal-ordered one will have the desirable feature that

$$N|0\rangle = 0, \quad e^{-iN\theta}|0\rangle = |0\rangle$$

Since we now want to treat fields, adding together an infinite number of such oscillator degrees of freedom, we will need the normal-ordered version in order to not get $\infty \cdot \frac{1}{2}$ as the number eigenvalue for the vacuum state.

In momentum space, we simply do the above for each value of p and sum, getting

$$\widehat{N} = \int_{-\infty}^{+\infty} a^\dagger(p) a(p) dp$$

where one needs to keep in mind that this is really an operator valued distribution, which must be integrated against some weighting function on momentum space to get a well-defined operator. What really makes sense is

$$\widehat{N}(f) = \int_{-\infty}^{+\infty} a^\dagger(p) a(p) f(p) dp$$

for a suitable class of functions f.

Instead of working with $a(p)$, the quantization of the Fourier transform of $\psi(x)$, one could work with $\psi(x)$ itself, and write

$$\widehat{N} = \int_{-\infty}^{+\infty} \widehat{\psi}^\dagger(x) \widehat{\psi}(x) dx$$

with the Fourier transform relating the two formulas for $\widehat{N}$. $\widehat{\psi}^\dagger(x)\widehat{\psi}(x)$ is also an operator valued distribution, with the interpretation of measuring the number density at x.

On field operators, $\widehat{N}$ satisfies

$$[\widehat{N}, \widehat{\psi}] = -\widehat{\psi}, \quad [\widehat{N}, \widehat{\psi}^\dagger] = \widehat{\psi}^\dagger$$

so $\widehat{\psi}$ acts on states by reducing the eigenvalue of N by one, while $\widehat{\psi}^\dagger$ acts on states by increasing the eigenvalue of N by one. Exponentiating, one has

$$e^{-i\theta\widehat{N}} \widehat{\psi} e^{i\theta\widehat{N}} = e^{i\theta}\widehat{\psi}, \quad e^{-i\theta\widehat{N}} \widehat{\psi}^\dagger e^{i\theta\widehat{N}} = e^{-i\theta}\widehat{\psi}^\dagger$$

which are the quantized versions of the $U(1)$ action on the phase space coordinates

$$\psi(x) \to e^{i\theta}\psi(x), \quad \overline{\psi}(x) \to e^{-i\theta}\overline{\psi}(x)$$

that we began our discussion with.

An important property of $\widehat{N}$ that can be straightforwardly checked is that

$$[\widehat{N}, \widehat{H}] = [\widehat{N}, \int_{-\infty}^{+\infty} \widehat{\psi}^\dagger(x) \frac{-1}{2m} \frac{\partial^2}{\partial x^2} \widehat{\psi}(x) dx] = 0$$

This implies that particle number is a conserved quantity: if we start out with a state with a definite particle number, this will remain constant. Note that the origin of this conservation law comes from the fact that $\widehat{N}$ is the quantized generator of the $U(1)$ symmetry of phase transformations on complex-valued fields ψ. If we start with any Hamiltonian function h on $\mathcal{H}_1$ that is invariant under the $U(1)$ (i.e. built out of terms with an equal number of ψs and $\overline{\psi}$s), then for such a theory $\widehat{N}$ will commute with $\widehat{H}$ and particle number will be conserved. Note though that one needs to take some care with arguments like this, which assume that symmetries of the classical phase space give rise to unitary representations in the quantum theory. The need to normal-order operator products, working with operators that differ from the most straightforward quantization by an infinite constant, can cause a failure of symmetries to be realized as expected in the quantum theory, a phenomenon known as an "anomaly" in the symmetry.

In quantum field theories, due to the infinite number of degrees of freedom, the Stone-von Neumann theorem does not apply, and one can have unitarily inequivalent representations of the algebra generated by the field operators, leading to new kinds of behavior not seen in finite dimensional quantum systems. In particular, one can have a space of states where the lowest energy state $|0\rangle$ does not have the property

$$\widehat{N}|0\rangle = 0, e^{-i\theta\widehat{N}}|0\rangle = |0\rangle$$

but instead gets taken by $e^{-i\theta\widehat{N}}$ to some other state, with

$$\widehat{N}|0\rangle \neq 0,\ e^{-i\theta\widehat{N}}|0\rangle \equiv |\theta\rangle \neq |0\rangle \quad (\text{for } \theta \neq 0)$$

In this case, the vacuum state is not an eigenstate of $\widehat{N}$ so does not have a well-defined particle number. If $[\widehat{N}, \widehat{H}] = 0$, the states $|\theta\rangle$ will all have the same energy as $|0\rangle$ and there will be a multiplicity of different vacuum states, labeled by θ. In such a case the $U(1)$ symmetry is said to be "spontaneously broken". This phenomenon occurs when non-relativistic quantum field theory is used to describe a superconductor. There the lowest energy state will be a state without a definite particle number, with electrons pairing up in a way that allows them to lower their energy, "condensing" in the lowest energy state.

36.1.2 $U(m)$ symmetry

By taking fields with values in $\mathbf{C}^m$, or, equivalently, m different species of complex-valued field $\psi_j,\ j = 1, 2, \ldots, m$, one can easily construct quantum field

theories with larger internal symmetry groups than $U(1)$. Taking as Hamiltonian function

$$h = \int_{-\infty}^{+\infty} \sum_{j=1}^{m} \overline{\psi}_j(x) \frac{-1}{2m} \frac{\partial^2}{\partial x^2} \psi_j(x) dx$$

one can see that this will be invariant not just under $U(1)$ phase transformations, but also under transformations

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_m \end{pmatrix} \to U \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_m \end{pmatrix}$$

where U is an m by m unitary matrix. The Poisson brackets will be

$$\{\psi_j(x), \overline{\psi}_k(x')\} = -i\delta(x - x')\delta_{jk}$$

and are also invariant under such transformations by $U \in U(m)$.

As in the $U(1)$ case, one can begin by considering the case of one particular value of p or of x, for which the phase space is $\mathbf{C}^m$, with coordinates $z_b, \overline{z}_b$. As we saw in section 23.1, the m^2 quadratic combinations $z_j \overline{z}_k$ for $j = 1, \ldots, m,\ k = 1, \ldots, m$ will generalize the role played by $z\overline{z}$ in the $m = 1$ case, with their Poisson bracket relations exactly the Lie bracket relations of the Lie algebra $\mathfrak{u}(m)$ (or, considering all complex linear combinations, $\mathfrak{gl}(m, \mathbf{C})$).

After quantization, these quadratic combinations become quadratic combinations in annihilation and creation operators $a_j, a_j^\dagger$ satisfying

$$[a_j, a_k^\dagger] = \delta_{jk}$$

Recall (theorem 23.2) that for m by m matrices X and Y one will have

$$[\sum_{j,k=1}^{m} a_j^\dagger X_{jk} a_k, \sum_{j,k=1}^{m} a_j^\dagger Y_{jk} a_k] = \sum_{j,k=1}^{m} a_j^\dagger [X, Y]_{jk} a_k$$

So, for each X in the Lie algebra $\mathfrak{gl}(m, \mathbf{C})$, quantization will give us a representation of $\mathfrak{gl}(m, \mathbf{C})$ where X acts as the operator

$$\sum_{j,k=1}^{m} a_j^\dagger X_{jk} a_k$$

When the matrices X are chosen to be skew-adjoint ($X_{jk} = -\overline{X_{kj}}$) this construction will give us a unitary representation of $\mathfrak{u}(m)$.

As in the $U(1)$ case, one gets an operator in the quantum field theory just by summing over either the $a(p)$ in momentum space, or the fields in configuration space, finding for each $X \in \mathfrak{u}(m)$ an operator

$$\widehat{X} = \int_{-\infty}^{+\infty} \sum_{j,k=1}^{m} \widehat{\psi}_j^\dagger(x) X_{jk} \widehat{\psi}_k(x) dx$$

that provides a representation of $\mathfrak{u}(m)$ and $U(m)$ on the quantum field theory state space. This representation takes

$$e^X \in U(m) \to U(e^X) = e^{\widehat{X}} = e^{\int_{-\infty}^{+\infty} \sum_{b,c=1}^{m} \widehat{\psi}_j^\dagger(x) X_{jk} \widehat{\psi}_k(x) dx}$$

When, as for the free-particle h we chose, the Hamiltonian is invariant under $U(m)$ transformations of the fields ψ_j, then we will have

$$[\widehat{X}, \widehat{H}] = 0$$

In this case, if $|0\rangle$ is invariant under the $U(m)$ symmetry, then energy eigenstates of the quantum field theory will break up into irreducible representations of $U(m)$ and can be labeled accordingly. As in the $U(1)$ case, the $U(m)$ symmetry may be spontaneously broken, with

$$\widehat{X}|0\rangle \neq 0$$

for some directions X in $\mathfrak{u}(m)$. When this happens, just as in the $U(1)$ case states did not have well-defined particle number, now they will not carry well-defined irreducible $U(m)$ representation labels.

36.2 Spatial symmetries

We saw in chapter 17 that the action of the group $E(3)$ on physical space $\mathbf{R}^3$ induces a unitary action on the space $\mathcal{H}_1$ of solutions to the free-particle Schrödinger equation. Quantization of this phase space with this group action produces a quantum field theory state space carrying a unitary representation of the group $E(3)$. There are three different actions of the group $E(3)$ that one needs to keep straight here. Given an element $(\mathbf{a}, R) \in E(3)$ one has:

1. an action on $\mathbf{R}^3$, preserving the inner product on $\mathbf{R}^3$

$$\mathbf{x} \to R\mathbf{x} + \mathbf{a}$$

2. A unitary action on $\mathcal{H}_1$ given by

$$\psi(\mathbf{x}) \to u(\mathbf{a}, R)\psi(\mathbf{x}) = \psi(R^{-1}(\mathbf{x} - \mathbf{a}))$$

on wavefunctions, or, on Fourier transforms by

$$\widetilde{\psi}(\mathbf{p}) \to \widetilde{u}(\mathbf{a}, R)\widetilde{\psi}(\mathbf{p}) = e^{-i\mathbf{a}\cdot R^{-1}\mathbf{p}}\widetilde{\psi}(R^{-1}\mathbf{p})$$

Recall that this is not an irreducible representation of $E(3)$, but one can get an irreducible representation by taking distributional wavefunctions $\widetilde{\psi}_E$ with support on the sphere $|\mathbf{p}|^2 = 2mE$.

For the case of two-component wavefunctions $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ satisfying the Pauli equation (see chapter 31), one has to use the double cover of $E(3)$, with elements $(\mathbf{a}, \Omega), \Omega \in SU(2)$ and on these the action is

$$\psi(\mathbf{x}) \to u(\mathbf{a}, \Omega)\psi(\mathbf{x}) = \Omega\psi(R^{-1}(\mathbf{x} - \mathbf{a}))$$

and

$$\widetilde{\psi}(\mathbf{p}) \to \widetilde{u}(\mathbf{a}, \Omega)\widetilde{\psi}(\mathbf{p}) = e^{-i\mathbf{a}\cdot R^{-1}\mathbf{p}}\Omega\widetilde{\psi}(R^{-1}\mathbf{p})$$

where $R = \Phi(\Omega)$ is the $SO(3)$ group element corresponding to Ω.

The infinitesimal version of this unitary action is given by the operators $-i\mathbf{P}$ and $-i\mathbf{L}$ (in the two-component case, instead of $-i\mathbf{L}$, one needs $-i\mathbf{J} = -i(\mathbf{L} + \mathbf{S})$).

3. The quantum field theory one gets by treating $\mathcal{H}_1$ as a classical phase space, and quantizing using an appropriate infinite-dimensional version of the Bargmann-Fock representation comes with another unitary representation $U(a, R)$, on the quantum field theory state space $\mathcal{H}$. This is because the representation $u(a, R)$ preserves the symplectic structure on $\mathcal{H}_1$, and the Bargmann-Fock construction gives a representation of the group of such symplectic transformations, of which $E(3)$ is a finite-dimensional subgroup.

It is the last of these that we want to understand here, and as usual for quantum field theory, we don't want to try and explicitly construct the state space $\mathcal{H}$ and see the $E(3)$ action on that construction, but instead want to use the analog of the Heisenberg picture in the time-translation case, taking the group to act on operators. For each $(\mathbf{a}, R) \in E(3)$ we want to find operators $U(a, R)$ that will be built out of the field operators, and act on the field operators as

$$\widehat{\psi}(\mathbf{x}) \to U(a, R)\widehat{\psi}(\mathbf{x})U(a, R)^{-1} = \widehat{\psi}(R\mathbf{x} + \mathbf{a}) \tag{36.1}$$

Note that here the way the group acts on the argument of the operator-valued distribution is opposite to the way that it acts on the argument of a solution in $\mathcal{H}_1$. This is because $\widehat{\psi}(\mathbf{x})$ is an operator associated not to an element of $\mathcal{H}_1$, but to a distribution on this space, in particular the distribution $\psi(\mathbf{x})$, here meaning "evaluation of the solution ψ at $\mathbf{x}$. The group will act oppositely on such linear functions on $\mathcal{H}_1$ to its action on elements of $\mathcal{H}_1$. For a more general distribution of the form

$$\psi(f) = \int_{\mathbf{R}^3} f(\mathbf{x})\psi(\mathbf{x})d^3\mathbf{x}$$

$E(3)$ will act on f by

$$f \to (\mathbf{a}, R) \cdot f(\mathbf{x}) = f(R^{-1}(\mathbf{x} - \mathbf{a}))$$

and on $\psi(f)$ by

$$\psi(f) \to (\mathbf{a}, R) \cdot \psi(f) = \int_{\mathbf{R}^3} f(R^{-1}(\mathbf{x} - \mathbf{a}))\psi(\mathbf{x})d^3\mathbf{x}$$

The distribution $\psi(\mathbf{x})$ corresponds to taking f as the delta-function, and it will transform as

$$\psi(\mathbf{x}) \to (\mathbf{a}, R) \cdot \psi(\mathbf{x}) = \psi(R\mathbf{x} + \mathbf{a}))$$

For spatial translations, we want to construct momentum operators $-i\widehat{\mathbf{P}}$ that give a Lie algebra representation of the translation group, and the operators

$$U(\mathbf{a}, \mathbf{1}) = e^{-i\mathbf{a}\cdot\widehat{\mathbf{P}}}$$

after exponentiation. Note that these are not the momentum operators $\mathbf{P}$ that act on $\mathcal{H}_1$, but are operators in the quantum field theory that will be built out of quadratic combinations of the field operators. By equation 36.1 we want

$$e^{-i\mathbf{a}\cdot\widehat{\mathbf{P}}}\widehat{\psi}(\mathbf{x})e^{i\mathbf{a}\cdot\widehat{\mathbf{P}}} = \widehat{\psi}(\mathbf{x} + \mathbf{a})$$

Such an operator $\widehat{\mathbf{P}}$ can be constructed in terms of quadratic operators in the fields in the same way as the Hamiltonian $\widehat{H}$ was in section 35.2, although there is an opposite choice of sign for time versus space translations ($-iH = \frac{\partial}{\partial t}$, and $-iP = -\frac{\partial}{\partial x}$) for reasons that appear when we combine space and time later in special relativity. The calculation proceeds by just replacing the single-particle Hamiltonian operator by the single-particle momentum operator $\mathbf{P} = -i\boldsymbol{\nabla}$. So one has

$$\widehat{\mathbf{P}} = \int_{\mathbf{R}^3} \widehat{\psi}^\dagger(\mathbf{x})(-i\boldsymbol{\nabla})\widehat{\psi}(\mathbf{x})d^3\mathbf{x}$$

In the last chapter we saw that, in terms of annihilation and creation operators, this operator is just

$$\widehat{\mathbf{P}} = \int_{\mathbf{R}^3} \mathbf{p}\ a^\dagger(\mathbf{p})a(\mathbf{p})d^3\mathbf{p}$$

which is just the integral over momentum space of the momentum times the number-density operator in momentum space.

For spatial rotations, we found in chapter 17 that these had generators the angular momentum operators

$$\mathbf{L} = \mathbf{X} \times \mathbf{P} = \mathbf{X} \times (-i\boldsymbol{\nabla})$$

acting on $\mathcal{H}_1$. Just as for energy and momentum, we can construct angular momentum operators in the quantum field theory as quadratic field operators by

$$\widehat{\mathbf{L}} = \int_{\mathbf{R}^3} \widehat{\psi}^\dagger(\mathbf{x})(\mathbf{x} \times (-i\boldsymbol{\nabla}))\widehat{\psi}(\mathbf{x})d^3\mathbf{x}$$

These will generate the action of rotations on the field operators. For instance, if $R(\theta)$ is a rotation about the x_3 axis by angle θ, we will have

$$\widehat{\psi}(R(\theta)\mathbf{x}) = e^{-i\theta\widehat{L}_3}\widehat{\psi}(\mathbf{x})e^{i\theta\widehat{L}_3}$$

Note that these constructions are infinite-dimensional examples of theorem 23.2 which showed how to take an action of the unitary group on phase space (preserving Ω) and produce a representation of this group on the state space of the quantum theory. In our study of quantum field theory, we will be continually exploiting this construction, for groups acting unitarily on the infinite-dimensional phase space $\mathcal{H}_1$ of solutions of some linear field equations.

36.3 Fermions

Everything that was done in this chapter carries over straightforwardly to the case of a fermionic non-relativistic quantum field theory of free particles. Field operators will in this case generate an infinite-dimensional Clifford algebra and the quantum state space will be an infinite-dimensional version of the spinor representation. All the symmetries considered in this chpter also appear in the fermionic case, and have Lie algebra representations constructed using quadratic combinations of the field operators in just the same way as in the bosonic case. In section 28.3 we saw in finite dimensions how unitary group actions on the fermionic phase space gave a unitary representation on the fermionic oscillator space, by the same method of annihilation and creation operators as in the bosonic case. The construction of the Lie algebra representation operators in the fermionic case is an infinite-dimensional example of that method.

36.4 For further reading

The material of this chapter is often developed in conventional quantum field theory texts in the context of relativistic rather than non-relativistic quantum field theory. Symmetry generators are also more often derived via Lagrangian methods (Noether's theorem) rather than the Hamiltonian methods used here. For an example of a detailed discussion relatively close to this one, see [23].

Chapter 37

Minkowski Space and the Lorentz Group

For the case of non-relativistic quantum mechanics, we saw that systems with an arbitrary number of particles, bosons or fermions, could be described by taking as the Hamiltonian phase space the state space $\mathcal{H}_1$ of the single-particle quantum theory (e.g. the space of complex-valued wavefunctions on $\mathbf{R}^3$ in the bosonic case). This phase space is infinite-dimensional, but it is linear and it can be quantized using the same techniques that work for the finite-dimensional harmonic oscillator. This is an example of a quantum field theory since it is a space of functions (fields, to physicists) that is being quantized.

We would like to find some similar way to proceed for the case of relativistic systems, finding relativistic quantum field theories capable of describing arbitrary numbers of particles, with the energy-momentum relationship $E^2 = |\mathbf{p}|^2c^2 + m^2c^4$ characteristic of special relativity, not the non-relativistic limit $|\mathbf{p}| \ll mc$ where $E = \frac{|\mathbf{p}|^2}{2m}$. In general, a phase space can be thought of as the space of initial conditions for an equation of motion, or equivalently, as the space of solutions of the equation of motion. In the non-relativistic field theory, the equation of motion is the first-order in time Schrödinger equation, and the phase space is the space of fields (wavefunctions) at a specified initial time, say $t = 0$. This space carries a representation of the time-translation group $\mathbf{R}$, the space-translation group $\mathbf{R}^3$ and the rotation group $SO(3)$. To construct a relativistic quantum field theory, we want to find an analog of this space. It will be some sort of linear space of functions satisfying an equation of motion, and we will then quantize by applying harmonic oscillator methods.

Just as in the non-relativistic case, the space of solutions to the equation of motion provides a representation of the group of space-time symmetries of the theory. This group will now be the Poincaré group, a ten-dimensional group which includes a four-dimensional subgroup of translations in space-time, and a six-dimensional subgroup (the Lorentz group), which combines spatial rotations and "boosts" (transformations mixing spatial and time coordinates).

The representation of the Poincaré group on the solutions to the relativistic wave equation will in general be reducible. Irreducible such representations will be the objects corresponding to elementary particles. Our first goal will be to understand the Lorentz group, in later sections we will find representations of this group, then move on to the Poincaré group and its representations.

37.1 Minkowski space

Special relativity is based on the principle that one should consider space and time together, and take them to be a four-dimensional space $\mathbf{R}^4$ with an indefinite inner product:

Definition (Minkowski space)**.** *Minkowski space M^4 is the vector space $\mathbf{R}^4$ with an indefinite inner product given by*

$$(x, y) \equiv x \cdot y = -x_0 y_0 + x_1 y_1 + x_2 y_2 + x_3 y_3$$

where (x_0, x_1, x_2, x_3) are the coordinates of $x \in \mathbf{R}^4$, (y_0, y_1, y_2, y_3) the coordinates of $y \in \mathbf{R}^4$.

Digression. *We have chosen to use the $-+++$ instead of the more common $+---$ sign convention for the following reasons:*

- *Analytically continuing the time variable x_0 to ix_0 gives a positive definite inner product.*
- *Restricting to spatial components, there is no change from our previous formulas for the symmetries of Euclidean space $E(3)$.*
- *Only for this choice will we have a purely real spinor representation (since $\text{Cliff}(3,1) = M(2^2, \mathbf{R}) \neq \text{Cliff}(1,3)$).*
- *Weinberg's quantum field theory textbook [71] uses this convention (although, unlike him, we'll put the 0 component first).*

This inner product will also sometimes be written using the matrix

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

as

$$x \cdot y = \sum_{\mu,\nu=0}^{3} \eta_{\mu\nu} x_\mu x_\nu$$

Digression (Upper and lower indices)**.** *In many physics texts it is conventional in discussions of special relativity to write formulas using both upper and lower indices, related by*

$$x_\mu = \sum_{\nu=0}^{3} \eta_{\mu\nu} x^\nu = \eta_{\mu\nu} x^\nu$$

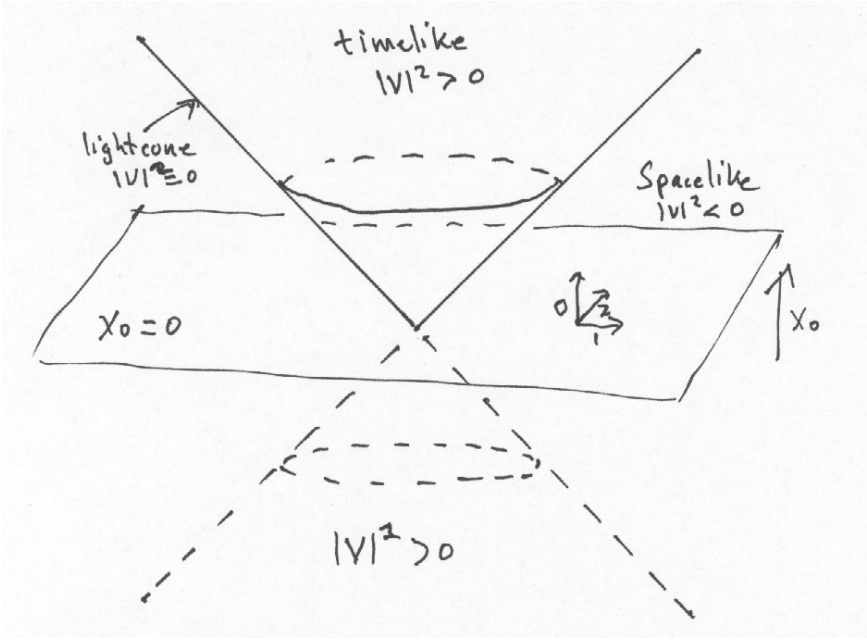
with the last form of this using the Einstein summation convention.

One motivation for introducing both upper and lower indices is that special relativity is a limiting case of general relativity, which is a fully geometrical theory based on taking space-time to be a manifold M with a metric g that varies from point to point. In such a theory it is important to distinguish between elements of the tangent space $T_x(M)$ at a point $x \in M$ and elements of its dual, the co-tangent space $T_x^*(M)$, while using the fact that the metric g provides an inner product on $T_x(M)$ and thus an isomorphism $T_x(M) \simeq T_x^*(M)$. In the special relativity case, this distinction between $T_x(M)$ and $T_x^*(M)$ just comes down to an issue of signs, but the upper and lower index notation is useful for keeping track of those.

A second motivation is that position and momenta naturally live in dual vector spaces, so one would like to distinguish between the vector space M^4 of positions and the dual vector space of momenta. In the case though of a vector space like M^4 which comes with a fixed inner product $\eta_{\mu\nu}$, this inner product gives a fixed identification of M^4 and its dual, an identification that is also an identification as representations of the Lorentz group. For simplicity, we will not here try and distinguish by notation whether a vector is in M^4 or its dual, so will just use lower indices, not both upper and lower indices.

The coordinates x_1, x_2, x_3 are interpreted as spatial coordinates, and the coordinate x_0 is a time coordinate, related to the conventional time coordinate t with respect to chosen units of time and distance by $x_0 = ct$ where c is the speed of light. Mostly we will assume units of time and distance have been chosen so that $c = 1$.

Vectors $v \in M^4$ such that $|v|^2 = v \cdot v > 0$ are called "spacelike", those with $|v|^2 < 0$ "time-like" and those with $|v|^2 = 0$ are said to lie on the "light-cone". Suppressing one space dimension, the picture to keep in mind of Minkowski space looks like this:



We can take Fourier transforms with respect to the four space-time variables, which will take functions of x_0, x_1, x_2, x_3 to functions of the Fourier transform variables p_0, p_1, p_2, p_3. The definition we will use for this Fourier transform will be

$$\begin{aligned}\widetilde{f}(p) =& \frac{1}{(2\pi)^2}\int_{M^4} e^{-ip\cdot x} f(x) d^4x \\ =& \frac{1}{(2\pi)^2}\int_{M^4} e^{-i(-p_0x_0+p_1x_1+p_2x_2+p_3x_3)} f(x) dx_0 d^3\mathbf{x}\end{aligned}$$

and the Fourier inversion formula is

$$f(x) = \frac{1}{(2\pi)^2}\int_{M^4} e^{ip\cdot x}\widetilde{f}(p) d^4p$$

Note that our definition puts one factor of $\frac{1}{\sqrt{2\pi}}$ with each Fourier (or inverse Fourier) transform with respect to a single variable. A common alternate convention among physicists is to put all factors of 2π with the p integrals (and thus in the inverse Fourier transform), none in the definition of $\widetilde{f}(p)$, the Fourier transform itself.

The reason why one conventionally defines the Hamiltonian operator as $i\frac{\partial}{\partial t}$ but the momentum operator with components $-i\frac{\partial}{\partial x_j}$ is due to the sign change between the time and space variables that occurs in this Fourier transform in the exponent of the exponential.

Discuss the sign conventions and the Fourier transform in more detail here.

37.2 The Lorentz group and its Lie algebra

Recall that in 3 dimensions the group of linear transformations of $\mathbf{R}^3$ preserving the standard inner product was the group $O(3)$ of 3 by 3 orthogonal matrices. This group has two disconnected components: $SO(3)$, the subgroup of orientation preserving (determinant $+1$) transformations, and a component of orientation reversing (determinant -1) transformations. In Minkowksi space, one has

Definition (Lorentz group)**.** *The Lorentz group $O(3,1)$ is the group of linear transformations preserving the Minkowski space inner product on $\mathbf{R}^4$.*

In terms of matrices, the condition for a 4 by 4 matrix Λ to be in $O(3,1)$ will be

$$\Lambda^T \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \Lambda = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The Lorentz group has four components, with the component of the identity a subgroup called $SO(3,1)$ (which some call $SO^+(3,1)$). The other three components arise by multiplication of elements in $SO(3,1)$ by P, T, PT where

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

is called the "parity" transformation, reversing the orientation of the spatial variables, and

$$T = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

reverses the time orientation.

The Lorentz group has a subgroup $SO(3)$ of transformations that just act on the spatial components, given by matrices of the form

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & & & \\ 0 & & R & \\ 0 & & & \end{pmatrix}$$

where R is in $SO(3)$. For each pair j, k of spatial directions one has the usual $SO(2)$ subgroup of rotations in the $j-k$ plane, but now in addition for each pair $0, j$ of the time direction with a spatial direction, one has $SO(1,1)$ subgroups

of matrices of transformations called "boosts" in the j direction. For example, for $j = 1$, one has the subgroup of $SO(3,1)$ of matrices of the form

$$\Lambda = \begin{pmatrix} \cosh\phi & \sinh\phi & 0 & 0 \\ \sinh\phi & \cosh\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

for $\phi \in \mathbf{R}$.

The Lorentz group is six-dimensional. For a basis of its Lie algebra one can take six matrices $M_{\mu\nu}$ for $\mu, \nu \in 0, 1, 2, 3$ and $j < k$. For the spatial indices, these are

$$M_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; M_{13} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \; M_{23} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

which correspond to the basis elements of the Lie algebra of $SO(3)$ that we saw in an earlier chapter. One can rename these using the same names as earlier

$$l_1 = M_{23}, \quad l_2 = M_{13}, \quad l_3 = M_{12}$$

and recall that these satisfy the $\mathfrak{so}(3)$ commutation relations

$$[l_1, l_2] = l_3, \quad [l_2, l_3] = l_1, \quad [l_3, l_1] = l_2$$

and correspond to infinitesimal rotations about the three spatial axes.

Taking the first index 0, one gets three elements corresponding to infinitesimal boosts in the three spatial directions

$$M_{01} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; M_{02} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; M_{03} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

These can be renamed as

$$k_1 = M_{01}, \quad k_2 = M_{02}, \quad k_3 = M_{03}$$

One can easily calculate the commutation relations between the k_j and l_j, which show that the k_j transform as a vector under infinitesimal rotations. For instance, for infinitesimal rotations about the x_1 axis, one finds

$$[l_1, k_1] = 0, \quad [l_1, k_2] = k_3, \quad [l_1, k_3] = -k_2$$

Commuting infinitesimal boosts, one gets infinitesimal spatial rotations

$$[k_1, k_2] = -l_3, \quad [k_3, k_1] = -l_2, \quad [k_2, k_3] = -l_1$$

Digression. *A more conventional notation in physics is to use $J_j = il_j$ for infinitesimal rotations, and $K_j = ik_j$ for infinitesimal boosts. The intention of the different notation used here is to start with basis elements of the real Lie algebra $\mathfrak{so}(3,1)$, (the l_j and k_j) which are purely real objects, before complexifying and considering representations of the Lie algebra.*

Taking the following complex linear combinations of the l_j and k_j

$$A_j = \frac{1}{2}(l_j + ik_j), \quad B_j = \frac{1}{2}(l_j - ik_j)$$

one finds

$$[A_1, A_2] = A_3, \quad [A_3, A_1] = A_2, \quad [A_2, A_3] = A_1$$

and

$$[B_1, B_2] = B_3, \quad [B_3, B_1] = B_2, \quad [B_2, B_3] = B_1$$

This construction of the A_j, B_j requires that we complexify (allow complex linear combinations of basis elements) the Lie algebra $\mathfrak{so}(3,1)$ of $SO(3,1)$ and work with the complex Lie algebra $\mathfrak{so}(3,1) \otimes \mathbf{C}$. It shows that this Lie algebra splits into a product of two sub-Lie algebras, which are each copies of the (complexified) Lie algebra of $SO(3)$, $\mathfrak{so}(3) \otimes \mathbf{C}$. Since

$$\mathfrak{so}(3) \otimes \mathbf{C} = \mathfrak{su}(2) \otimes \mathbf{C} = \mathfrak{sl}(2, \mathbf{C})$$

we have

$$\mathfrak{so}(3,1) \otimes \mathbf{C} = \mathfrak{sl}(2, \mathbf{C}) \times \mathfrak{sl}(2, \mathbf{C})$$

In the next section we'll see the origin of this phenomenon at the group level.

37.3 Spin and the Lorentz group

Just as the groups $SO(n)$ have double covers $Spin(n)$, the group $SO(3,1)$ has a double cover, which we will show can be identified with the group $SL(2, \mathbf{C})$ of 2 by 2 complex matrices with unit determinant. This group will have the same Lie algebra as the $SO(3,1)$, and we will sometimes refer to either group as the "Lorentz group".

Recall that for $SO(3)$ the spin double cover $Spin(3)$ can be identified with either $Sp(1)$ (the unit quaternions) or $SU(2)$, and then the action of $Spin(3)$ as $SO(3)$ rotations of $\mathbf{R}^3$ was given by conjugation of imaginary quaternions or certain 2 by 2 complex matrices respectively. In the $SU(2)$ case this was done explicitly by identifying

$$(x_1, x_2, x_3) \leftrightarrow \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix}$$

and then showing that conjugating this matrix by an element of $SU(2)$ was a linear map leaving invariant

$$\det \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} = -(x_1^2 + x_2^2 + x_3^2)$$

and thus a rotation in $SO(3)$.

The same sort of thing works for the Lorentz group case. Now we identify $\mathbf{R}^4$ with the space of 2 by 2 complex self-adjoint matrices by

$$(x_0, x_1, x_2, x_3) \leftrightarrow \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix}$$

and observe that

$$\det \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} = x_0^2 - x_1^2 - x_2^2 - x_3^2$$

This provides a very useful way to think of Minkowski space: as complex self-adjoint 2 by 2 matrices, with norm-squared minus the determinant of the matrix.

The linear transformation

$$\begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \to \tilde{\Lambda} \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \tilde{\Lambda}^\dagger$$

for $\tilde{\Lambda} \in SL(2, \mathbf{C})$ preserves the determinant and thus the inner-product, since

$$\begin{aligned} \det(\tilde{\Lambda} \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \tilde{\Lambda}^\dagger) =& (\det \tilde{\Lambda}) \det \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} (\det \tilde{\Lambda}^\dagger) \\ =& x_0^2 - x_1^2 - x_2^2 - x_3^2 \end{aligned}$$

It also takes self-adjoint matrices to self-adjoints, and thus $\mathbf{R}^4$ to $\mathbf{R}^4$, since

$$\begin{aligned} (\tilde{\Lambda} \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \tilde{\Lambda}^\dagger)^\dagger =& (\tilde{\Lambda}^\dagger)^\dagger \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix}^\dagger \tilde{\Lambda}^\dagger \\ =& \tilde{\Lambda} \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \tilde{\Lambda}^\dagger \end{aligned}$$

Note that both $\tilde{\Lambda}$ and $-\tilde{\Lambda}$ give the same linear transformation when they act by conjugation like this. One can show that all elements of $SO(3,1)$ arise as such conjugation maps, by finding appropriate $\tilde{\Lambda}$ that give rotations or boosts in the $\mu - \nu$ planes, since these generate the group.

Recall that the double covering map

$$\Phi : SU(2) \to SO(3)$$

was given for $\Omega \in SU(2)$ by taking $\Phi(\Omega)$ to be the linear transformation in $SO(3)$

$$\begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \to \Omega \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \Omega^{-1}$$

We have found an extension of this map to a double covering map from $SL(2, \mathbf{C})$ to $SO(3,1)$. This restricts to Φ on the subgroup $SU(2)$ of $SL(2, \mathbf{C})$ matrices satisfying $\tilde{\Lambda}^\dagger = \tilde{\Lambda}^{-1}$.

Digression (The complex group $Spin(4,\mathbf{C})$ and its real forms)**.** *Recall that we found that $Spin(4) = Sp(1) \times Sp(1)$, with the corresponding $SO(4)$ transformation given by identifying $\mathbf{R}^4$ with the quaternions $\mathbf{H}$ and taking not just conjugations by unit quaternions, but both left and right multiplication by distinct unit quaternions. Rewriting this in terms of complex matrices instead of quaternions, we have $Spin(4) = SU(2) \times SU(2)$, and a pair Ω_1, Ω_2 of $SU(2)$ matrices acts as an $SO(4)$ rotation by*

$$\begin{pmatrix} x_0 - ix_3 & -x_2 - ix_1 \\ x_2 - ix_1 & x_0 + ix_3 \end{pmatrix} \to \Omega_1 \begin{pmatrix} x_0 - ix_3 & -x_2 - ix_1 \\ x_2 - ix_1 & x_0 + ix_3 \end{pmatrix} \Omega_2$$

preserving the determinant $x_0^2 + x_1^2 + x_2^2 + x_3^2$.

For another example, consider the identification of $\mathbf{R}^4$ with 2 by 2 real matrices given by

$$(x_0, x_1, x_2, x_3) \leftrightarrow \begin{pmatrix} x_0 + x_3 & x_2 + x_1 \\ x_2 - x_1 & x_0 - x_3 \end{pmatrix}$$

Given a pair of matrices Ω_1, Ω_2 in $SL(2,\mathbf{R})$, the linear transformation

$$\begin{pmatrix} x_0 + x_3 & x_2 + x_1 \\ x_2 - x_1 & x_0 - x_3 \end{pmatrix} \to \Omega_1 \begin{pmatrix} x_0 + x_3 & x_2 + x_1 \\ x_2 - x_1 & x_0 - x_3 \end{pmatrix} \Omega_2$$

preserves the reality condition on the matrix, and preserves

$$\det \begin{pmatrix} x_0 + x_3 & x_2 + x_1 \\ x_2 - x_1 & x_0 - x_3 \end{pmatrix} = x_0^2 + x_1^2 - x_2^2 - x_3^2$$

so gives an element of $SO(2,2)$ and we see that $Spin(2,2) = SL(2,\mathbf{R}) \times SL(2,\mathbf{R})$.

The three different examples

$$Spin(4) = SU(2) \times SU(2), \quad Spin(3,1) = SL(2,\mathbf{C})$$

and

$$Spin(2,2) = SL(2,\mathbf{R}) \times SL(2,\mathbf{R})$$

that we have seen are all so-called "real forms" of a fact about complex groups that one can get by complexifying any of the examples, i.e. considering elements $(x_0, x_1, x_2, x_3) \in \mathbf{C}^4$, not just in $\mathbf{R}^4$. For instance, in the $Spin(4)$ case, taking the x_0, x_1, x_2, x_3 in the matrix

$$\begin{pmatrix} x_0 - ix_3 & -x_2 - ix_1 \\ x_2 - ix_1 & x_0 + ix_3 \end{pmatrix}$$

to have arbitrary complex values z_0, z_1, z_2, z_3 one gets arbitrary 2 by 2 complex matrices, and the transformation

$$\begin{pmatrix} z_0 - iz_3 & -z_2 - iz_1 \\ z_2 - iz_1 & z_0 + iz_3 \end{pmatrix} \to \Omega_1 \begin{pmatrix} z_0 - iz_3 & -z_2 - iz_1 \\ z_2 - iz_1 & z_0 + iz_3 \end{pmatrix} \Omega_2$$

preserves this space as well as the determinant $(z_0^2+z_1^2+z_2^2+z_3^2)$ *for* Ω_1 *and* Ω_2 *not just in* $SU(2)$*, but in the larger group* $SL(2,\mathbf{C})$*. So we find that the group* $SO(4,\mathbf{C})$ *of complex orthogonal transformations of* $\mathbf{C}^4$ *has spin double cover*

$$Spin(4,\mathbf{C}) = SL(2,\mathbf{C}) \times SL(2,\mathbf{C})$$

Since $\mathfrak{spin}(4,\mathbf{C}) = \mathfrak{so}(3,1) \otimes \mathbf{C}$*, this relation between complex Lie groups corresponds to the Lie algebra relation*

$$\mathfrak{so}(3,1) \otimes \mathbf{C} = \mathfrak{sl}(2,\mathbf{C}) \times \mathfrak{sl}(2,\mathbf{C})$$

we found explicitly earlier when we showed that by taking complex coefficients of generators l_j *and* k_j *of* $\mathfrak{so}(3,1)$ *we could find generators* A_j *and* B_j *of two different* $\mathfrak{sl}(2,\mathbf{C})$ *sub-algebras.*

37.4 For further reading

Those not familiar with special relativity should consult a textbook on the subject for the physics background necessary to appreciate the significance of Minkowski space and its Lorentz group of invariances. An example of a suitable such book aimed at mathematics students is Woodhouse's *Special Relativity* [76].

Most quantum field theory textbooks have some sort of discussion of the Lorentz group and its Lie algebra, although the issue of its complexification is often not treated. A typical example is Peskin-Schroeder [46], see the beginning of Chapter 3. Another example is *Quantum Field Theory in a Nutshell* by Tony Zee, see Chapter II.3 [77] (and test your understanding by interpreting properly some of the statements included there such as "The mathematically sophisticated say the algebra $SO(3,1)$ is isomorphic to $SU(2) \otimes SU(2)$").

Chapter 38

Representations of the Lorentz Group

Having seen the importance in quantum mechanics of understanding the representations of the rotation group $SO(3)$ and its double cover $Spin(3) = SU(2)$ one would like to also understand the representations of the Lorentz group. We'll consider this question for the double cover $SL(2, \mathbf{C})$. As in the three-dimensional case, only some of these will also be representations of $SO(3, 1)$. One difference from the $SO(3)$ case is that these will be non-unitary representations, so do not by themselves provide physically sensible state spaces. All finite-dimensional irreducible representations of the Lorentz group are non-unitary (except for the trivial representation). The Lorentz group does have unitary irreducible representations, but these are infinite-dimensional and a topic we will not cover.

38.1 Representations of the Lorentz group

In the $SU(2)$ case we found irreducible unitary representations (π_n, V^n) of dimension $n+1$ for $n = 0, 1, 2, \ldots$. These could also be labeled by $s = \frac{n}{2}$, called the "spin" of the representation, and we will do that from now on. These representations can be realized explicitly as homogeneous polynomials of degree $n = 2s$ in two complex variables z_1, z_2. For the case of $Spin(4) = SU(2) \times SU(2)$, the irreducible representation will just be tensor products

$$V^{s_1} \otimes V^{s_2}$$

of $SU(2)$ irreducibles, with the first $SU(2)$ acting on the first factor, the second on the second factor. The case $s_1 = s_2 = 0$ is the trivial representation, $s_1 = \frac{1}{2}, s_2 = 0$ is one of the half-spinor representations of $Spin(4)$ on $\mathbf{C}^2$, $s_1 = 0, s_2 = \frac{1}{2}$ is the other, and $s_1 = s_2 = \frac{1}{2}$ is the representation on four-dimensional (complexified) vectors.

Turning now to $Spin(3, 1) = SL(2, \mathbf{C})$, one can take the $SU(2)$ matrices acting on homogeneous polynomials to instead be $SL(2, \mathbf{C})$ matrices and still

have irreducible representations of dimension $2s+1$ for $s = 0, \frac{1}{2}, 1, \ldots$. These will now be representations (π_s, V^s) of $SL(2, \mathbf{C})$. There are several things that are different though about these representations:

- They are not unitary (except in the case of the trivial representation). For example, for the defining representation $V^{\frac{1}{2}}$ on $\mathbf{C}^2$ and the Hermitian inner product $< \cdot, \cdot >$

$$< \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} >= \begin{pmatrix} \overline{\psi_1} & \overline{\psi_2} \end{pmatrix} \cdot \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} = \overline{\psi_1}\psi'_1 + \overline{\psi_2}\psi'_2$$

  is invariant under $SU(2)$ transformations Ω since

$$< \Omega \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \Omega \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} >= \begin{pmatrix} \overline{\psi_1} & \overline{\psi_2} \end{pmatrix} \Omega^\dagger \cdot \Omega \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix}$$

  and $\Omega^\dagger \Omega = 1$ by unitarity. This is no longer true for $\Omega \in SL(2, \mathbf{C})$.

- The condition that matrices $\Omega \in SL(2, \mathbf{C})$ do satisfy is that they have determinant 1. It turns out that Ω having determinant one is equivalent to the condition that Ω preserves the antisymmetric bilinear form on $\mathbf{C}^2$, i.e.

$$\Omega^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

  To see this, take

$$\Omega = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

  and calculate

$$\Omega^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Omega = \begin{pmatrix} 0 & \alpha\delta - \beta\gamma \\ \beta\gamma - \alpha\delta & 0 \end{pmatrix} = (\det \Omega) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

  As a result, on representations $V^{\frac{1}{2}}$ of $SL(2, \mathbf{C})$ we do have a non-degenerate bilinear form

$$(\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix}) \to \begin{pmatrix} \psi_1 & \psi_2 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} = \psi_1\psi'_2 - \psi_2\psi'_1$$

  that is invariant under the $SL(2, \mathbf{C})$ action on $V^{\frac{1}{2}}$ and can be used to identify the representation and its dual.

  Such a non-degenerate bilinear form is called a "symplectic form", and we have already made extensive use of these as a fundamental structure that occurs on a Hamiltonian phase space. For the simplest case of the phase space $\mathbf{R}^2$ for one degree of freedom, such a form is given with respect to a basis as the same matrix

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

that we find here giving the symplectic form on a representation space $\mathbf{C}^2$ of $SL(2,\mathbf{C})$. In the phase space case, everything was real, and the invariance group of ϵ was the real symplectic group $Sp(2,\mathbf{R}) = SL(2,\mathbf{R})$. What occurs here is just the complexification of this story, with the symplectic form now on $\mathbf{C}^2$, and the invariance group now $SL(2,\mathbf{C})$.

- In the case of $SU(2)$ representations, the complex conjugate representation one gets by taking as representation matrices $\overline{\pi(g)}$ instead of $\pi(g)$ is equivalent to the original representation (the same representation, with a different basis choice, so matrices changed by a conjugation). To see this for the spin-$\frac{1}{2}$ representation, note that $SU(2)$ matrices are of the form

$$\Omega = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

and one has

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} \overline{\alpha} & \overline{\beta} \\ -\beta & \alpha \end{pmatrix}$$

so the matrix

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is the change of basis matrix relating the representation and its complex conjugate.

This is no longer true for $SL(2,\mathbf{C})$. One cannot complex conjugate arbitrary 2 by 2 complex matrices of unit determinant by a change of basis, and representations π_s will not be equivalent to their complex conjugates $\overline{\pi}_s$.

To add: show that this is true

The classification of irreducible finite dimensional $SU(2)$ representation was done earlier in this course by considering its Lie algebra $\mathfrak{su}(2)$, complexified to give us raising and lowering operators, and this complexification is $\mathfrak{sl}(2,\mathbf{C})$. If you take a look at that argument, you see that it mostly also applies to irreducible finite-dimensional $\mathfrak{sl}(2,\mathbf{C})$ representations. There is a difference though: now flipping positive to negative weights (which corresponds to change of sign of the Lie algebra representation matrices, or conjugation of the Lie group representation matrices) no longer takes one to an equivalent representation. It turns out that to get all irreducibles, one must take both the representations we already know about and their complex conjugates. Using the fact that the tensor product of one of each type of irreducible is still an irreducible, one can show (we won't do this here) that the complete list of irreducible representations of $\mathfrak{sl}(2,\mathbf{C})$ is given by

Theorem (Classification of finite dimensional $\mathfrak{sl}(2,\mathbf{C})$ representations)**.** *The irreducible representations of* $\mathfrak{sl}(2,\mathbf{C})$ *are labeled by* (s_1, s_2) *for* $s_j = 0, \frac{1}{2}, 1, \ldots$.

These representations are built out of the representations (π_s, V^s) *with the irreducible* (s_1, s_2) *given by*

$$(\pi_{s_1} \otimes \overline{\pi}_{s_2}, V^{s_1} \otimes V^{s_2})$$

and having dimension $(2s_1 + 1)(2s_2 + 1)$.

All these representations are also representations of the group $SL(2, \mathbf{C})$ and one has the same classification theorem for the group, although we will not try and prove this. We will also not try and study these representations in general, but will restrict attention to the four cases of most physical interest.

- $(0, 0)$: The trivial representation on $\mathbf{C}$, also called the "spin 0" or scalar representation.
- $(\frac{1}{2}, 0)$: These are called left-handed (for reasons we will see later on) "Weyl spinors". We will often denote the representation space $\mathbf{C}^2$ in this case as S_L, and write an element of it as ψ_L.
- $(0, \frac{1}{2})$: These are called right-handed Weyl spinors. We will often denote the representation space $\mathbf{C}^2$ in this case as S_R, and write an element of it as ψ_R.

  Note that the representations of $SL(2, C)$ on S_L and S_R are described explicitly below.
- $(\frac{1}{2}, \frac{1}{2})$: This is called the "vector" representation since it is the complexification of the action of $SL(2, \mathbf{C})$ as $SO(3, 1)$ transformations of space-time vectors that we saw earlier. Recall that for $\Omega \in SL(2, \mathbf{C})$ this action was

  $$\begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \to \Omega \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} \Omega^\dagger$$

  Since $\Omega^\dagger$ is the conjugate transpose this is the action of $SL(2, \mathbf{C})$ on the representation $S_L \otimes S_R$.

  add an explicit identification of matrices and the tensor product

  This representation is on a vector space $\mathbf{C}^4 = M(2, \mathbf{C})$, but preserves the subspace of self-adjoint matrices that we have identified with the Minkowski space $\mathbf{R}^4$.

The reducible 4 complex dimensional representation $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$ is known as the representation on "Dirac spinors". As explained earlier, of these representations, only the trivial one is unitary. Only the trivial and vector representations are representations of $SO(3, 1)$ as well as $SL(2, \mathbf{C})$.

One can manipulate these Weyl spinor representations $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ in a similar way to the treatment of tangent vectors and their duals in tensor analysis. Just like in that formalism, one can distinguish between a representation space and its dual by upper and lower indices, in this case using not the metric but the $SL(2, \mathbf{C})$ invariant bilinear form ϵ to raise and lower indices. With complex conjugates and duals, there are four kinds of irreducible $SL(2, \mathbf{C})$ representations on $\mathbf{C}^2$ to keep track of

- S_L: This is the standard defining representation of $SL(2,\mathbf{C})$ on $\mathbf{C}^2$, with $\Omega \in SL(2,\mathbf{C})$ acting on $\psi_L \in S_L$ by

$$\psi_L \to \Omega\psi_L$$

A standard index notation for such things is called the "van der Waerden notation". It uses a lower index α taking values $1, 2$ to label the components

$$\psi_L = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \psi_\alpha$$

and in this notation Ω acts by

$$\psi_\alpha \to \Omega_\alpha^\beta \psi_\beta$$

For instance, the element

$$\Omega = e^{-i\frac{\theta}{2}\sigma_3}$$

that acts on vectors by a rotation by an angle θ around the z-axis acts on S_L by

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \to e^{-i\frac{\theta}{2}\sigma_3}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$$

- S_L^*: This is the dual of the defining representation, with $\Omega \in SL(2,\mathbf{C})$ acting on $\psi_L^* \in S_L^*$ by

$$\psi_L^* \to (\Omega^{-1})^T \psi_L^*$$

This is a general property of representations: given any finite-dimensional representation $(\pi(g), V)$, the pairing between V and its dual V^* is preserved by acting on V^* by matrices $(\pi(g)^{-1})^T$, and these provide a representation $((\pi(g)^{-1})^T, V^*)$. In van der Waerden notation, one uses upper indices and writes

$$\psi^\alpha \to ((\Omega^{-1})^T)_\beta^\alpha \psi^\beta$$

Writing elements of the dual as row vectors, our example above of a particular Ω acts by

$$\begin{pmatrix}\psi_1 & \psi_2\end{pmatrix} \to \begin{pmatrix}\psi_1 & \psi_2\end{pmatrix} e^{i\frac{\theta}{2}\sigma_3}$$

Note that the matrix ϵ gives an isomorphism of representations between S_L and S_L^*, given in index notation by

$$\psi^\alpha = \epsilon^{\alpha\beta}\psi_\beta$$

where

$$\epsilon^{\alpha\beta} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

- S_R: This is the complex conjugate representation to S_L, with $\Omega \in SL(2,\mathbf{C})$ acting on $\psi_R \in S_R$ by
$$\psi_R \to \overline{\Omega}\psi_R$$
The van der Waerden notation uses a separate set of dotted indices for these, writing this as
$$\psi_{\dot\alpha} \to \overline{\Omega}^{\dot\beta}_{\dot\alpha}\psi_{\dot\beta}$$
Another common notation among physicists puts a bar over the ψ to denote that the vector is in this representation, but we'll reserve that notation for complex conjugation. The Ω corresponding to a rotation about the z-axis acts as
$$\begin{pmatrix}\psi_{\dot 1}\\ \psi_{\dot 2}\end{pmatrix} \to e^{i\frac{\theta}{2}\sigma_3}\begin{pmatrix}\psi_{\dot 1}\\ \psi_{\dot 2}\end{pmatrix}$$

- S_R^*: This is the dual representation to S_R, with $\Omega \in SL(2,\mathbf{C})$ acting on $\psi_R^* \in S_R^*$ by
$$\psi_R^* \to (\overline{\Omega}^{-1})^T\psi_R^*$$
and the index notation uses raised dotted indices
$$\psi^{\dot\alpha} \to ((\overline{\Omega}^{-1})^T)^{\dot\alpha}_{\dot\beta}\psi^{\dot\beta}$$
Our standard example of a Ω acts by
$$\begin{pmatrix}\psi_{\dot 1} & \psi_{\dot 2}\end{pmatrix} \to \begin{pmatrix}\psi_{\dot 1} & \psi_{\dot 2}\end{pmatrix} e^{-i\frac{\theta}{2}\sigma_3}$$
Another copy of ϵ
$$\epsilon^{\dot\alpha\dot\beta} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$
gives the isomorphism of S_R and S_R^* as representations, by
$$\psi^{\dot\alpha} = \epsilon^{\dot\alpha\dot\beta}\psi_{\dot\beta}$$

Restricting to the $SU(2)$ subgroup of $SL(2,\mathbf{C})$, all these representations are unitary, and equivalent. As $SL(2,\mathbf{C})$ representations, they are not unitary, and while the representations are equivalent to their duals, S_L and S_R are inequivalent (since as we have seen one cannot complex conjugate $SL(2,\mathbf{C})$ matrices by a conjugation).

38.2 Dirac γ matrices and Cliff$(3,1)$

In our discussion of the fermionic version of the harmonic oscillator, we defined the Clifford algebra Cliff(r,s) and found that elements quadratic in its generators gave a basis for the Lie algebra of $\mathfrak{so}(r,s) = \mathfrak{spin}(r,s)$. Exponentiating these gave an explicit construction of the group $Spin(r,s)$. We can apply that general

theory to the case of Cliff$(3,1)$ and this will give us explicitly the representations $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$.

If we complexify our $\mathbf{R}^4$, then its Clifford algebra becomes just the algebra of 4 by 4 complex matrices

$$\text{Cliff}(3,1)\otimes\mathbf{C}=\text{Cliff}(4,\mathbf{C})=M(4,\mathbf{C})$$

We will represent elements of Cliff$(3,1)$ as such 4 by 4 matrices, but should keep in mind that we are working in the complexification of the Clifford algebra that corresponds to the Lorentz group, so there is some sort of condition on the matrices that should be kept track of. There are several different choices of how to explicitly represent these matrices, and for different purposes, different ones are most convenient. The one we will begin with and mostly use is sometimes called the chiral or Weyl representation, and is the most convenient for discussing massless charged particles. We will try and follow the conventions used for this representation in [71].

Digression. *Note that the A_j and B_j we constructed using the l_j and k_j were also complex 4 by 4 matrices, but they were acting on complex vectors (the complexification of the vector representation $(\frac{1}{2},\frac{1}{2})$). Now we want 4 by 4 matrices for something different, putting together the spinor representations $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$.*

Writing 4 by 4 matrices in 2 by 2 block form and using the Pauli matrices σ_j we assign the following matrices to Clifford algebra generators

$$\gamma_0=-i\begin{pmatrix}0&1\\1&0\end{pmatrix},\gamma_1=-i\begin{pmatrix}0&\sigma_1\\-\sigma_1&0\end{pmatrix},\gamma_2=-i\begin{pmatrix}0&\sigma_2\\-\sigma_2&0\end{pmatrix},\gamma_3=-i\begin{pmatrix}0&\sigma_3\\-\sigma_3&0\end{pmatrix}$$

One can easily check that these satisfy the Clifford algebra relations for generators of Cliff$(1,3)$: they anticommute with each other and

$$\gamma_0^2=-1,\quad \gamma_1^2=\gamma_2^2=\gamma_3^2=1$$

The quadratic Clifford algebra elements $-\frac{1}{2}\gamma_j\gamma_k$ for $j<k$ satisfy the commutation relations of $\mathfrak{so}(3,1)$. These are explicitly

$$-\frac{1}{2}\gamma_1\gamma_2=-\frac{i}{2}\begin{pmatrix}\sigma_3&0\\0&\sigma_3\end{pmatrix},\ -\frac{1}{2}\gamma_1\gamma_3=-\frac{i}{2}\begin{pmatrix}\sigma_2&0\\0&\sigma_2\end{pmatrix},\ -\frac{1}{2}\gamma_2\gamma_3=-\frac{i}{2}\begin{pmatrix}\sigma_1&0\\0&\sigma_1\end{pmatrix}$$

and

$$-\frac{1}{2}\gamma_0\gamma_1=\frac{1}{2}\begin{pmatrix}-\sigma_1&0\\0&\sigma_1\end{pmatrix},\ -\frac{1}{2}\gamma_0\gamma_2=\frac{1}{2}\begin{pmatrix}-\sigma_2&0\\0&\sigma_2\end{pmatrix},\ -\frac{1}{2}\gamma_0\gamma_3=\frac{1}{2}\begin{pmatrix}-\sigma_3&0\\0&\sigma_3\end{pmatrix}$$

They provide a representation $(\pi',\mathbf{C}^4)$ of the Lie algebra $\mathfrak{so}(3,1)$ with

$$\pi'(l_1)=-\frac{1}{2}\gamma_2\gamma_3,\ \pi'(l_2)=-\frac{1}{2}\gamma_1\gamma_3,\ \pi'(l_3)=-\frac{1}{2}\gamma_1\gamma_2$$

and

$$\pi'(k_1) = -\frac{1}{2}\gamma_0\gamma_1,\ \pi'(k_2) = -\frac{1}{2}\gamma_0\gamma_2,\ \pi'(k_3) = -\frac{1}{2}\gamma_0\gamma_3$$

Note that the $\pi'(l_j)$ are skew-adjoint, since this representation of the $\mathfrak{so}(3) \subset \mathfrak{so}(3,1)$ sub-algebra is unitary. The $\pi'(k_j)$ are self-adjoint and this representation π' of $\mathfrak{so}(3,1)$ is not unitary.

On the two commuting $SL(2,\mathbf{C})$ subalgebras of $\mathfrak{so}(3,1) \otimes \mathbf{C}$ with bases

$$A_j = \frac{1}{2}(l_j + ik_j),\quad B_j = \frac{1}{2}(l_j - ik_j)$$

this representation is

$$\pi'(A_1) = -\frac{i}{2}\begin{pmatrix}\sigma_1 & 0\\ 0 & 0\end{pmatrix},\ \pi'(A_2) = -\frac{i}{2}\begin{pmatrix}\sigma_2 & 0\\ 0 & 0\end{pmatrix},\ \pi'(A_3) = -\frac{i}{2}\begin{pmatrix}\sigma_3 & 0\\ 0 & 0\end{pmatrix}$$

and

$$\pi'(B_1) = -\frac{i}{2}\begin{pmatrix}0 & 0\\ 0 & \sigma_1\end{pmatrix},\ \pi'(B_2) = -\frac{i}{2}\begin{pmatrix}0 & 0\\ 0 & \sigma_2\end{pmatrix},\ \pi'(B_3) = -\frac{i}{2}\begin{pmatrix}0 & 0\\ 0 & \sigma_3\end{pmatrix}$$

We see explicitly that the action of the quadratic elements of the Clifford algebra on the spinor representation $\mathbf{C}^4$ is reducible, decomposing as the direct sum $S_L \oplus S_R^*$ of two inequivalent representations on $\mathbf{C}^2$

$$\Psi = \begin{pmatrix}\psi_L\\ \psi_R^*\end{pmatrix}$$

with complex conjugation (interchange of A_j and B_j) relating the $\mathfrak{sl}(2,\mathbf{C})$ actions on the components. The A_j act just on S_L, the B_j just on S_R^*. An alternative standard notation to the two-component van der Waerden notation is to use the four components of $\mathbf{C}^4$ with the action of the γ matrices. The relation between the two notations is given by

$$\Psi_\alpha \leftrightarrow \begin{pmatrix}\psi_\alpha\\ \phi^{\dot\alpha}\end{pmatrix}$$

where the index α on the left takes values $1,2,3,4$ and the indices $\alpha, \dot\alpha$ on the right each take values $1,2$.

An important element of the Clifford algebra is constructed by multiplying all of the basis elements together. Physicists traditionally multiply this by i to make it self-adjoint and define

$$\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$$

This can be used to produce projection operators from the Dirac spinors onto the left and right-handed Weyl spinors

$$\frac{1}{2}(1-\gamma_5)\Psi = \psi_L,\quad \frac{1}{2}(1+\gamma_5)\Psi = \psi_R^*$$

There are two other commonly used representations of the Clifford algebra relations, related to the one above by a change of basis. The Dirac representation is useful to describe massive charged particles, especially in the non-relativistic limit. Generators are given by

$$\gamma_0^D = -i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \gamma_1^D = -i\begin{pmatrix}0 & \sigma_1\\ -\sigma_1 & 0\end{pmatrix}$$

$$\gamma_2^D = -i\begin{pmatrix}0 & \sigma_2\\ -\sigma_2 & 0\end{pmatrix}, \gamma_3^D = -i\begin{pmatrix}0 & \sigma_3\\ -\sigma_3 & 0\end{pmatrix}$$

and the projection operators for Weyl spinors are no longer diagonal, since

$$\gamma_5^D = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

A third representation, the Majorana representation, is given by (now no longer writing in 2 by 2 block form, but as 4 by 4 matrices)

$$\gamma_0^M = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}, \quad \gamma_1^M = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}$$

$$\gamma_2^M = \begin{pmatrix}0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\\ 0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}, \quad \gamma_3^M = \begin{pmatrix}0 & -1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}$$

with

$$\gamma_5^M = i\begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix}$$

The importance of the Majorana representation is that it shows the interesting possibility of having (in signature $(3,1)$) a spinor representation on a real vector space $\mathbf{R}^4$, since one sees that the Clifford algebra matrices can be chosen to be real. One has

$$\gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix}$$

and

$$(\gamma_0\gamma_1\gamma_2\gamma_3)^2 = -1$$

The Majorana spinor representation is on $S_M = \mathbf{R}^4$, with $\gamma_0\gamma_1\gamma_2\gamma_3$ a real operator on this space with square -1, so it provides a complex structure on S_M. Recall that a complex structure on a real vector space gives a splitting of

the complexification of the real vector space into a sum of two complex vector spaces, related by complex conjugation. In this case this corresponds to

$$S_M \otimes \mathbf{C} = S_L \oplus S_R^*$$

the fact that complexifying Majorana spinors gives the two kinds of Weyl spinors.

38.3 For further reading

Most quantum field theory textbook have extensive discussions of spinor representations of the Lorentz group and gamma matrices, although most use the opposite convention for the signature of the Minkowski metric. Typical examples are Peskin-Schroeder [46] and *Quantum Field Theory in a Nutshell* by Tony Zee, see Chapter II.3 and Appendix E [77].

Chapter 39

The Poincaré Group and its Representations

In the previous chapter we saw that one can take the semi-direct product of spatial translations and rotations and that the resulting group has infinite-dimensional unitary representations on the state space of a quantum free particle. The free particle Hamiltonian plays the role of a Casimir operator: to get irreducible representations one fixes the eigenvalue of the Hamiltonian (the energy), and then the representation is on the space of solutions to the Schrödinger equation with this energy. This is a non-relativistic procedure, treating time and space (and correspondingly the Hamiltonian and the momenta) differently. For a relativistic analog, we will use instead the semi-direct product of space-time translations and Lorentz transformations. Irreducible representations of this group will be labeled by a continuous parameter (the mass) and a discrete parameter (the spin or helicity), and these will correspond to possible relativistic elementary particles.

In the non-relativistic case, the representation occurred as a space of solutions to a differential equation, the Schrödinger equation. There is an analogous description of the irreducible Poincaré group representations as spaces of solutions of relativistic wave equations, but we will put off that story until succeeding chapters.

39.1 The Poincaré group and its Lie algebra

Definition (Poincaré group)**.** *The Poincaré group is the semi-direct product*

$$\mathcal{P} = \mathbf{R}^4 \rtimes SO(3,1)$$

with double-cover

$$\tilde{\mathcal{P}} = \mathbf{R}^4 \rtimes SL(2,\mathbf{C})$$

The action of $SO(3,1)$ or $SL(2,\mathbf{C})$ on $\mathbf{R}^4$ is the action of the Lorentz group on Minkowski space.

We will refer to both of these groups as the "Poincaré group", meaning by this the double-cover only when we need it because spinor representations of the Lorentz group are involved. The two groups have the same Lie algebra, so the distinction is not needed in discussions that only need the Lie algebra. Elements of the group $\mathcal{P}$ will be written as pairs (a, Λ), with $a \in \mathbf{R}^4$ and $\Lambda \in SO(3,1)$. The group law is

$$(a_1, \Lambda_1)(a_2, \Lambda_2) = (a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2)$$

The Lie algebra $Lie\mathcal{P} = Lie\tilde{\mathcal{P}}$ has dimension 10, with basis

$$t_0, t_1, t_2, t_3, l_1, l_2, l_3, k_1, k_2, k_3$$

where the first four elements are a basis of the Lie algebra of the translation group, and the next six are a basis of $\mathfrak{so}(3,1)$, with the l_j giving the subgroup of spatial rotations, the k_j the boosts. We already know the commutation relations for the translation subgroup, which is commutative so

$$[t_j, t_k] = 0$$

We have seen that the commutation relations for $\mathfrak{so}(3,1)$ are

$$[l_1, l_2] = l_3, \quad [l_2, l_3] = l_1, \quad [l_3, l_1] = l_2$$

$$[k_1, k_2] = -l_3, \quad [k_3, k_1] = -l_2, \quad [k_2, k_3] = -l_1$$

and that the commutation relations between the l_j and k_j correspond to the fact that the k_j transform as a vector under spatial rotations, so for example commuting the k_j with l_1 gives an infinitesimal rotation about the 1-axis and

$$[l_1, k_1] = 0, \quad [l_1, k_2] = k_3, \quad [l_1, k_3] = -k_2$$

The Poincaré group is a semi-direct product group of the sort discussed in chapter 16 and it can be represented as a group of 5 by 5 matrices in much the same way as elements of the Euclidean group $E(3)$ could be represented by 4 by 4 matrices (see chapter 17). Writing out this isomorphism explicitly for a basis of the Lie algebra, we have

$$l_1 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad l_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad l_3 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$k_1 \leftrightarrow \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad k_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad k_3 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$t_0 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad t_1 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$t_2 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad t_3 \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

We can use this explicit matrix representation to compute the commutators of the infinitesimal translations t_j with the infinitesimal rotations and boosts (l_j, k_j). t_0 commutes with the l_j and t_1, t_2, t_3 transform as a vector under rotations, For instance, for infinitesimal rotations about the 1-axis

$$[l_1, t_1] = 0, \quad [l_1, t_2] = t_3, \ [l_1, t_3] = -t_2$$

with similar relations for the other axes.

For boosts one has

$$[k_j, t_0] = t_j, \quad [k_j, t_j] = t_0, \quad [k_j, t_k] = 0 \text{ if } j \neq k, \ k \neq 0$$

Note that infinitesimal boosts do not commute with infinitesimal time translation, so after quantization boost will not commute with the Hamiltonian and thus are not the sort of symmetries which act on spaces of energy eigenstates, preserving the energy.

39.2 Representations of the Poincaré group

We want to find unitary irreducible representations of the Poincaré group. These will be infinite dimensional, so given by operators $\pi(g)$ on a Hilbert space $\mathcal{H}$, which will have an interpretation as a single-particle relativistic quantum state space. The standard physics notation for the operators giving the representation is $U(a, \Lambda)$, with the U emphasizing their unitarity. To classify these representations, we recall from chapter 18 that irreducible representations of semi-direct products $N \rtimes K$ are associated with pairs of a K-orbit $\mathcal{O}_\alpha$ in the space $\hat{N}$ and an irreducible representation of the corresponding little group K_α.

For the Poincaré group, $\hat{N} = \mathbf{R}^4$ is the space of characters (one-dimensional representations) of the translation group of Minkowski space. These are labeled by an element $p = (p_0, p_1, p_2, p_3)$ that has a physical interpretation as the energy-momentum vector of the state such that $\pi(x)$ (for x in the translation group N) acts as multiplication by

$$e^{i(-p_0 x_0 + p_1 x_1 + p_2 x_2 + p_3 x_3)}$$

Equivalently, the p_0, p_1, p_2, p_3 are the eigenvalues of the energy and momentum operators

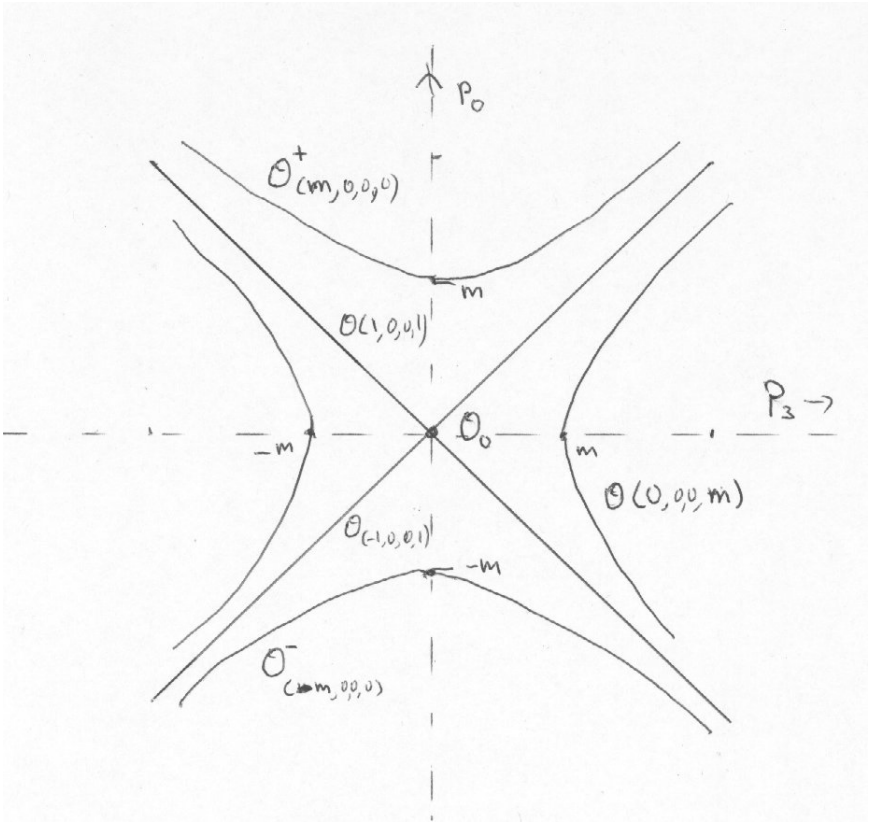
$$P_0 = -i\pi'(t_0), P_1 = i\pi'(t_1), P_2 = i\pi'(t_2), P_3 = i\pi'(t_3)$$

that give the representation of the translation part of the Poincaré group Lie algebra on the states.

The Lorentz group acts on this $\mathbf{R}^4$ by

$$p \to \Lambda p$$

and, restricting attention to the $p_0 - p_3$ plane, the picture of the orbits looks like this



Unlike the Euclidean group case, here there are several different kinds of orbits $\mathcal{O}_\alpha$. We'll examine them and the corresponding stabilizer groups K_α each in turn, and see what can be said about the associated representations. One way to understand the equations describing these orbits is to note that the different orbits correspond to different eigenvalues of the Poincaré group Casimir operator

$$P^2 = -P_0^2 + P_1^2 + P_2^2 + P_3^2$$

This operator commutes with all the generators of the Lie algebra of the Poincaré group, so by Schur's lemma it must act as a scalar times the identity on an irreducible representation (recall that the same phenomenon occurs for $SU(2)$ representations, which can be characterized by the eigenvalue $j(j+1)$ of the Casmir operator $\mathbf{J}^2$ for $SU(2)$). At a point $p = (p_0, p_1, p_2, p_3)$ in energy-momentum space, the P_j operators are diagonalized and P^2 will act by the scalar

$$-p_0^2 + p_1^2 + p_2^2 + p_3^2$$

which can be positive, negative, or zero, so given by $m^2, -m^2, 0$ for various m. The value of the scalar will be the same everywhere on the orbit, so in energy-momentum space orbits will satisfy one of the three equations

$$-p_0^2 + p_1^2 + p_2^2 + p_3^2 = \begin{cases} -m^2 \\ m^2 \\ 0 \end{cases}$$

Note that in this chapter we are just classifying Poincaré group representations, not actually constructing them. It is possible to construct these representations using the data we will find that classifies them, but this would require introducing some techniques (for so-called "induced representations") that go beyond the scope of this course. In later chapters we will explicitly construct these representations in certain specific cases as solutions to certain relativistic wave equations.

39.2.1 Positive energy time-like orbits

One way to get negative values $-m^2$ of the Casimir P^2 is to take the vector $p = (m, 0, 0, 0)$, $m > 0$ and generate an orbit $\mathcal{O}_{m,0,0,0}$ by acting on it with the Lorentz group. This will be the upper, positive energy, hyperboloid of the hyperboloid of two sheets

$$-p_0^2 + p_1^2 + p_2^2 + p_3^2 = -m^2$$

so

$$p_0 = \sqrt{p_1^2 + p_2^2 + p_3^2 + m^2}$$

The stabilizer group of $K_{m,0,0,0}$ is the subgroup of $SO(3,1)$ of elements of the form

$$\begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \Omega \end{pmatrix}$$

where $\Omega \in SO(3)$, so $K_{m,0,0,0} = SO(3)$. Irreducible representations of this group are classified by the spin. For spin 0, points on the hyperboloid can be identified with positive energy solutions to a wave equation called the Klein-Gordon equation and functions on the hyperboloid both correspond to the space of all solutions of this equation and carry an irreducible representation of the Poincaré group. In the next chapter we will study the Klein-Gordon equation,

as well as the quantization of the space of its solutions by quantum field theory methods.

We will later study the case of spin $\frac{1}{2}$, where one must use the double cover $SU(2)$ of $SO(3)$. The Poincaré group representation will be on functions on the orbit that take values in two copies of the spinor representation of $SU(2)$. These will correspond to solutions of a wave equation called the massive Dirac equation.

For choices of higher spin representations of the stabilizer group, one can again find appropriate wave equations and construct Poincaré group representations on their space of solutions, but we will not enter into this topic.

39.2.2 Negative energy time-like orbits

Starting instead with the energy-momentum vector $p = (-m, 0, 0, 0)$, $m > 0$, the orbit $\mathcal{O}_{-m,0,0,0}$ one gets is the lower, negative energy component of the hyperboloid

$$-p_0^2 + p_1^2 + p_2^2 + p_3^2 = -m^2$$

satisfying

$$p_0 = -\sqrt{p_1^2 + p_2^2 + p_3^2 + m^2}$$

Again, one has the same stabilizer group $K_{-m,0,0,0} = SO(3)$ and the same constuctions of wave equations of various spins and Poincaré group representations on their solution spaces as in the positive energy case. Since negative energies lead to unstable, unphysical theories, we will see that these representations are treated differently under quantization, corresponding physically not to particles, but to antiparticles.

39.2.3 Space-like orbits

One can get positive values m^2 of the Casimir P^2 by considering the orbit $\mathcal{O}_{0,0,0,m}$ of the vector $p = (0, 0, 0, m)$. This is a hyperboloid of one sheet, satisfying the equation

$$-p_0^2 + p_1^2 + p_2^2 + p_3^2 = m^2$$

It is not too difficult to see that the stabilizer group of the orbit is $K_{0,0,0,m} = SO(2, 1)$. This is isomorphic to the group $SL(2, \mathbf{R})$, and it has no finite-dimensional unitary representations. These orbits correspond physically to "tachyons", particles that move faster than the speed of light, and there is no known way to consistently incorporate them in a conventional theory.

39.2.4 The zero orbit

The simplest case where the Casimir P^2 is zero is the trivial case of a point $p = (0, 0, 0, 0)$. This is invariant under the full Lorentz group, so the orbit $\mathcal{O}_{0,0,0,0}$ is just a single point and the stabilizer group $K_{0,0,0,0}$ is the entire Lorentz

group $SO(3,1)$. For each finite-dimensional representation of $SO(3,1)$, one gets a corresponding finite dimensional representation of the Poincaré group, with translations acting trivially. These representations are not unitary, so not usable for our purposes.

39.2.5 Positive energy null orbits

One has $P^2 = 0$ not only for the zero-vector in momentum space, but for a three-dimensional set of energy-momentum vectors, called the null-cone. By the term "cone" one means that if a vector is in the space, so are all products of the vector times a positive number. Vectors $p = (p_0, p_1, p_2, p_3)$ are called "light-like" or "null" when they satisfy

$$|p|^2 = -p_0^2 + p_1^2 + p_2^2 + p_3^2 = 0$$

One such vector is $p = (1, 0, 0, 1)$ and the orbit of the vector under the action of the Lorentz group will be the upper half of the full null-cone, the half with energy $p_0 > 0$, satisfying

$$p_0 = \sqrt{p_1^2 + p_2^2 + p_3^2}$$

The stabilizer group $K_{1,0,0,1}$ of $p = (1, 0, 0, 1)$ includes rotations about the x_3 axis, but also boosts in the other two directions. It is isomorphic to the Euclidean group $E(2)$. Recall that this is a semi-direct product group, and it has two sorts of irreducible representations

- Representations such that the two translations act trivially. These are irreducible representations of $SO(2)$, so one-dimensional and characterized by an integer n (half-integers when one uses the Poincaré group double cover).
- Infinite dimensional irreducible representations on a space of functions on a circle of radius r

The first of these two gives irreducible representations of the Poincaré group on certain functions on the positive energy null-cone, labeled by the integer n, which is called the "helicity" of the representation. We will in later chapters consider the cases $n = 0$ (massless scalars, wave-equation the Klein-Gordon equation), $n = \pm\frac{1}{2}$ (Weyl spinors, wave equation the Weyl equation), and $n = \pm 1$ (photons, wave equation the Maxwell equations).

The second sort of representation of $E(2)$ gives representations of the Poincaré group known as "continuous spin" representations, but these seem not to correspond to any known physical phenomena.

39.2.6 Negative energy null orbits

Looking instead at the orbit of $p = (-1, 0, 0, 1)$, one gets the negative energy part of the null-cone. As with the time-like hyperboloids of non-zero mass m, these will correspond to antiparticles instead of particles, with the same classification as in the positive energy case.

39.3 For further reading

The Poincaré group and its Lie algebra is discussed in pretty much any quantum field theory textbook. Weinberg [71] (Chapter 2) has some discussion of the representations of the Poincaré group on single particle state spaces that we have classified here. Folland [20] (Chapter 4.4) and Berndt [7] (Chapter 7.5) discuss the actual construction of these representations using the induced representation methods that we have chosen not to try and explain here.

Chapter 40

The Klein-Gordon Equation and Scalar Quantum Fields

In the non-relativistic case we found that it was possible to build a quantum theory describing arbitrary numbers of particles by "second quantization" of the standard quantum theory of a free particle. This was done by taking as classical phase space the space of solutions to the free particle Schrödinger equation, a space which carries a unitary representation of the Euclidean group $E(3)$. This is an infinite dimensional space of functions (the space of solutions can be identified with the space of initial conditions, which is the space of wavefunctions at a fixed time), but one can quantize it using analogous methods to the case of the finite-dimensional harmonic oscillator (annihilation and creation operators). After such quantization we get a quantum field theory, with a state space that describes an arbitrary number of particles. Such a state space provides a unitary representation of the $E(3)$ group and we saw how to construct the momentum and angular momentum operators that generate it.

To make the same sort of construction for relativistic systems, we want to start with an irreducible unitary representation not of $E(3)$, but of the Poincaré group $\mathcal{P}$. In the last chapter we saw that such things were classified by orbits $\mathcal{O}_\alpha$ of the Lorentz group on momentum space, together with a choice of representation of the stabilizer group K_α of the orbit. The simplest case will be the orbits $\mathcal{O}_{m,0,0,0}$, and the choice of the trivial spin-zero representation of the stabilizer group $K_{m,0,0,0} = SO(3)$. These orbits are characterized by a positive real number m, and are hyperboloids in energy-momentum space. Points on these orbits correspond to solutions of a relativistic analog of the Schrödinger representation, the Klein-Gordon equation, so we will begin by studying this equation and its solutions.

40.1 The Klein-Gordon equation and its solutions

Recall that a condition characterizing the orbit in momentum space that we want to study was that the Casimir operator P^2 of the Poincaré group acts on the representation corresponding to the orbit as the scalar m^2. So, we have the operator equation

$$P^2 = -P_0^2 + P_1^2 + P_2^2 + P_3^2 = -m^2$$

characterizing the Poincaré group representation we are interested in. Interpreting the P_j as the standard differentiation operators $-i\frac{\partial}{\partial x_j}$ on a space of wavefunctions, generating the infinitesimal action of the translation group on such wavefunctions, we get the following differential equation for wavefunctions:

Definition (Klein-Gordon equation)**.** *The Klein-Gordon equation is the second-order partial differential equation*

$$(-\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2})\phi = m^2\phi$$

or

$$(-\frac{\partial^2}{\partial t^2} + \Delta - m^2)\phi = 0$$

for functions $\phi(x)$ on Minkowski space (which may be real or complex valued).

This equation is the simplest Lorentz-invariant wave equation to try, and historically was the one Schrödinger first tried (he then realized it could not account for atomic spectra and instead used the non-relativistic equation that bears his name). Taking Fourier transforms

$$\widetilde{\phi}(p) = \frac{1}{(2\pi)^2}\int d^4x e^{-i(-p_0x_0+\mathbf{p}\cdot\mathbf{x})}\phi(x)$$

the Klein-Gordon equation becomes

$$(p_0^2 - p_1^2 - p_2^2 - p_3^2 - m^2)\widetilde{\phi}(p) = 0$$

Solutions to this will be functions $\widetilde{\phi}(p)$ that are non-zero only on the hyperboloid

$$p_0^2 - p_1^2 - p_2^2 - p_3^2 - m^2 = 0$$

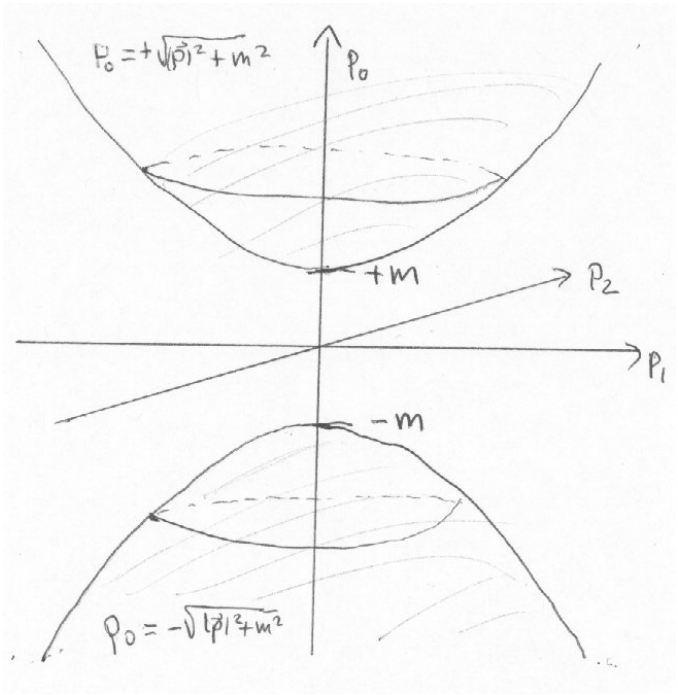
in energy-momentum space $\mathbf{R}^4$. This hyperboloid has two components, with positive and negative energy

$$p_0 = \pm\omega_{\mathbf{p}}$$

where

$$\omega_{\mathbf{p}} = \sqrt{p_1^2 + p_2^2 + p_3^2 + m^2}$$

Ignoring one dimension these look like



In the non-relativistic case, a continuous basis of solutions of the Schrödinger equation labeled by $\mathbf{p} \in \mathbf{R}^3$ was given by the functions

$$e^{i\mathbf{p}\cdot\mathbf{x}} e^{-i\frac{|\mathbf{p}|^2}{2m}t}$$

with a general solution a superposition of these with coefficients $\widetilde{\psi}(\mathbf{p})$ given by the Fourier inversion formula

$$\psi(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} \widetilde{\psi}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} e^{-i\frac{|\mathbf{p}|^2}{2m}t} d^3\mathbf{x}$$

The complex values $\widetilde{\psi}(\mathbf{p})$ gave coordinates on our single-particle space $\mathcal{H}_1$, and we had actions on this of the group of time translations (generated by the Hamiltonian) and the Euclidean group $E(3)$ (generated by momentum and angular momentum).

In the relativistic case we want to study the corresponding single-particle space $\mathcal{H}_1$ of solutions to the Klein-Gordon equation, but parametrized in a way that makes clear the action of the Poincaré group on this space. Coordinates on the space of such solutions will now be given by complex-valued functions $\widetilde{\phi}(p)$ on the energy-momentum space $\mathbf{R}^4$, supported on the two-component hyperboloid (here $p = (p_0, \mathbf{p})$). The Fourier inversion formula giving a general solution in terms of these coordinates will be

$$\phi(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{M^4} \delta(p_0^2 - \omega_{\mathbf{p}}^2) \widetilde{\phi}(p) e^{i(\mathbf{p}\cdot\mathbf{x} - p_0 t)} d^4p$$

with the integral over the 3d hyperboloid expressed as a 4d integral over $\mathbf{R}^4$ with a delta-function on the hyperboloid in the argument.

The delta function distribution with argument a function $f(x)$ depends only on the zeros of f, and if $f' \neq 0$ at such zeros, one has

$$\delta(f(x)) = \sum_{x_j : f(x_j)=0} \delta(f'(x_j)(x - x_j)) = \frac{1}{|f'(x_j)|}\delta(x - x_j)$$

For each $\mathbf{p}$, one can apply this to the case of the function of p_0 given by

$$f = p_0^2 - \omega_{\mathbf{p}}^2$$

on $\mathbf{R}^4$, and using

$$\frac{d}{dp_0}(p_0^2 - \omega_{\mathbf{p}}^2) = 2p_0 = \pm 2\omega_{\mathbf{p}}$$

one finds

$$\begin{aligned}\phi(\mathbf{x}, t) =& \frac{1}{(2\pi)^{3/2}} \int_{M^4} \frac{1}{2\omega_{\mathbf{p}}}(\delta(p_0 - \omega_{\mathbf{p}}) + \delta(p_0 + \omega_{\mathbf{p}}))\widetilde{\phi}(p)e^{i(\mathbf{p}\cdot\mathbf{x} - p_0 t)}dp_0 d^3\mathbf{p} \\ =& \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (\widetilde{\phi}_+(\mathbf{p})e^{-i\omega_{\mathbf{p}}t} + \widetilde{\phi}_-(\mathbf{p})e^{i\omega_{\mathbf{p}}t})e^{i\mathbf{p}\cdot\mathbf{x}}\frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}}\end{aligned}$$

Here

$$\widetilde{\phi}_+(\mathbf{p}) = \widetilde{\phi}(\omega_{\mathbf{p}}, \mathbf{p}), \quad \widetilde{\phi}_-(\mathbf{p}) = \widetilde{\phi}(-\omega_{\mathbf{p}}, \mathbf{p})$$

are the values of $\widetilde{\phi}$ on the positive and negative energy hyperboloids. We see that instead of thinking of the Fourier transforms of solutions as taking values on energy-momentum hyperboloids, we can think of them as taking values just on the space $\mathbf{R}^3$ of momenta (just as in the non-relativistic case), but we do have to use both positive and negative energy Fourier components, and to get a Lorentz invariant measure need to use

$$\frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}}$$

instead of $d^3\mathbf{p}$.

A general complex-valued solution to the Klein-Gordon equation will be given by the two complex-valued functions $\widetilde{\phi}_+$, $\widetilde{\phi}_-$, but we can impose the condition that the solution be real-valued, in which case one can check that the pair of functions must satisfy the condition

$$\widetilde{\phi}_-(\mathbf{p}) = \overline{\widetilde{\phi}}_+(-\mathbf{p})$$

Real-valued solutions of the Klein-Gordon equation thus correspond to arbitrary complex-valued functions $\widetilde{\phi}_+$ defined on the positive energy hyperboloid, which fixes the value of the other function $\widetilde{\phi}_-$.

40.2 Classical relativistic scalar field theory

We would like to set up the Hamiltonian formalism, finding a phase space $\mathcal{H}_1$ and a Hamiltonian function h on it such that Hamilton's equations will give us the Klein-Gordon equation as equation of motion. Such a phase space will be an infinite-dimensional function space and the Hamiltonian will be a functional. We will here blithely ignore the analytic difficulties of working with such spaces, and use physicist's methods, with formulas that can be given a legitimate interpretation by being more careful and using distributions. Note that now we will take the fields ϕ to be real-valued, this is the so-called real scalar field.

Since the Klein-Gordon equation is second order in time, solutions will be parametrized by initial data which, unlike the non-relativistic case now requires the specification at $t = 0$ of not one, but two functions,

$$\phi(\mathbf{x}) = \phi(\mathbf{x}, 0), \quad \dot{\phi}(\mathbf{x}) = \frac{\partial}{\partial t}\phi(\mathbf{x}, t)_{|t=0}$$

the values of the field and its first time derivative.

We will take as our phase space $\mathcal{H}_1$ the space of pairs of functions (ϕ, π), with coordinates $\phi(\mathbf{x}), \pi(\mathbf{x})$ and Poisson brackets

$$\{\phi(\mathbf{x}), \pi(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}'), \quad \{\phi(\mathbf{x}), \phi(\mathbf{x}')\} = \{\pi(\mathbf{x}), \pi(\mathbf{x}')\} = 0$$

We want to get the Klein-Gordon equation for $\phi(\mathbf{x}, t)$ as the following pair of first order equations

$$\frac{\partial}{\partial t}\phi = \pi, \quad \frac{\partial}{\partial t}\pi = (\Delta - m^2)\phi$$

which together imply

$$\frac{\partial^2}{\partial t^2}\phi = (\Delta - m^2)\phi$$

To get these as equations of motion, we just need to find a Hamiltonian function h on the phase space $\mathcal{H}_1$ such that

$$\begin{aligned}\frac{\partial}{\partial t}\phi &= \{\phi, h\} = \pi \\ \frac{\partial}{\partial t}\pi &= \{\pi, h\} = (\Delta - m^2)\phi\end{aligned}$$

One can check that two choices of Hamiltonian function that will have this property are

$$h = \int_{\mathbf{R}^3} \mathcal{H}(\mathbf{x}) d^3\mathbf{x}$$

where

$$\mathcal{H} = \frac{1}{2}(\pi^2 - \phi\Delta\phi + m^2\phi^2) \quad \text{or} \quad \mathcal{H} = \frac{1}{2}(\pi^2 + (\nabla\phi)^2 + m^2\phi^2)$$

where the two different integrands $\mathcal{H}(\mathbf{x})$ are related (as in the non-relativistic case) by integration by parts so these just differ by boundary terms that are assumed to vanish.

To be added: work out one of the two above Poisson brackets

One could instead have taken as starting point the Lagrangian formalism, with an action

$$S = \int_{M^4} \mathcal{L}\ d^4x$$

where

$$\mathcal{L} = \frac{1}{2}((\frac{\partial}{\partial t}\phi)^2 - (\nabla\phi)^2 - m^2\phi^2)$$

This action is a functional now of fields on Minkowski space M^4 and is Lorentz invariant. The Euler-Lagrange equations give as equation of motion the Klein-Gordon equation

$$(\Box - m^2)\phi = 0$$

One recovers the Hamiltonian formalism by seeing that the canonical momentum for ϕ is

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}$$

and the Hamiltonian density is

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L} = \frac{1}{2}(\pi^2 + (\nabla\phi)^2 + m^2\phi^2)$$

Besides the position-space Hamiltonian formalism, we would like to have one for the momentum space components of the field, since for a free field it is these that will decouple into an infinite collection of harmonic oscillators. For a real solution to the Klein-Gordon equation we have

$$\begin{aligned}\phi(\mathbf{x},t) =& \frac{1}{(2\pi)^{3/2}}\int_{\mathbf{R}^3}(\widetilde{\phi}_+(\mathbf{p})e^{-i\omega_{\mathbf{p}}t} + \overline{\widetilde{\phi}}_+(-\mathbf{p})e^{i\omega_{\mathbf{p}}t})e^{i\mathbf{p}\cdot\mathbf{x}}\frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}} \\ =& \frac{1}{(2\pi)^{3/2}}\int_{\mathbf{R}^3}(\widetilde{\phi}_+(\mathbf{p})e^{-i\omega_{\mathbf{p}}t}e^{i\mathbf{p}\cdot\mathbf{x}} + \overline{\widetilde{\phi}}_+(\mathbf{p})e^{i\omega_{\mathbf{p}}t}e^{-i\mathbf{p}\cdot\mathbf{x}})\frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}}\end{aligned}$$

where we have used the symmetry of the integration over $\mathbf{p}$ to integrate over $-\mathbf{p}$ instead of $\mathbf{p}$.

We can choose a new way of normalizing Fourier coefficients, one that reflects the fact that the Lorentz-invariant notion is that of integrating over the energy-momentum hyperboloid rather than momentum space

$$\alpha(\mathbf{p}) = \frac{\widetilde{\phi}_+(\mathbf{p})}{\sqrt{2\omega_{\mathbf{p}}}}$$

and in terms of these we have

$$\phi(\mathbf{x},t) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbf{R}^3}(\alpha(\mathbf{p})e^{-i\omega_{\mathbf{p}}t}e^{i\mathbf{p}\cdot\mathbf{x}} + \overline{\alpha}(\mathbf{p})e^{i\omega_{\mathbf{p}}t}e^{-i\mathbf{p}\cdot\mathbf{x}})\frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

The $\alpha(\mathbf{p}), \overline{\alpha}(\mathbf{p})$ will have the same sort of Poisson bracket relations as the $z, \overline{z}$ for a single harmonic oscillator, or the $\alpha(\mathbf{p}), \overline{\alpha}(\mathbf{p})$ Fourier coefficients in the case of the non-relativistic field:

$$\{\alpha(\mathbf{p}), \overline{\alpha}(\mathbf{p}')\} = -i\delta^3(\mathbf{p} - \mathbf{p}'), \quad \{\alpha(\mathbf{p}), \alpha(\mathbf{p}'))\} = \{\overline{\alpha}(\mathbf{p}), \overline{\alpha}(\mathbf{p}'))\} = 0$$

To see this, one can compute the Poisson brackets for the fields as follows. We have

$$\pi(\mathbf{x}) = \frac{\partial}{\partial t}\phi(\mathbf{x}, t)_{|t=0} = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (-i\omega_{\mathbf{p}})(\alpha(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} - \overline{\alpha}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

and

$$\phi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (\alpha(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} + \overline{\alpha}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

so

$$\begin{aligned}
\{\phi(\mathbf{x}), \pi(\mathbf{x}')\} =& \frac{1}{2(2\pi)^3} \int_{\mathbf{R}^3 \times \mathbf{R}^3} (\{\alpha(\mathbf{p}), i\overline{\alpha}(\mathbf{p}')\} e^{i(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\mathbf{x}')} \\
& - \{i\overline{\alpha}(\mathbf{p}), \alpha(\mathbf{p}')\} e^{i(-\mathbf{p}\cdot\mathbf{x} + \mathbf{p}'\mathbf{x}')}) d^3\mathbf{p} d^3\mathbf{p}' \\
=& \frac{1}{2(2\pi)^3} \int_{\mathbf{R}^3 \times \mathbf{R}^3} \delta^3(\mathbf{p} - \mathbf{p}')(e^{i(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\mathbf{x}')} + e^{i(-\mathbf{p}\cdot\mathbf{x} + \mathbf{p}'\mathbf{x}')}) d^3\mathbf{p} d^3\mathbf{p}' \\
=& \frac{1}{2(2\pi)^3} \int_{\mathbf{R}^3} (e^{i\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')} + e^{-i\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')}) d^3\mathbf{p} \\
=& \delta^3(\mathbf{x} - \mathbf{x}')
\end{aligned}$$

As in the non-relativistic case, one really should work elements of $\mathcal{H}_1^*$ of the form (for appropriately chosen class of functions f, g)

$$\phi(f) + \pi(g) = \int_{\mathbf{R}^3} (f(\mathbf{x})\phi(\mathbf{x}) + g(\mathbf{x})\pi(\mathbf{x})) d^3\mathbf{x}$$

getting Poisson bracket relations

$$\{\phi(f_1) + \pi(g_1), \phi(f_2) + \pi(g_2)\} = \int_{\mathbf{R}^3} (f_1(\mathbf{x})g_2(\mathbf{x}) - f_2(\mathbf{x})g_1(\mathbf{x})) d^3\mathbf{x}$$

This is just the infinite-dimensional analog of the Poisson bracket of two linear combinations of the q_j, p_j, with the right-hand side the symplectic form Ω on $\mathcal{H}_1^*$.

40.3 The complex structure on the space of Klein-Gordon solutions

Recall from chapter 21 that if we intend to quantize a classical phase space M by the Bargmann-Fock method, we need to choose a complex structure J on that phase space (or on the dual phase space $\mathcal{M} = M^*$). Then

$$\mathcal{M} \otimes \mathbf{C} = \mathcal{M}_J^+ \oplus \mathcal{M}_J^-$$

where $\mathcal{M}_J^+$ is the $+i$ eigenspace of J, $\mathcal{M}_J^-$ the $-i$ eigenspace. The quantum state space will be the space of polynomials on the dual of $\mathcal{M}_J^+$. The choice of J corresponds to a choice of distinguished state $|0\rangle_J \in \mathcal{H}$, the Bargmann-Fock state given by the constant polynomial function 1.

In the non-relativistic quantum field theory case we saw that basis elements of $\mathcal{M}$ could be taken to be either the linear functionals $\psi(x)$ and their conjugates $\overline{\psi}(x)$ or, Fourier transforming, the linear functionals $\alpha(p)$ and their conjugates $\overline{\alpha}(p)$. These coordinates are not real-valued, but complex-valued, and as a result $\mathcal{M}$ came with a distinguished natural complex structure J, which is $+i$ on the $\psi(x)$ or the $\alpha(p)$, and $-i$ on their conjugates.

In the relativistic scalar field theory, we must do something very different. The solutions to the Klein-Gordon equation we are considering are real-valued, not complex-valued functions, and give a real phase space $\mathcal{M}$ to be quantized (what happens when we consider a theory with configuration space complex valued fields will be discussed in chapter 41). When we complexify and look at the space $\mathcal{M} \otimes \mathbf{C}$, it naturally decomposes as a representation of the Poincaré group into two pieces: $\mathcal{M}^+$, the complex functions on the positive energy hyperboloid and $\mathcal{M}^-$, the complex functions on the negative energy hyperboloid. More explicitly, we can decompose a complexified solution $\phi(\mathbf{x}, t)$ of the Klein-Gordon equation as $\phi = \phi_+ + \phi_-$, where

$$\phi_+(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} \alpha(\mathbf{p}) e^{-i\omega_{\mathbf{p}} t} e^{i\mathbf{p}\cdot\mathbf{x}} \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

and

$$\phi_-(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} \overline{\alpha}(\mathbf{p}) e^{i\omega_{\mathbf{p}} t} e^{-i\mathbf{p}\cdot\mathbf{x}} \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

We will take as complex structure the operator J that is $+i$ on positive energy wavefunctions and $-i$ on negative energy wavefunctions. Complexified classical fields in $\mathcal{M}^+$ get quantized as annihilation operators, those in $\mathcal{M}^-$ as creation operators. Since conjugation interchanges $\mathcal{M}^+$ and $\mathcal{M}^-$, non-zero real-valued classical fields have components in both $\mathcal{M}^+$ and $\mathcal{M}^-$ since they are their own conjugates.

One motivation for this particular choice of J is that it leads to a state space with states of non-negative energy. Theories with states of arbitrarily negative energy are considered undesirable since they will tend to have no stable vacuum state (since any supposed vacuum state could potentially decay into states of large positive and large negative energy, while preserving total energy). To see the mechanism for non-negative energy, first consider again the non-relativistic case, where the Hamiltonian is (for $d = 1$)

$$h = \frac{1}{2m} \int_{-\infty}^{+\infty} |\frac{d}{dx}\psi(x)|^2 dx = \int_{-\infty}^{\infty} \frac{p^2}{2m} |\alpha(p)|^2 dp$$

This is positive definite, either on $\mathcal{M}^+$ (the ψ) or $\mathcal{M}^-$ (the $\overline{\psi}$). Quantization takes

$$h \to \widehat{H} = \int_{-\infty}^{\infty} \frac{p^2}{2m} a^\dagger(p) a(p) dp$$

which is an operator with positive eigenvalues (this is in normal-ordered form, but the non-normal-ordered version is still positive, although adding an infinite positive constant).

WARNING: HAVEN'T FINISHED REWRITING REST OF THIS SECTION.

The Hamiltonian function h is the quadratic polynomial function of the coordinates $\phi(\mathbf{x}), \pi(\mathbf{x})$

$$h = \int_{\mathbf{R}^3} \frac{1}{2}(\pi^2 + (\nabla\phi)^2 + m^2\phi^2)d^3\mathbf{x}$$

and by laborious calculation one can substitute the above expressions for ϕ, π in terms of $\alpha(\mathbf{p}), \overline{\alpha}(\mathbf{p})$ to find h as a quadratic polynomial in these coordinates on the momentum space fields. A quicker way to find the correct expression is to use the fact that different momentum components of the field decouple, and we know the time-dependence of such components, so just need to find the right h that generates this.

If, as in the non-relativistic case, we interpret ϕ as a single-particle wavefunction, Hamilton's equation of motion says

$$\{\phi, h\} = \frac{\partial}{\partial t}\phi$$

and applying this to the component of ϕ_+ with momentum $\mathbf{p}$, we just get multiplication by $-i\omega_{\mathbf{p}}$. The energy of such a wavefunction would be $\omega_{\mathbf{p}}$, the eigenvalue of $i\frac{\partial}{\partial t}$. These are called "positive frequency" or "positive energy" wavefunctions. In the case of momentum components of ϕ_-, the eigenvalue is $-\omega_{\mathbf{p}}$, and one has "negative frequency" or "negative energy" wavefunctions.

An expression for h in terms of momentum space field coordinates that will have the right Poisson brackets on ϕ_+, ϕ_- is

$$h = \int_{\mathbf{R}^3} \omega_{\mathbf{p}}\alpha(p)\overline{\alpha}(p)d^3\mathbf{p}$$

and this is the same expression one could have gotten by a long direct calculation.

In the non-relativistic case, the eigenvalues of the action of $i\frac{\partial}{\partial t}$ on the wavefunctions ψ were non-negative ($\frac{|\mathbf{p}|^2}{2m}$) so the single-particle states had non-negative energy. Here we find instead eigenvalues $\pm\omega_{\mathbf{p}}$ of both signs, so single-particle states can have arbitrarily negative energies. This makes a physically sensible interpretation of $\mathcal{H}_1$ as a space of wavefunctions describing a single relativistic particle difficult if not impossible. We will however see in the next section that there is a way to quantize this $\mathcal{H}_1$ as a phase space, getting a sensible multi-particle theory with a stable ground state.

40.4 Quantization of the real scalar field

Given the description we have found in momentum space of a real scalar field satisfying the Klein-Gordon equation, it is clear that one can proceed to quan-

tize the theory in exactly the same way as was done with the non-relativistic Schrödinger equation, taking momentum components of fields to operators by replacing

$$\alpha(\mathbf{p}) \to a(\mathbf{p}), \quad \overline{\alpha}(\mathbf{p}) \to a^\dagger(\mathbf{p})$$

where $a(\mathbf{p}), a^\dagger(\mathbf{p})$ are operator valued distributions satisfying the commutation relations

$$[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = \delta^3(\mathbf{p} - \mathbf{p}')$$

For the Hamiltonian we take the normal-ordered form

$$\widehat{H} = \int_{\mathbf{R}^3} \omega_{\mathbf{p}} a^\dagger(\mathbf{p}) a(\mathbf{p}) d^3\mathbf{p}$$

Starting with a vacuum state $|0\rangle$, by applying creation operators one can create arbitary positive energy multiparticle states of free relativistic particles with single-particle states having the energy momentum relation

$$E(\mathbf{p}) = \omega_{\mathbf{p}} = \sqrt{|\mathbf{p}|^2 + m^2}$$

If we try and consider not momentum eigenstates, but position eigenstates, in the non-relativistic case we could define a position space complex-valued field operator by

$$\widehat{\psi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} a(p) e^{i\mathbf{p}\cdot\mathbf{x}} d^3\mathbf{p}$$

which has an interpretation as an annhilation operator for a particle localized at $\mathbf{x}$. Solving the dynamics of the theory gave the time-dependence of the field operator

$$\widehat{\psi}(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} a(p) e^{-i\frac{p^2}{2m}t} e^{i\mathbf{p}\cdot\mathbf{x}} d^3\mathbf{p}$$

For the relativistic case we must do something somewhat different, defining

Definition (Real scalar quantum field)**.** *The real scalar quantum field operators are the operator-valued distributions defined by*

$$\widehat{\phi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (a(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}} \tag{40.1}$$

$$\widehat{\pi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (-i\omega_{\mathbf{p}})(a(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} - a^\dagger(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}} \tag{40.2}$$

By essentially the same computation as for Poisson brackets, one can compute commutators, finding

$$[\widehat{\phi}(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = i\delta^3(\mathbf{x} - \mathbf{x}'), \quad [\widehat{\phi}(\mathbf{x}), \widehat{\phi}(\mathbf{x}')] = [\widehat{\pi}(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = 0$$

These can be interpreted as the relations of a unitary representation of a Heisenberg Lie algebra, now the infinite dimensional Lie algebra corresponding to the phase space $\mathcal{H}_1$ of solutions of the Klein-Gordon equation.

The Hamiltonian operator will be quadratic in the field operators and can be chosen to be

$$\widehat{H} = \int_{\mathbf{R}^3} \frac{1}{2} : (\widehat{\pi}(\mathbf{x})^2 + (\nabla\widehat{\phi}(\mathbf{x}))^2 + m^2\widehat{\phi}(\mathbf{x})^2) : d^3\mathbf{x}$$

This operator is normal ordered, and a computation (see for instance [10]) shows that in terms of momentum space operators this is just

$$\widehat{H} = \int_{\mathbf{R}^3} \omega_{\mathbf{p}} a^\dagger(\mathbf{p}) a(\mathbf{p}) d^3\mathbf{p}$$

the Hamiltonian operator discussed earlier.

The dynamical equations of the quantum field theory are now

$$\frac{\partial}{\partial t}\widehat{\phi} = [\widehat{\phi}, -i\widehat{H}] = \widehat{\pi}$$

$$\frac{\partial}{\partial t}\widehat{\pi} = [\widehat{\pi}, -i\widehat{H}] = (\Delta - m^2)\widehat{\phi}$$

which have as solution the following equation for the time-dependent field operator:

$$\widehat{\phi}(\mathbf{x}, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (a(\mathbf{p})e^{-i\omega_{\mathbf{p}}t}e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(\mathbf{p})e^{i\omega_{\mathbf{p}}t}e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

This is a superposition of annihilation operators for momentum eigenstates of positive energy and creation operators for momentum eigenstates of negative energy. Note that, unlike the non-relativistic case, here the quantum field operator is self-adjoint. In the next chapter we will see what happens in the case of a complex scalar quantum field, where the operator and its adjoint are distinct.

It is a characteristic feature of relativistic field theory that what one is quantizing is not just a space of positive energy wavefunctions, but a space that includes both positive and negative energy wavefunctions, assigning creation operators to one sign of the energy, annihilation operators to the other, and by this mechanism getting a Hamiltonian operator with spectrum bounded below. In more complicated quantum field theories there will be other operators (for instance, a charge operator) that can distinguish between "particle" states that correspond to wavefunctions of positive energy and "antiparticle" states that correspond to wavefunctions of negative energy. The real scalar field case is rather special in that there are no such operators and one says that here "a particle is its own antiparticle."

40.5 The propagator

As explained in the non-relativistic case, in quantum field theory explicitly dealing with states and their time-dependence is awkward, so we work in the Heisenberg picture, expressing everything in terms of a fixed, unchangeable

state $|0\rangle$ and time-dependent operators. For the free scalar field theory, we have explicitly solved for the time-dependence of the field operators. A basic quantity needed for describing the propagation of quanta of a quantum field theory is the propagator:

Definition (Green's function or propagator, scalar field theory)**.** *The Green's function or propagator for a scalar field theory is the amplitude, for $t > t'$*

$$G(\mathbf{x}, t, \mathbf{x}', t') = \langle 0|\widehat{\phi}(\mathbf{x}, t)\widehat{\phi}(\mathbf{x}', t')|0\rangle$$

By translation invariance, the propagator will only depend on $t - t'$ and $\mathbf{x} - \mathbf{x}'$, so we can just evaluate the case $(\mathbf{x}', t') = (\mathbf{0}, 0)$, using the formula for the time dependent field to get

$$\begin{aligned} G(\mathbf{x}, t, \mathbf{0}, 0) =& \frac{1}{(2\pi)^3} \int_{\mathbf{R}^3 \times \mathbf{R}^3} \langle 0|(a(\mathbf{p})e^{-i\omega_{\mathbf{p}} t} e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(\mathbf{p})e^{i\omega_{\mathbf{p}} t} e^{-i\mathbf{p}\cdot\mathbf{x}}) \\ & \qquad (a(\mathbf{p}') + a^\dagger(\mathbf{p}'))|0\rangle \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}} \frac{d^3\mathbf{p}'}{\sqrt{2\omega_{\mathbf{p}'}}} \\ =& \int_{\mathbf{R}^3 \times \mathbf{R}^3} \delta^3(\mathbf{p} - \mathbf{p}') e^{-i\omega_{\mathbf{p}} t} e^{i\mathbf{p}\cdot\mathbf{x}} \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}} \frac{d^3\mathbf{p}'}{\sqrt{2\omega_{\mathbf{p}'}}} \\ =& \int_{\mathbf{R}^3} e^{-i\omega_{\mathbf{p}} t} e^{i\mathbf{p}\cdot\mathbf{x}} \frac{d^3\mathbf{p}}{2\omega_{\mathbf{p}}} \end{aligned}$$

For $t > 0$, this gives the amplitude for propagation of a particle in time t from the origin to the point $\mathbf{x}$.

Plan to expand this section. Compare to non-relativistic propagator. Compute commutator of fields at arbitrary space-time separations, show that commutator of fields at space-like separations vanishes.

40.6 Fermionic scalars

Explain nature of problems. Non-positivity of the Hamiltonian. Commutator at space-like separations does not vanish.

40.7 For further reading

Pretty much every quantum field theory textbook has a treatment of the relativistic scalar field with more details than here, and significantly more physical motivation. A good example with some detailed versions of the calculations done here is chapter 5 of [10]. See Folland [20], chapter 5 for a mathematically more careful treatment of the distributional nature of the scalar field operators.

Chapter 41

Symmetries and Relativistic Scalar Quantum Fields

Just as for non-relativistic quantum fields, the theory of free relativistic scalar quantum fields starts by taking as phase space an infinite dimensional space of solutions of an equation of motion. Quantization of this phase space involves constructing field operators which provide a representation of the corresponding Heisenberg Lie algebra, by an infinite dimensional version of the Bargmann-Fock construction. The equation of motion has its own representation-theoretical significance: it is an eigenvalue equation for a Casimir operator of a group of space-time symmetries, picking out an irreducible representation of that group. In this case the Casimir operator is the Klein-Gordon operator, and the space-time symmetry group is the Poincaré group. The Poincaré group acts on the phase space of solutions to the Klein-Gordon equation, preserving the Poisson bracket. One can thus use the same methods as in the finite-dimensional case to get a representation of the Poincaré group by intertwining operators for the Heisenberg Lie algebra representation (that representation is given by the field operators). These methods give a representation of the Lie algebra of the Poincaré group in terms of quadratic combinations of the field operators.

We'll begin with the case of an even simpler group action on the phase space, that coming from an "internal symmetry" one gets if one takes multi-component scalar fields, with an orthogonal group or unitary group acting on the real or complex vector space in which the classical fields take their values.

41.1 Internal symmetries

The real scalar field theory of chapter 40 lacks one feature of the non-relativistic theory, which is an action of the group $U(1)$ by phase changes on complex fields. This is needed to provide a notion of "charge" and allow the introduction of electromagnetism into the theory. In the real scalar field theory there is no distinction between states describing particles and states describing antiparticles.

To get a theory with such a distinction we need to introduce fields with more components. Two possibilities are to consider real fields with m components, in which case we will have a theory with $SO(m)$ symmetry, and $U(1) = SO(2)$ the $m = 2$ special case, or to consider complex fields with m components, in which case we have theories with $U(m)$ symmetry, and $m = 1$ the $U(1)$ special case.

41.1.1 $SO(m)$ symmetry and real scalar fields

Taking as single particle phase space $\mathcal{H}_1$ the space of pairs ϕ_1, ϕ_2 of real solutions to the Klein-Gordon equation, elements $g(\theta)$ of the group $SO(2)$ will act on the dual phase space $\mathcal{H}_1^*$ of coordinates on such solutions by

$$\begin{pmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \end{pmatrix} \to g(\theta) \cdot \begin{pmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \end{pmatrix}$$

$$\begin{pmatrix} \pi_1(\mathbf{x}) \\ \pi_2(\mathbf{x}) \end{pmatrix} \to g(\theta) \cdot \begin{pmatrix} \pi_1(\mathbf{x}) \\ \pi_2(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \pi_1(\mathbf{x}) \\ \pi_2(\mathbf{x}) \end{pmatrix}$$

Here $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \pi_1(\mathbf{x}), \pi_2(\mathbf{x})$ are the coordinates for initial values at $t = 0$ of a Klein-Gordon solution. The Fourier transforms of solutions behave in the same manner.

This group action on $\mathcal{H}_1$ breaks up into a direct sum of an infinite number (one for each value of $\mathbf{x}$) of identical cases of rotations in a configuration space plane, as discussed in section 18.2.2. We will use the calculation there, where we found that for a basis element L of the Lie algebra of $SO(2)$ the corresponding quadratic function on the phase space with coordinates q_1, q_2, p_1, p_2 was

$$\mu_L = q_1 p_2 - q_2 p_1$$

For the case here, we just take

$$q_1, q_2, p_1, p_2 \to \phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \pi_1(\mathbf{x}), \pi_2(\mathbf{x})$$

To get a quadratic functional on the fields that will have the desired Poisson bracket with the fields for each value of $\mathbf{x}$, we need to just integrate the analog of μ_L over $\mathbf{R}^3$. We will denote the result by Q, since it is an observable that will have a physical interpretation as electric charge when this theory is coupled to the electromagnetic field (see chapter 42):

$$Q = \int_{\mathbf{R}^3} (\pi_2(\mathbf{x})\phi_1(\mathbf{x}) - \pi_1(\mathbf{x})\phi_2(\mathbf{x}))d^3\mathbf{x}$$

One can use the field Poisson bracket relations

$$\{\phi_j(\mathbf{x}), \pi_k(\mathbf{x}')\} = \delta_{jk}\delta(\mathbf{x} - \mathbf{x}')$$

to check that

$$\{Q, \begin{pmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \end{pmatrix}\} = \begin{pmatrix} -\phi_2(\mathbf{x}) \\ \phi_1(\mathbf{x}) \end{pmatrix}, \quad \{Q, \begin{pmatrix} \pi_1(\mathbf{x}) \\ \pi_2(\mathbf{x}) \end{pmatrix}\} = \begin{pmatrix} -\pi_2(\mathbf{x}) \\ \pi_1(\mathbf{x}) \end{pmatrix}$$

Quantization of the classical field theory gives us a unitary representation U of $SO(2)$, with

$$U'(L) = -i\widehat{Q} = -i\int_{\mathbf{R}^3} (\widehat{\pi}_2(\mathbf{x})\widehat{\phi}_1(\mathbf{x}) - \widehat{\pi}_1(\mathbf{x})\widehat{\phi}_2(\mathbf{x}))d^3\mathbf{x}$$

The operator

$$U(\theta) = e^{-i\theta\widehat{Q}}$$

will act by conjugation on the fields:

$$U(\theta)\begin{pmatrix}\widehat{\phi}_1(\mathbf{x})\\ \widehat{\phi}_2(\mathbf{x})\end{pmatrix}U(\theta)^{-1} = \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\widehat{\phi}_1(\mathbf{x})\\ \widehat{\phi}_2(\mathbf{x})\end{pmatrix}$$

$$U(\theta)\begin{pmatrix}\widehat{\pi}_1(\mathbf{x})\\ \widehat{\pi}_2(\mathbf{x})\end{pmatrix}U(\theta)^{-1} = \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\widehat{\pi}_1(\mathbf{x})\\ \widehat{\pi}_2(\mathbf{x})\end{pmatrix}$$

It will also give a representation of $SO(2)$ on states, with the state space decomposing into sectors each labeled by the integer eigenvalue of the operator $\widehat{Q}$ (which will be called the "charge" of the state).

Using the definitions of $\widehat{\phi}$ and $\widehat{\pi}$ (40.1 and 40.2) one can compute $\widehat{Q}$ in terms of annihilation and creation operators, with the result

$$\widehat{Q} = i\int_{\mathbf{R}^3} (a_2^\dagger(\mathbf{p})a_1(\mathbf{p}) - a_1^\dagger(\mathbf{p})a_2(\mathbf{p}))d^3\mathbf{p} \tag{41.1}$$

One expects that since the time evolution action on the classical field space commutes with the $SO(2)$ action, the operator $\widehat{Q}$ should commute with the Hamiltonian operator $\widehat{H}$. This can readily be checked by computing $[\widehat{H}, \widehat{Q}]$ using

$$\widehat{H} = \int_{\mathbf{R}^3} \omega_{\mathbf{p}}(a_1^\dagger(\mathbf{p})a_1(\mathbf{p}) + a_2^\dagger(\mathbf{p})a_2(\mathbf{p}))d^3\mathbf{p}$$

Note that the vacuum state $|0\rangle$ is an eigenvector for $\widehat{Q}$ and $\widehat{H}$ with eigenvalue 0: it has zero energy and zero charge. States $a_1^\dagger(\mathbf{p})|0\rangle$ and $a_2^\dagger(\mathbf{p})|0\rangle$ are eigenvectors of $\widehat{H}$ with eigenvalue and thus energy $\omega_{\mathbf{p}}$, but these are not eigenvectors of $\widehat{Q}$, so do not have a well-defined charge.

All of this can be generalized to the case of $m > 2$ real scalar fields, with a larger group $SO(m)$ now acting instead of the group $SO(2)$. The Lie algebra is now multi-dimensional, with a basis the elementary antisymmetric matrices ϵ_{jk}, with $j, k = 1, 2, \cdots, m$ and $j < k$, which correspond to infinitesimal rotations in the $j-k$ planes. Group elements can be constructed by multiplying rotations $e^{\theta\epsilon_{jk}}$ in different planes. Instead of a single operator $\widehat{Q}$, we get multiple operators

$$-i\widehat{Q}_{jk} = -i\int_{\mathbf{R}^3} (\widehat{\pi}_k(\mathbf{x})\widehat{\phi}_j(\mathbf{x}) - \widehat{\pi}_j(\mathbf{x})\widehat{\phi}_k(\mathbf{x}))d^3\mathbf{x}$$

and conjugation by

$$U_{jk}(\theta) = e^{-i\theta\widehat{Q}_{jk}}$$

rotates the field operators in the $j-k$ plane. These also provide unitary operators on the state space, and, taking appropriate products of them, a unitary representation of the full group $SO(m)$ on the state space. The $\widehat{Q}_{jk}$ commute with the Hamiltonian, so the energy eigenstates of the theory break up into irreducible representations of $SO(m)$ (a subject we haven't discussed for $m > 3$).

41.1.2 $U(1)$ symmetry and complex scalar fields

Instead of describing a scalar field system with $SO(2)$ symmetry using a pair ϕ_1, ϕ_2 of real fields, it is more covenient to identify the $\mathbf{R}^2$ that the fields take values in with $\mathbf{C}$, and work with complex scalar fields and a $U(1)$ symmetry. This will allow us to work with a set of annihilation and creation operators for particle states with a definite value of the charge observable. Note that we were already forced to introduce a complex structure (given by the splitting of complexified solutions of the Klein-Gordon equation into positive and negative energy solutions) as part of the Bargmann-Fock quantization. This is a second and independent source of complex numbers in the theory.

We express a pair of real-valued fields as complex-valued fields using

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2), \quad \pi = \frac{1}{\sqrt{2}}(\pi_1 - i\pi_2)$$

These can be thought of as initial-value data parametrizing complex solutions of the Klein-Gordon equation, giving a phase space that is infinite-dimensional, with four real dimensions for each value of $\mathbf{x}$. Instead of

$$\phi_1(\mathbf{x}), \phi_1(\mathbf{x}), \pi_1(\mathbf{x}), \pi_2(\mathbf{x})$$

we can think of the complex-valued fields and their complex conjugates

$$\phi(\mathbf{x}), \overline{\phi}(\mathbf{x}), \pi(\mathbf{x}), \overline{\pi}(\mathbf{x})$$

as providing a real basis of the coordinates on phase space.

The Poisson bracket relations on such complex fields will be

$$\{\phi(\mathbf{x}), \overline{\phi}(\mathbf{x}')\} = \{\pi(\mathbf{x}), \overline{\pi}(\mathbf{x}')\} = \{\phi(\mathbf{x}), \overline{\pi}(\mathbf{x}')\} = \{\overline{\phi}(\mathbf{x}), \pi(\mathbf{x}')\} = 0$$

$$\{\phi(\mathbf{x}), \pi(\mathbf{x}')\} = \{\overline{\phi}(\mathbf{x}), \overline{\pi}(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}')$$

and the classical Hamiltonian is

$$h = \int_{\mathbf{R}^3} (|\pi|^2 + |\nabla\phi|^2 + m^2|\phi|^2) d^3\mathbf{x}$$

Note that introducing complex fields in a theory like this with field equations that are second-order in time means that for each $\mathbf{x}$ we have a phase space with two complex dimensions ($\phi(\mathbf{x})$ and $\pi(\mathbf{x})$). Using Bargmann-Fock methods requires complexifying one's phase space, which is a bit confusing here since the phase space is already is given in terms of complex fields. We can however proceed to find the operator that generates the $U(1)$ symmetry as follows.

In terms of complex fields, the $SO(2)$ transformations on the pair ϕ_1, ϕ_2 of real fields become $U(1)$ phase transformations, with Q now given by

$$Q = -i \int_{\mathbf{R}^3} (\pi(\mathbf{x})\phi(\mathbf{x}) - \overline{\pi}(\mathbf{x})\overline{\phi}(\mathbf{x}))d^3\mathbf{x}$$

satisfying

$$\{Q, \phi(\mathbf{x})\} = i\phi(\mathbf{x}), \quad \{Q, \overline{\phi}(\mathbf{x})\} = -i\overline{\phi}(\mathbf{x})$$

Quantization of the classical field theory gives a representation of the infinite dimensional Heisenberg algebra with commutation relations

$$[\widehat{\phi}(\mathbf{x}), \widehat{\phi}(\mathbf{x}')] = [\widehat{\pi}(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = [\widehat{\phi}^\dagger(\mathbf{x}), \widehat{\phi}^\dagger(\mathbf{x}')] = [\widehat{\pi}^\dagger(\mathbf{x}), \widehat{\pi}^\dagger(\mathbf{x}')] = 0$$

$$[\widehat{\phi}(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = [\widehat{\phi}^\dagger(\mathbf{x}), \widehat{\pi}^\dagger(\mathbf{x}')] = i\delta^3(\mathbf{x} - \mathbf{x}')$$

Quantization of the quadratic functional Q of the fields is done with the normal-ordering prescription, to get

$$\widehat{Q} = -i \int_{\mathbf{R}^3} : (\widehat{\pi}(\mathbf{x})\widehat{\phi}(\mathbf{x}) - \widehat{\pi}^\dagger(\mathbf{x})\widehat{\phi}^\dagger(\mathbf{x})) : d^3\mathbf{x}$$

Taking $L = i$ as a basis element for $\mathfrak{u}(1)$, one gets a unitary representation U of $U(1)$ using

$$U'(L) = -i\widehat{Q}$$

and

$$U(\theta) = e^{-i\theta\widehat{Q}}$$

U acts by conjugation on the fields:

$$U(\theta)\widehat{\phi}U(\theta)^{-1} = e^{-i\theta}\widehat{\phi}, \quad U(\theta)\widehat{\phi}^\dagger U(\theta)^{-1} = e^{i\theta}\widehat{\phi}^\dagger$$

$$U(\theta)\widehat{\pi}U(\theta)^{-1} = e^{i\theta}\widehat{\pi}, \quad U(\theta)\widehat{\pi}^\dagger U(\theta)^{-1} = e^{-i\theta}\widehat{\pi}^\dagger$$

It will also give a representation of $U(1)$ on states, with the state space decomposing into sectors each labeled by the integer eigenvalue of the operator $\widehat{Q}$.

In the Bargmann-Fock quantization of this theory, we can express quantum fields now in terms of a different set of two annihilation and creation operators

$$a(\mathbf{p}) = \frac{1}{\sqrt{2}}(a_1(\mathbf{p}) + ia_2(\mathbf{p})), \quad a^\dagger(\mathbf{p}) = \frac{1}{\sqrt{2}}(a_1^\dagger(\mathbf{p}) - ia_2^\dagger(\mathbf{p}))$$

$$b(\mathbf{p}) = \frac{1}{\sqrt{2}}(a_1(\mathbf{p}) - ia_2(\mathbf{p})), \quad b^\dagger(\mathbf{p}) = \frac{1}{\sqrt{2}}(a_1^\dagger(\mathbf{p}) + ia_2^\dagger(\mathbf{p}))$$

The only non-zero commutation relations between these operators will be

$$[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}'), \quad [b(\mathbf{p}), b^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}')$$

so we see that we have, for each $\mathbf{p}$, two independent sets of standard annihilation and creation operators, which will act on a tensor product of two standard harmonic oscillator state spaces. The states created and annihilated by the $a^\dagger(\mathbf{p})$ and $a(\mathbf{p})$ operators will have an interpretation as particles of momentum $\mathbf{p}$, whereas those created and annihilated by the $b^\dagger(\mathbf{p})$ and $b(\mathbf{p})$ operators will be antiparticles of momentum $\mathbf{p}$. The vacuum state will satisfy

$$a(\mathbf{p})|0\rangle = b(\mathbf{p})|0\rangle = 0$$

Using these creation and annihilation operators, the definition of the complex field operators is

Definition (Complex scalar quantum field)**.** *The complex scalar quantum field operators are the operator-valued distributions defined by*

$$\widehat{\phi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (a(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} + b^\dagger(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

$$\widehat{\phi}^\dagger(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (b(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

$$\widehat{\pi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (-i\omega_{\mathbf{p}})(a(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} - b^\dagger(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

$$\widehat{\pi}^\dagger(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} (-i\omega_{\mathbf{p}})(b(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}} - a^\dagger(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}) \frac{d^3\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}$$

These operators provide a representation of the infinite-dimensional Heisenberg algebra given by the linear functions on the phase space of solutions to the complexified Klein-Gordon equation. This representation will be on a state space describing both particles and antiparticles. The commutation relations are

$$[\widehat{\phi}(\mathbf{x}), \widehat{\phi}(\mathbf{x}')] = [\widehat{\pi}(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = [\widehat{\phi}^\dagger(\mathbf{x}), \widehat{\phi}^\dagger(\mathbf{x}')] = [\widehat{\pi}^\dagger(\mathbf{x}), \widehat{\pi}^\dagger(\mathbf{x}')] = 0$$

$$[\widehat{\phi}^\dagger(\mathbf{x}), \widehat{\pi}(\mathbf{x}')] = [\widehat{\phi}(\mathbf{x}), \widehat{\pi}^\dagger(\mathbf{x}')] = i\delta^3(\mathbf{x} - \mathbf{x}')$$

The Hamiltonian operator will be

$$\begin{aligned}\widehat{H} &= \int_{\mathbf{R}^3} :(\widehat{\pi}^\dagger(\mathbf{x})\widehat{\pi}(\mathbf{x}) + (\nabla\widehat{\phi}^\dagger(\mathbf{x}))(\nabla\widehat{\phi}(\mathbf{x})) + m^2\widehat{\phi}^\dagger(\mathbf{x})\widehat{\phi}(\mathbf{x})): d^3\mathbf{x} \\ &= \int_{\mathbf{R}^3} \omega_{\mathbf{p}}(a^\dagger(\mathbf{p})a(\mathbf{p}) + b^\dagger(\mathbf{p})b(\mathbf{p}))d^3\mathbf{p}\end{aligned}$$

Note that the classical solutions to the Klein-Gordon equation have both positive and negative energy, but the quantization is chosen so that negative energy solutions correspond to antiparticle annihilation and creation operators, and all states of the quantum theory have non-negative energy.

41.2 Poincaré symmetry and scalar fields

Momentum and energy operators, angular momentum operators. Discuss action of Lorentz boosts.

The Poincaré group action on the coordinates $\widetilde{\phi}(p)$ on $\mathcal{H}_1$ will be given by

$$u(a,\Lambda)\widetilde{\phi}(p) = e^{-ipa}\widetilde{\phi}(\Lambda^{-1}p)$$

41.3 For further reading

Chapter 42

$U(1)$ Gauge Symmetry and Coupling to the Electromagnetic Field

We have now constructed both relativistic and non-relativistic quantum field theories for free scalar particles. In the non-relativistic case we had to use complex valued fields, and found that the theory came with an action of a $U(1)$ group, the group of phase transformations on the fields. In the relativistic case real-valued fields could be used, but if we took complex-valued ones (or used pairs of real-valued fields), again there was an action of a $U(1)$ group of phase transformations. This is the simplest example of a so-called "internal symmetry" and it is reflected in the existence of an operator Q called the "charge".

In this chapter we'll see to to go beyond the theory of free particles by introducing classical electromagnetic forces acting on quantized particles. We will see that this can be done using the $U(1)$ group action, with Q now having the interpetation of "electric charge": the strength of the coupling between the particle and the electric field. This requires a new sort of space-time dependent field, called the "vector potential", and by using this field one finds quantum theories with a large, infinite-dimensional group of symmetries, a group called the "gauge group". In this chapter we'll study this new symmetry and see how to use it and the vector potential to get quantum field theories describing particles interacting with electromagnetic fields. In the next chapter we'll go on to study the question of how to quantize the vector potential field, leading to a quantum field-theoretic description of photons.

42.1 $U(1)$ gauge symmetry

In sections 36.1.1 and 41.1 we saw that the existence of a $U(1)$ group action by overall phase transformations on the field values led to the existence of an

operator with certain commutation relations with the field operators, acting with integral eigenvalues on the space of states. Instead of just multiplying fields by a constant phase $e^{i\varphi}$, one can imagine multiplying by a phase that varies with the coordinates x, so

$$\psi(x) \to e^{i\varphi(x)}\psi(x)$$

(so φ will be a function, taking values in $\mathbf{R}/2\pi$). By doing this, we are making a huge group of transformations act on the theory. Elements of this group are called gauge transformations:

Definition (Gauge group)**.** *The group $\mathcal{G}$ of functions on $\mathbf{R}^4$ with values in the unit circle $U(1)$, with group law given by point-wise multiplication*

$$e^{i\varphi_1(\mathbf{x})} \cdot e^{i\varphi_2(\mathbf{x})} = e^{i(\varphi_1(\mathbf{x})+\varphi_2(\mathbf{x}))}$$

is called the $U(1)$ gauge group, or group of $U(1)$ gauge transformations.

This is an infinite-dimensional group, and new methods are needed to study its representations (although we will mainly be interested in invariant states, so just the trivial representation of the group).

Terms in the Hamiltonian that just involve $\overline{\psi}(\mathbf{x})\psi(\mathbf{x})$ will be invariant under the group $\mathcal{G}$, but terms with derivatives such as

$$|\nabla\psi|^2$$

will not, since when

$$\psi \to e^{i\varphi(x)}\psi(x)$$

one has the inhomogeneous behavior

$$\partial_\mu\psi(x) \to \partial_\mu(e^{i\varphi(x)}\psi(x)) = e^{i\varphi(x)}(i\partial_\mu\varphi(x) + \partial_\mu)\psi(x)$$

To deal with this problem, one introduces a new degree of freedom

Definition (Connection or vector potential)**.** *A $U(1)$ connection (mathematician's terminology) or vector potential (physicist's terminology) is a function A on space-time $\mathbf{R}^4$ taking values in $\mathbf{R}^4$, with its components denoted*

$$A_\mu(x)$$

and such that the gauge group $\mathcal{G}$ acts on the space of $U(1)$ connections by

$$A_\mu(x) \to A_\mu(x) + i\partial_\mu\varphi(x)$$

With this new object one can define a new sort of derivative which will have homogeneous transformation properties

Definition (Covariant derivative)**.** *Given a connection A, the associated covariant derivative in the μ direction is the operator*

$$(D_A)_\mu = \partial_\mu - iA_\mu(x)$$

Note that under a gauge tranformation, one has

$$(D_A)_\mu \psi \to e^{i\varphi(x)}(D_A)_\mu \psi$$

and terms in a Hamiltonian such as

$$\sum_{j=1}^{3}((D_A)_j\overline{\psi})((D_A)_j\psi)$$

will be invariant under the infinite-dimensional group $\mathcal{G}$.

Write out Hamiltonian version of Schrodinger and KG, coupled to a vector potential

Digression. *Explain the path-integral formalism, weighting of paths. Lagrangian form, just minimal coupling.*

42.2 Electric and magnetic fields

While the connection A is the fundamental geometrical quantity needed to construct theories with gauge symmetry, one often wants to work instead with quantities derived from A which describe the information contained in A that does not change when one acts by a gauge transformation. To a mathematician, this is the curvature of a connection, to a physicist, it is the field strengths derived from a vector potential.

Digression. *If one is familiar with differential forms, the definition of the curvature F of a connection A is most simply made by thinking of A as an element of $\Omega(\mathbf{R}^4)$, the space of 1-forms on space-time $\mathbf{R}^4$. Then the curvature of A is simply the 2-form $F = dA$, where d is the de Rham differential. The gauge group acts on connections by*

$$A \to A + d\varphi$$

The curvature or field strength of a vector potential is defined by:

Definition (Curvature or field strength)**.** *To a connection $A_\mu(x)$ one can associate the curvature*

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

This is a set of functions on $\mathbf{R}^4$ depending on two indices μ, ν that can each take values $0, 1, 2, 3$.

The 6 independent components of $F_{\mu\nu}$ are often written in terms of two vectors $\mathbf{E}, \mathbf{B}$ with components

$$E_j = -F_{0j} = -\frac{\partial A_j}{\partial t} + \frac{\partial A_0}{\partial x_j} \text{ or } \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} + \boldsymbol{\nabla} A_0$$

$$B_j = \epsilon_{jkl}(\frac{\partial A_l}{\partial x_k} - \frac{\partial A_k}{\partial x_l}) \text{ or } \mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$$

E *is called the electric field,* **B** *the magnetic field.*

42.3 The Pauli-Schrödinger equation in an electromagnetic field

The Pauli-Schrödinger equation (31.1) describes a free spin-half non-relativistic quantum particle. One can couple it to a vector potential by the "minimal coupling" prescription of replacing derivatives by covariant derivatives, with the result

$$i(\frac{\partial}{\partial t} - iA_0) \begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix} = -\frac{1}{2m}(\sigma \cdot (\boldsymbol{\nabla} - i\mathbf{A}))^2 \begin{pmatrix} \psi_1(\mathbf{q}) \\ \psi_2(\mathbf{q}) \end{pmatrix}$$

Give examples of an external magnetic field, and of a Coulomb potential.

42.4 Non-abelian gauge symmetry

42.5 For further reading

Chapter 43

Quantization of the Electromagnetic Field: the Photon

Understanding the classical field theory of coupled scalar fields and vector potentials is rather difficult, with the quantized theory even more so, due to the fact that the Hamiltonian is no longer quadratic in the field variables. If one simplifies the problem by ignoring the scalar fields and just considering the vector potentials, one does get a theory with quadratic Hamiltonian that can be readily understood and quantized. The classical equations of motion are the Maxwell equation in a vacuum, with solutions electromagnetic waves. The quantization will be a relativistic theory of free, massless particles of helicity ± 1, the photons.

To get a sensible, unitary theory of photons, one must take into account the infinite dimensional gauge group $\mathcal{G}$ that acts on the classical phase space of solutions to the Maxwell equations. We will see that there are various ways of doing this, each with its own subtleties.

43.1 Maxwell's equations

First using differential forms:

$$dF = 0, \quad d * F = 0$$

Then in components.

Show that gauge transform of a solution is a solution, gauge group acts on the solution space.

43.2 Hamiltonian formalism for electromagnetic fields

Equations in Hamiltonian form. Hamiltonian is $E^2 + B^2$.

First problem: data at fixed t does not give a unique solution. Deal with this by going to temporal gauge $A_0 = 0$.

Second problem: no Gauss's law. Have remaining symmetry under time-independent gauge transformations. Compute moment map for time-independent gauge transformation.

43.3 Quantization

Two general philosophies: impose constraints on states, or on the space one quantizes.

43.4 Field operators for the vector potential

Relate to the helicity one irreps of Poincare.

43.5 For further reading

Chapter 44

The Dirac Equation and Spin-1/2 Fields

The space of solutions to the Klein-Gordon equation gives an irreducible representation of the Poincaré group corresponding to a relativistic particle of mass m and spin zero. Elementary matter particles (quarks and leptons) are spin 1/2 particles, and we would like to have a relativistic wave equation that describes them, suitable for building a quantum field theory. This is provided by a remarkable construction that uses the Clifford algebra and its action on spinors to find a square root of the Klein-Gordon equation. The result, the Dirac equation, requires that our fields take not just real or complex values, but values in a spinor $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$ representation of the Lorentz group. In the massless case, the Dirac equation decouples into two separate Weyl equations, for left-handed ($(\frac{1}{2}, 0)$ representation of the Lorentz group) and right-handed ($(0, \frac{1}{2})$ representation) Weyl spinor fields. As with the scalar fields discussed earlier, for now we are just considering free quantum fields, which describe non-interacting particles. In following chapters we will see how to couple these fields to $U(1)$ gauge fields, allowing a description of electromagnetic particle interactions.

44.1 The Dirac and Weyl Equations

Recall from our discussion of supersymmetric quantum mechanics that we found that in n-dimensions the operator

$$\sum_{j=1}^{n} P_j^2$$

has a square root, given by

$$\sum_{j=1}^{n} \gamma_j P_j$$

where the γ_j are generators of the Clifford algebra Cliff(n). The same thing is true for Minkowski space, where one takes the Clifford algebra Cliff$(3,1)$ which is generated by elements $\gamma_0, \gamma_1, \gamma_2, \gamma_3$ satisfying

$$\gamma_0^2 = -1, \quad \gamma_1^2 = \gamma_2^2 = \gamma_3^2 = +1, \quad \gamma_j\gamma_k + \gamma_k\gamma_j = 0 \text{ for} j \neq k$$

which we have seen can be realized in various ways an an algebra of 4 by 4 matrices.

We have seen that $-P_0^2 + P_1^2 + P_2^2 + P_3^2$ is a Casimir operator for the Poincaré group, and that we get irreducible representations of the Poincaré group by using the condition that this acts as a scalar $-m^2$

$$-P_0^2 + P_1^2 + P_2^2 + P_3^2 = m^2$$

Using the Clifford algebra generators, we find that this Casimir operator has a square root

$$\pm(-\gamma_0 P_0 + \gamma_1 P_1 + \gamma_2 P_2 + \gamma_3 P_3)$$

so one could instead look for solutions to

$$\pm(-\gamma_0 P_0 + \gamma_1 P_1 + \gamma_2 P_2 + \gamma_3 P_3) = im$$

If the operators P_j continue to act on functions $\phi(x)$ on Minkowski space as $-i\frac{\partial}{\partial x_j}$, then this square root of the Casimir acts on the tensor product of the spinor space $S \simeq \mathbf{C}^4$ and a space of functions on Minkowski space. We will denote such objects by Ψ; they are $\mathbf{C}^4$-valued functions on Minkowski space. Taking the negative square root, we have

Definition (Dirac operator and the Dirac equation)**.** *The Dirac operator is the operator*

$$\not{D} = -\gamma_0\frac{\partial}{\partial x_0} + \gamma_1\frac{\partial}{\partial x_1} + \gamma_2\frac{\partial}{\partial x_2} + \gamma_3\frac{\partial}{\partial x_3}$$

and the Dirac equation is the equation

$$\not{D}\Psi = m\Psi$$

This rather simple looking equation contains an immense amount of non-trivial mathematics and physics, providing a spectacularly successful description of the behavior of physical elementary particles. Writing it more explicitly requires a choice of a specific representation of the γ_j as complex matrices, and we will use the chiral or Weyl representation, here written as 2 by 2 blocks

$$\gamma_0 = -i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \gamma_1 = -i\begin{pmatrix} 0 & \sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}, \gamma_2 = -i\begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix}, \gamma_3 = -i\begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix}$$

which act on

$$\Psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

(recall that using γ-matrices this way, ψ_L transforms under the Lorentz group as the S_L representation, ψ_R as the dual of the S_R representation).

The Dirac equation is then

$$\begin{pmatrix} 0 & (\frac{\partial}{\partial x_0} - \sigma \cdot \boldsymbol{\nabla}) \\ (\frac{\partial}{\partial x_0} + \sigma \cdot \boldsymbol{\nabla}) & 0 \end{pmatrix} \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = m \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

or, in components

$$(\frac{\partial}{\partial x_0} - \sigma \cdot \boldsymbol{\nabla})\psi_R = m\psi_L$$

$$(\frac{\partial}{\partial x_0} + \sigma \cdot \boldsymbol{\nabla})\psi_L = m\psi_R$$

In the case that $m = 0$, these equations decouple and we get

Definition (Weyl equations)**.** *The Weyl wave equations for two-component spinors are*

$$(\frac{\partial}{\partial x_0} - \sigma \cdot \boldsymbol{\nabla})\psi_R = 0, \quad (\frac{\partial}{\partial x_0} + \sigma \cdot \boldsymbol{\nabla})\psi_L = 0$$

To find solutions to these equations we Fourier transform, using

$$\psi(x_0, \mathbf{x}) = \frac{1}{(2\pi)^2} \int d^4p \; e^{i(-p_0 x_0 + \mathbf{p}\cdot\mathbf{x})} \tilde{\psi}(p_0, \mathbf{p})$$

and see that the Weyl equations are

$$(p_0 + \sigma \cdot \mathbf{p})\tilde{\psi}_R = 0$$

$$(p_0 - \sigma \cdot \mathbf{p})\tilde{\psi}_L = 0$$

Since

$$(p_0 + \sigma \cdot \mathbf{p})(p_0 - \sigma \cdot \mathbf{p}) = p_0^2 - (\sigma \cdot \mathbf{p})^2 = p_0^2 - |\mathbf{p}|^2$$

both $\tilde{\psi}_R$ and $\tilde{\psi}_L$ satisfy

$$(p_0^2 - |\mathbf{p}|^2)\tilde{\psi} = 0$$

so are functions with support on the positive ($p_0 = |\mathbf{p}|$) and negative ($p_0 = -|\mathbf{p}|$) energy null-cone. These are Fourier transforms of solutions to the massless Klein-Gordon equation

$$(-\frac{\partial^2}{\partial x_0^2} + \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2})\psi = 0$$

Recall that our general analysis of irreducible representations of the Poincaré group showed that we expected to find such representations by looking at functions on the positive and negative energy null-cones, with values in representations of $SO(2)$, the group of rotations preserving the vector $\mathbf{p}$. Acting on the spin-1/2 representation, the generator of this group is given by the following operator:

Definition (Helicity)**.** *The operator*

$$h = \frac{\sigma \cdot \mathbf{p}}{|\mathbf{p}|}$$

is called the helicity operator. It has eigenvalues $\pm\frac{1}{2}$*, and its eigenstates are said to have helicity* $\pm\frac{1}{2}$*. States with helicity* $+\frac{1}{2}$ *are called "left-handed", those with helicity* $-\frac{1}{2}$ *are called "right-handed".*

We see that a continuous basis of solutions to the Weyl equation for ψ_L is given by the positive energy ($p_0 = |\mathbf{p}|$) solutions

$$u_L(\mathbf{p})e^{i(-p_0x_0+\mathbf{p}\cdot\mathbf{x})}$$

where $u_L \in \mathbf{C}^2$ satisfies

$$hu_L = +\frac{1}{2}u_L$$

so the helicity is $+\frac{1}{2}$, and negative energy ($p_0 = -|\mathbf{p}|$) solutions

$$u_L(\mathbf{p})e^{i(-p_0x_0+\mathbf{p}\cdot\mathbf{x})}$$

with helicity $-\frac{1}{2}$. After quantization, this wave equation gives a field theory describing masslessleft-handed particles and right-handed antiparticles. The Weyl equation for ψ_R will give a description of massless right-handed particles and left-handed antiparticles.

Show Lorentz covariance.

Canonical formalism Hamiltonian, Lagrangian

Separate sub-sections for the Dirac and Majorana cases

44.2 Quantum Fields

Start by recalling fermionic harmonic oscillator

Write down expressions for the quantum fields in the various cases

44.3 Symmetries

Write down formulas for Poincaré and internal symmetry actions.

44.4 The propagator

44.5 For further reading

Maggiore

Chapter 45

An Introduction to the Standard Model

45.1 Non-Abelian gauge fields

Explain non-abelian case.
Note no longer quadratic.
Asymptotic freedom.
Why these groups and couplings?

45.2 Fundamental fermions

mention the possibility of a right-handed neutrino
$SO(10)$ spinor.
Problem, why these representations? Why three generations

45.3 Spontaneous symmetry breaking

Explain general idea with $U(1)$ case. Mention superconductors.
Higgs potential.
Mass terms. Kobayashi-Maskawa.

45.4 For further reading

Chapter 46

Further Topics

There's a long list of topics that should be covered in a quantum mechanics course that aren't discussed here due to lack of time in the class and lack of energy of the author. Two important ones are:

- Scattering theory. Here one studies solutions to Schrödinger's equation that in the far past and future correspond to free-particle solutions, with a localized interaction with a potential occuring at finite time. This is exactly the situation analyzed experimentally through the study of scattering processes. Use of the representation theory of the Euclidean group, the semi-direct product of rotations and translations in $\mathbf{R}^3$ provides insight into this problem and the various functions that occur, including spherical Bessel functions.

- Perturbation methods. Rarely can one find exact solutions to quantum mechanical problems, so one needs to have at hand an array of approximation techniques. The most important is perturbation theory, the study of how to construct series expansions about exact solutions. This technique can be applied to a wide variety of situations, as long as the system in question is not too dramatically of a different nature than one for which an exact solution exists.

More advanced topics where representation theory is important:

- Conformal geometry. For theories with massless particles, conformal group as extension of Poincaré group. Twistors.

- Infinite dimensional non-abelian groups: loop groups and affine Lie algebras, the Virasoro algebra. Conformal quantum field theories.

Appendix A

Conventions

I've attempted to stay close to the conventions used in the physics literature, leading to the choices listed here. Units have been chosen so that $\hbar = 1$.

To get from the self-adjoint operators used by physicists as generators of symmetries, multiply by $-i$ to get a skew-adjoint operator in a unitary representation of the Lie algebra, for example

- The Lie bracket on the space of functions on phase space M is given by the Poisson bracket, determined by

  $$\{q, p\} = 1$$

  Quantization takes $1, q, p$ to self-adjoint operators $\mathbf{1}, Q, P$. To make this a unitary representation of the Heisenberg Lie algebra $\mathfrak{h}_3$, multiply the self-adjoint operators by $-i$, so they satisfy

  $$[-iQ, -iP] = -i\mathbf{1}, \quad \text{or} \quad [Q, P] = i\mathbf{1}$$

  In other words, our quantization map is the unitary representation of $\mathfrak{h}_3$ that satisfies

  $$\Gamma'(q) = -iQ, \quad \Gamma'(p) = -iP, \quad \Gamma'(1) = -i\mathbf{1}$$

- The classical expressions for angular momentum quadratic in q_j, p_j, for example

  $$l_1 = q_2 p_3 - q_3 p_2$$

  under quantization go to the self-adjoint operator

  $$L_1 = Q_2 P_3 - Q_3 P_2$$

  and $-iL_1$ will be the skew-adjoint operator giving a unitary representation of the Lie algebra $\mathfrak{so}(3)$. The three such operators will satisfy the Lie bracket relations of $\mathfrak{so}(3)$, for instance

  $$[-iL_1, -iL_2] = -iL_3$$

For the spin $\frac{1}{2}$ representation, the self-adjoint operators are $S_j = \frac{\sigma_j}{2}$, the $X_j = -i\frac{\sigma_j}{2}$ give the Lie algebra representation. Unlike the integer spin representations, this representation does not come from the bosonic quantization map Γ.

Given a unitary Lie algebra representation $\pi'(X)$, the unitary group action on states is given by

$$|\psi\rangle \to \pi(e^{\theta X})|\psi\rangle = e^{\theta\pi'(X)}|\psi\rangle$$

Instead of considering the action on states, one can consider the action on operators by conjugation

$$\mathcal{O} \to \mathcal{O}(\theta) = e^{-\theta\pi'(X)}\mathcal{O}e^{\theta\pi'(X)}$$

or the infinitesimal version of this

$$\frac{d}{d\theta}\mathcal{O}(\theta) = [\mathcal{O}, \pi'(X)]$$

If a group G acts on a space M, the representation one gets on functions on M is given by

$$\pi(g)(f(x)) = f(g^{-1} \cdot x)$$

Examples include

- Space translation ($q \to q + a$). On states one has

  $$|\psi\rangle \to e^{-iaP}|\psi\rangle$$

  which in the Schrödinger representation is

  $$e^{-ia(-i\frac{d}{dq})}\psi(q) = e^{-a\frac{d}{dq}}\psi(q) = \psi(q - a)$$

  So, the Lie algebra action is given by the operator $-iP = -\frac{d}{dq}$. On operators one has

  $$\mathcal{O}(a) = e^{iaP}\mathcal{O}e^{-iaP}$$

  or infinitesimally

  $$\frac{d}{da}\mathcal{O}(a) = [\mathcal{O}, -iP]$$

- Time translation ($t \to t - a$). The convention for the Hamiltonian H is opposite that for the momentum P, with the Schrödinger equation saying that

  $$-iH = \frac{d}{dt}$$

  On states, time evolution is translation in the positive time direction, so states evolve as

  $$|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle$$

Operators in the Heisenberg picture satisfy

$$\mathcal{O}(t) = e^{itH}\mathcal{O}e^{-itH}$$

or infinitesimally

$$\frac{d}{dt}\mathcal{O}(t) = [\mathcal{O}, -iH]$$

which is the quantization of the Poisson bracket relation in Hamiltonian mechanics

$$\frac{d}{dt}f = \{f, h\}$$

Conventions for special relativity.

Conventions for representations on field operators.

Conventions for anticommuting variables. for unitary and odd super Lie algebra actions.

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