Spectral Decomposition of Quantum-Mechanical Operators

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Abstract

In this work, applications of the spectral theorem for self-adjoint operators in quantum mechanics are examined. While classical physics provides differential equations (in the form of Newton's laws) that describe deterministic evolution of phase space variables, quantum mechanics evolves the more abstract wavefunction, an element of the quantum Hilbert space. To find measurement probabilities for a phase space variable (an "observable"), the observable is identified with a self-adjoint operator on the corresponding Hilbert space. The spectral decomposition of the quantized operator gives information on the values possible for such an observable. Furthermore, the different parts of the spectrum of a quantum observable will be shown to correspond to different types of states, an idea which will be demonstrated with concrete examples. Finally, different formulations of the spectral theorem are explored, including the projection-valued measure and direct integral approach. These different formulations will yield further insights into physical understandings of quantum mechanical states.

1 A First Pass at Quantum

The early 1900's brought about a distinct revolution in our understanding of physics. Certain issues in small-scale thermal physics were becoming more apparent as the experiments and the theory became more precise. The total energy emitted by a black body radiator in the framework of classical theory was infinite, while observations guaranteed that the average iron rod was not, in fact, a source of infinite energy. Furthermore, the photoelectric effect, a phenomenon in which a metal subjected to certain frequencies of light would emit electrons, was not well-understood. It was thought at the time that these small problems were the last remaining questions to be answered in physics, but they would prove to be signs of a much greater misunderstanding of the physical world.

Planck's solution to the black-body problem was intriguing. He achieved finite predictions to black body energy radiation by assuming that the energy of the radiation came in discrete quantized packets of energy, $E = h\nu$, where h is Planck's constant, and ν is the frequency of the light emitted. While Planck used this method merely as a calculation tool, Einstein showed that such an assumption has a more physical interpretation.

The problem with the photoelectric effect was as follows: the electrons that eject from the metal have energy values that only depend on the *frequency*, not the intensity, of the light impinging on them. Furthermore, below a certain color frequency, no electrons would be emitted at all, regardless of intensity. In the classical theory, light is modeled as a continuous electromagnetic wave. In this model, the average power of a pure EM wave is given as

$$P_{avg} = \frac{Af}{2}$$

where A is the amplitude, and f is the frequency of the light. In this model, any frequency of light–given a high enough amplitude–can deliver enough energy to ionize the electrons in the metal. However, experiments showed that this was not the case. Below a certain frequency, electrons would not be ionized by the impinging light, regardless of intensity.

Einstein's solution to the problem was to assume that the energy delivered to the metal was not continuously delivered–it came in discrete quantized

packets he called photons with energy $E = h\nu$. In this interpretation, the intensity of light describes how many of these photons are emitted per second, and the frequency of the light describes the amount of energy contained in a single photon. The dynamics of the photoelectric effect are determined by the interactions of the individual photons with the metal. This explains why the frequency of light, not the intensity, dictated the energy of the electrons emitted.

Both Planck's black body solution and Einstein's photoelectric solution hint at a more complicated physical model than the classical theory described. As it turns out, these complications are more than just changes in the form of equations of motion: they require an entirely new mathematical system to describe the theory.

For more information on the experimental development of quantum mechanics, see [3, p. 1-16].

1.1 The Rules of Quantum Mechanics

In this section, we will introduce the basic rules that describe the mathematical system of quantum mechanics, as well as its connection to the physical world. To make things simple, only systems of a single particle will be considered. Rules one and two describe the objects that make up the theory, rules three and four describe how they behave to produce physical results, and rule five describes how these objects evolve in time. [3, p. 64]

Rule 1: The state of a quantum system is given by a unit vector (usually denoted ψ) in some Hilbert space $\mathbf{H}$. Furthermore, two unit vectors ψ_1 and ψ_2 are equivalent (in the sense that they represent the same physical state) iff $\psi_1 = c\psi_2$ for some $c \in \mathbb{C}$.

While the Hilbert space used will often change from system to system, it is usually taken to be L^2 on some appropriate domain. In the simple case of a particle moving in $\mathbb{R}^1$, for example, the Hilbert space associated with such a system is $L^2(\mathbb{R})$. Unit vectors in the Hilbert space are known as wavefunctions and multiplication by a complex scalar is known as a phase shift.

Rule 2: For each function f on the classical phase space there is associated a self-adjoint operator $\hat{f}$ on the quantum Hilbert space $\mathbf{H}$. Such an operator is known as a quantum observable.

The process of obtaining $\hat{f}$ from f is known as quantization. For the most part, it is not necessary to consider quantizations of all possible phase space functions, but only of a few key variables like position, momentum, and energy. While there are known methods for quantization of arbitrary functions, such methods are beyond the scope of current investigation (see [3, p.255-275] for a more complete discussion of quantization schemes). The key quantization results are those for position and momentum. For position, $\hat{x} = M_x$, the operator of multiplication by x. For momentum, $\hat{p} = -i\hbar\frac{d}{dx}$.

In most cases, the operator $\hat{f}$ will be unbounded. This arises from the fact that the position and momentum operators, which will be explored in detail in the next section, are themselves usually unbounded. For unbounded operators, the notion of self-adjointness becomes a bit more complicated, but will be explored in detail later on.

Rule 3: The probability distribution for the measurement of some observable $\hat{f}$ for a quantum state ψ satisfies

$$\langle f \rangle = \langle \psi, \hat{f}\psi \rangle$$

where $\langle f \rangle$ is the expectation value of f.

Finding the probability distribution for an observable is the main objective of a quantum mechanics problem, and is typically done with the linear algebra tools of diagonalization, or spectral decomposition.

Consider a specific state ψ_λ such that $\hat{f}\psi_\lambda = \lambda\psi_\lambda$. In this case, the expectation value of f is given as

$$\begin{aligned}\langle f \rangle &= \langle \psi_\lambda, \hat{f}\psi_\lambda \rangle \\ &= \langle \psi_\lambda, \lambda\psi_\lambda \rangle \\ &= \lambda\langle \psi_\lambda, \psi_\lambda \rangle \\ &= \lambda.\end{aligned}$$

As it turns out, the only probability distribution that satisfies these conditions is the δ distribution at λ. In other words, measurement of the variable

f on the state ψ_λ will always result in λ.

Ideally, one would find a complete set of such eigenstates. Then, each quantum state in the system could be expressed as a linear combination of eigenstates $\psi = \sum_n c_n \psi_{\lambda_n}$. The probability of measuring λ_n for the variable f would then be given as $|c_n|^2$. While this assertion is not directly derivable from the previous results [3, p. 67], it is a very reasonable assumption to make. Since ψ is a unit vector, $\sum |c_n|^2 = 1$, and the expectation value for f is readily seen to be consistent with this assumption.

Extending this method from the case of discrete eigenvalues to a continuous spectrum is possible, and will be extensively explored later in this paper.

Rule 4: Suppose ψ represents an initial state of a quantum system, and suppose a state variable f is measured to have a value $\lambda \in \mathbb{R}$. Then, immediately following the measurement, the system will be in a new state ψ' satisfying

$$\hat{f}\psi' = \lambda\psi'.$$

The transition of the wavefunction from ψ to ψ' is known as the collapse of the wavefunction. This rule makes intuitive sense: measuring a variable twice in rapid succession should yield very similar, if not identical, results. Collapse is frequently used to set up quantum mechanical systems. If one desires a wavefunction in a particular eigenstate ψ_λ of an observable f, one could construct and ensemble of identical systems, and measure f on each system until the measurement yields λ (for further discussion of such a setup, see [2]). For observables whose eigenstates are stationary in time, the wavefunction is then guaranteed to stay in the state ψ_λ.

Rule 5: The time evolution of a state ψ is governed by the Schrodinger equation:

$$\partial_t \psi = \frac{1}{i\hbar}\hat{H}\psi$$

where $\hat{H}$ is the observable obtained from the classical Hamiltonian of the system.

It is not difficult to see that this differential equation is solved with

$$\psi(t) = e^{\frac{-it\hat{H}}{\hbar}}\psi_0.$$

(For an exploration of this *operator valued exponential* , see [3, p. 74,208]). In the case that $\hat{H}$ has eigenfunctions e_n and eigenvalues E_n that form an orthonormal basis for $\mathbf{H}$, the exponential becomes

$$e^{\frac{-it\hat{H}}{\hbar}}e_n = e^{\frac{-iE_nt}{\hbar}}e_n$$

which extends linearly to arbitrary states

$$\psi = \sum_n c_n e_n$$
$$e^{\frac{-it\hat{H}}{\hbar}}\psi = \sum_n c_n e^{\frac{-iE_nt}{\hbar}}e_n.$$

Of course, it is unreasonable to expect $\hat{H}$, which is only guaranteed to be self-adjoint, to have an orthonormal basis of eigenfunctions. However, we will see that the spectral theorem gives a way to generalize the notion of eigenfunction such that we can define $e^{\frac{-it\hat{H}}{\hbar}}$ for any Hamiltonian.

The eigenvalues of $\hat{H}$ hold special significance in quantum mechanics, as they govern how the system evolves in time. Solving the Schrodinger equation, in light of this result, usually boils down to solving the time-independent Schrodinger equation

$$\hat{H}\psi = E\psi$$

or more generally, finding the spectral decomposition of $\hat{H}$.

1.2 An Example: The Infinite Square Well

The most pertinent difference between classical physics and quantum physics lies in the discretization of certain state variables of the system. To illustrate

this difference, consider the simple setup of a particle of mass m in a one-dimensional infinite square well potential

$$V(x) = \begin{cases} 0 & \text{if } x \in [0, a] \\ \infty & \text{else} \end{cases}$$

The relevant Hilbert space for this problem is $L^2(\mathbb{R})$, although the wavefunctions for this problem will be required to be zero outside $[0, a]$. The Hamiltonian for the system is the free particle Hamiltonian, given as

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

inside the well.

The standard quantization of kinetic energy uses the identity

$$KE = \frac{p^2}{2m}$$

which implies that

$$\widehat{KE} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

Since the Hamiltonian is the sum of the kinetic and potential energy of the particle, and the particle has no potential energy inside the well, it follows that the Hamiltonian is as we stated.

Our goal is to decompose an arbitrary state into eigenstates of this Hamiltonian. This will tell us the allowed energy values for the specified potential. To do so, let's set up the time-independent Schrodinger equation $\hat{H}\psi = E\psi$. This leads to the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$$

Solving this second order differential equation yields

$$\psi_E(x) = A\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) + B\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right).$$

Now, we can impose boundary conditions. By requiring that the wavefunction be zero at the ends of the well when the potential is infinite, the following conclusions can be made:

$$\begin{aligned} \psi(0) = 0 &\implies B = 0 \\ \psi(a) = 0 &\implies E = \tfrac{n^2\pi^2\hbar^2}{2ma^2} \end{aligned}$$

The condition on E gives us a characterization of the spectrum of $\hat{H}$.

Furthermore, the wavefunction is required to have unit length. This means

$$\langle \psi, \psi \rangle = 1$$

or

$$\int_{[0,a]} A \sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) \overline{A \sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)} dx = 1$$

which restricts A to the value of $\sqrt{\frac{2}{a}}$.

Thus, we have a complete characterization of the eigenstates of the Hamiltonian:

$$\psi_E(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

It is a standard result ([1, p. 89]) that such functions are dense in the solution space $L^2([0,a]) \subset L^2(\mathbb{R})$. So any wavefunction $\psi(x)$ can be written as

$$\psi(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

with coefficients given by

$$c_n = \int_{[0,a]} \psi(x) \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) dx$$

Furthermore, given an initial state $\Psi(x,0) = \psi(x)$, the full time-evolution solution to this potential is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n e^{\frac{-iE_n t}{\hbar}} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

with $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ for $n \in \mathbb{N}$.

Classically, one could imagine a particle in a box with any arbitrary kinetic energy. However, in quantum this is not the case. Notice how the allowed energy states are quantized: values like $E = \frac{17\pi^2\hbar^2}{2ma^2}$ do not show up in the spectrum of $\hat{H}$, so they will not be measured. The particle cannot have any arbitrary definite energy.

1.3 The Finite Square Well: Continuous vs Discrete Spectra

Consider a similar potential function, the finite square well

$$V(x) = \begin{cases} -V_0 & \text{if } x \in [-a, a] \\ 0 & \text{else} \end{cases}$$

for some positive potential height V_0.

This time, the Hamiltonian is piecewise defined as

$$\hat{H}(x) = \begin{cases} \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} - V_0 & \text{if } x \in [-a, a] \\ \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} & \text{else} \end{cases}$$

which will operate on the Hilbert space $L^2(\mathbb{R})$.

Again, our goal is to find the eigenfunctions (or a more general spectral decomposition) of this Hamiltonian on $L^2(\mathbb{R})$. The complicating factor here is the fact that the Hamiltonian is actually unbounded on $L^2(\mathbb{R})$. For example, there are many functions in $L^2(\mathbb{R})$ that do not have square-integrable second derivatives, so $\hat{H}$ cannot act on them. Therefore, it is necessary to impose stricter conditions on our solutions. Namely, ψ is required to be continuous with a continuous first derivative. Note that ψ may not have a defined second derivative at the points of discontinuity $x = a, x = -a$, but since this is a set of measure zero, the second derivative can still be computed in L^2 space.

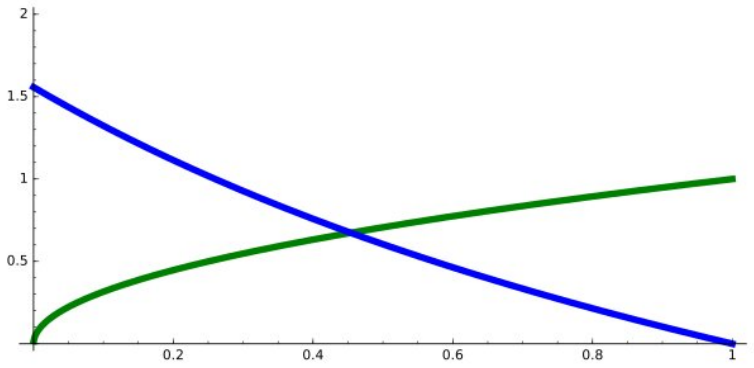

Figure 1: A plot of the functions $f(x) = \sqrt{x}$ and $g(x) = \sqrt{1-x}\tan(\sqrt{1-x})$. Their intersection point marks a solution to the transcendental equation $\sqrt{x} = \sqrt{1-x}\tan(\sqrt{1-x})$.

If we assume $E < 0$, we find that

$$\psi(x) = \begin{cases} C_1 e^{\sqrt{\epsilon}x} & \text{if } x \in (-\infty, -a] \\ C_2 \cos(\sqrt{v-\epsilon}) & \text{if } x \in [-a, a] \\ C_3 e^{-\sqrt{\epsilon}x} & \text{if } x \in [a, \infty) \end{cases}$$

Where $\epsilon = -\frac{2mE}{\hbar^2}$ and $v = \frac{2mV_0}{\hbar^2}$.

Applying the continuity conditions necessary for ψ to be in the domain of the Hamiltonian and applying some basic algebra, we find that

$$\sqrt{\epsilon} = \sqrt{v-\epsilon}\tan(\sqrt{v-\epsilon}a)$$

This equation is transcendental, so there are no closed-form solutions to ϵ, but the existence of solutions can be seen by graphing $\sqrt{\epsilon}$ and $\sqrt{v-\epsilon}\tan(\sqrt{v-\epsilon}a)$ (see [2, p. 78-80]). However, there are only finitely many ϵ for which this is true. That is, there are only finitely many energy states that are "bound" to the potential.

What if we restrict attention instead to the case $E > 0$? Applying a similar analysis to what was done in the infinite square well case, the solutions can be found to be linear combinations of complex exponentials. There is no inherent restriction on the energies allowed in this case, since there are

no boundary conditions to match. However, a single complex exponential $\psi(x) = e^{ikx}$ is not in $L^2(\mathbb{R})$, since the integral $\int_{\mathbb{R}} e^{ikx}\overline{e^{ikx}}dx$ diverges to infinity, and thus is not in the domain of the Hamiltonian.

While a single complex exponential may not be square-integrable, an infinite sum of them might be. Using some elementary results from Fourier analysis(see [6, Thm. 8.4.1]), it can be shown that the function

$$\psi(x) = \int_{\mathbb{R}} \phi(k)e^{ikx}dx$$

is square-integrable for ϕ a Schwartz function (a function that rapidly decays to zero).

In this sense, the state e^{ikx} is a sort of "pseudo-eigenstate". By itself, the state is not in $L^2(\mathbb{R})$, but a continuous sum of these states, which physicists refer to as a "wave packet", can be in $L^2(\mathbb{R})$. This concept will be made much more complete with the tools of the spectral theorem.

For a more detailed derivation of these results, see [3, p. 109-120] and [2, p. 78-82].

2 Hilbert Space Basics

In quantum mechanics, each system has an associated Hilbert space where the states live, and each observable has an associated (potentially unbounded) operator on that Hilbert space. It is necessary, then, to understand what Hilbert spaces are and how to work with them.

2.1 Hilbert Space Definitions

A *complex Hilbert space* $\mathbf{H}$ is a vector space over $\mathbb{C}$ along with an inner product such that $\mathbf{H}$ is complete with respect to the induced metric

$$d(x, y) = \langle x - y, x - y \rangle$$

[7, p. 8]

Here, $\mathbf{H}$ being complete means that every Cauchy sequence in $\mathbf{H}$ converges in $\mathbf{H}$. This condition is important, as it allows for limits to be taken without worry of accidentally leaving the space.

The requirement that the vector space be over $\mathbb{C}$ is not necessary for a general Hilbert space, but most Hilbert spaces encountered in quantum mechanics will be over $\mathbb{C}$.

Most familiar vector spaces are, in fact, Hilbert spaces. The familiar vector space $\mathbb{C}^n$ is a vector space over $\mathbb{C}$ that is complete with respect to its inner product, since $\mathbb{C}$ itself is complete, and the metric on $\mathbb{C}^n$ respects the standard metric on $\mathbb{C}$. However, a Hilbert space need not be finite dimensional.

Example 2.1.1 (L^2 as a Hilbert Space)**.** An important class of Hilbert spaces is the L^2 spaces of square integrable functions. Given a positive measure space (X, μ), let $L^2(X, \mu)$ be the collection of all equivalence classes of measurable functions $f : X \to \mathbb{C}$ that satisfy

$$\int_X |f|^2 d\mu < \infty$$

where $f \sim g$ if and only if $\int_X |f-g|^2 d\mu = 0$. As a consequence of this, changing f on a set of measure zero will not change its equivalence class.

To define an inner product on $L^2(X, \mu)$, we set

$$\langle f, g \rangle = \int_X f \overline{g} d\mu$$

For a more detailed construction of L^2 spaces, see [6, p. 181-185].

2.1.1 Orthonormal Bases

A natural way to express elements of a Hilbert space is in reference to a basis. Preferably, this basis should also reflect the inner product structure of the Hilbert space, and the most useful way to do so is by using an orthonormal basis.

An orthonormal set is a set $\mathscr{E}$ of vectors in a Hilbert space $\mathbf{H}$ where

- $\forall e \in \mathscr{E}, |e| = 1$
- $\forall e, f \in \mathscr{E}, \langle e, f \rangle = \delta_{ef}$

where δ_{ef} is the Kronecker Delta on e and f.

An orthonormal basis is defined as a maximal orthonormal set. A quick application of Zorn's lemma ([7, p. 19, 50]) shows that every Hilbert space has an orthonormal basis.

For an arbitrary vector ψ in $\mathbf{H}$ with ONB $\{e_n\}$, its ONB expansion in terms of $\{e_n\}$ is

$$\psi = \sum_{n=0}^{\infty} \langle \psi, e_n \rangle e_n$$

2.2 Hilbert Space Duality: Functionals and Representation

Every vector space V has a corresponding dual space of linear functionals on V, denoted V^*. This is the space of all linear functions $\phi : V \to \mathbb{R}$. In the case of a vector space with norms, it is additionally required that the function be bounded with respect to the norm

$$||\phi|| = \sup_{x \in V} \{|\phi(x)| : |x| \leq 1\}$$

When studying Hilbert spaces, it is important to understand the structure of its dual space. To that end, the Riesz representation theorem will give an easy way to understand the dual space of a Hilbert space in terms of the Hilbert space itself.

Theorem 2.2.1 (Riesz Representation)**.** *Any linear functional on a Hilbert space* $\boldsymbol{H}$ *is given by an inner product with a unique fixed vector* $h_0 \in \boldsymbol{H}$ *:* $\phi(x) = \langle h_0, x \rangle$*, and the norm of the functional is* $||h_0||$*.*

[7, p. 17]

In other words, there is an isometric isomorphism between H and H^*. Because of this, Hilbert spaces are said to be *self-dual*.

2.3 Operators on a Hilbert Space

For any pair X and Y of Hilbert spaces, there is another normed vector space that is of great importance: the space of bounded linear operators from X to Y. For an operator $T : X \to Y$ to be linear, it must satisfy

$$T(\alpha x_1 + \beta x_2) = \alpha T(x_1) + \beta T(x_2)$$

for vectors x_1, x_2 and scalars α, β. Furthermore, for T to be bounded, there must exist some positive constant C such that

$$||T(x)||_Y \leq C||x||_X$$

Bounded linear operators are a natural generalization of the matrix operators seen in a linear algebra course, but also include many other useful operators, such as integral operators, multiplication operators, and other such linear objects. (See [7, p. 32-34] for more examples).

Example 2.3.1. Consider a matrix $M \in \mathbb{R}^{n\times m}$ as a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$ defined as $M(x) = Mx$. This is a bounded linear operator from $\mathbb{R}^n$ to $\mathbb{R}^m$. Linearity is obvious from the definition of matrix multiplication, since $M(x+y) = Mx + My$. Furthermore, the matrix is also bounded, since $\forall x \in X$ we have

$$||Mx|| \leq ||M||||x||$$

where the vector norm is the standard Euclidean norm, and the matrix norm is the induced norm, which is guaranteed to be finite.

Example 2.3.2. Consider the operator $T : L^2([0,1]) \to L^2([0,1])$ given by $Tf(x) = \int_0^x f(y)dy$. This operator is easily seen to be both bounded and linear. More generally, given a measurable function $k : X \times X \to \mathbb{C}$ on a measure space (X, μ), the *integral operator*

$$\int_X k(x,y)f(y)d\mu(y)$$

from $L^2(X)$ to itself is a bounded linear operator. Thus, the familiar integral operator from differential equations is just a special case of a bounded linear operator on some Hilbert space.

Example 2.3.3. The derivative operator $\frac{d}{dx}$ on $L^2([0,1])$ is a linear operator, since

$$\frac{d}{dx}(\alpha f + \beta g) = \alpha\frac{df}{dx} + \beta\frac{dg}{dx}.$$

However, this operator is not bounded. In fact, it's only defined on a (dense) subset of $L^2([0,1])$, the space of differentiable functions with a square-integrable derivative. For a detailed treatment of this operator, see [3, p. 127-128, Ch. 9].

2.4 Adjoints of Operators

Given a Hilbert space, there is a natural symmetry present in the inner product. For a bounded operator A from a Hilbert space $\mathbf{H}$ to itself, we

define the *adjoint of* A to be the unique bounded operator A^* such that, $\forall x, y \in \mathbf{H}$,

$$\langle Ax, y\rangle = \langle x, A^* y\rangle$$

Such a unique bounded operator is guaranteed to exist as a consequence of Riesz Representation (see [7, Thm. 2.12]). In the case of $A = A^*$, the operator is said to be *self-adjoint*, and in the case of $AA^* = A^*A$, the operator is said to be *normal*. The condition of normality is a powerful property, and will be the condition necessary for an operator to satisfy the spectral theorem. Furthermore, we have already seen that every quantum observable is self-adjoint, and thus is normal. The rest of this paper will focus on normal operators.

3 Spectral Analysis of Linear Operators

In finite dimensional linear algebra, diagonalization is a powerful tool used to understand linear operators. One of the key results in linear algebra is the spectral theorem, which gives a method of diagonalizing a matrix in terms of its eigenvalues and eigenvectors. Since the study of quantum mechanics focuses on finding eigenvalues of the quantized linear operators, it is natural to ask whether or not the spectral theorem still holds in the infinite-dimensional case. While infinite dimensionality introduces some difficulties, there are a few equivalent statements of the spectral theorem that work in infinite dimensions, and each will provide further insight into the nature of the "eigenvalues" of linear operators.

3.1 The Spectrum of an Operator

In finite dimensions, the *spectrum* of a matrix is the set of eigenvalues associated to that matrix. That is, for a matrix $A \in \mathbb{R}^{n\times n}$, the spectrum of A is given as

$$\sigma(A) = \{\lambda \in \mathbb{C} : Ax = \lambda x \text{ for some } x \in \mathbb{R}^n\}$$

Another way of restating this is that $\sigma(A)$ is the set of all (complex) scalars λ such that the matrix $A - \lambda I$ has nontrivial kernel.

Of course, in finite dimensions, having a nontrivial kernel is equivalent to being noninvertible, so the spectrum of a matrix A is best described as the set of all λ such that $A - \lambda I$ is not invertible. By defining the spectrum in terms of invertibility, it is easy to extend the concept to arbitrary Hilbert spaces.

For a general operator $T \in \mathscr{B}(H)$ (where $\mathscr{B}(H)$ is the set of bounded linear operators on a Hilbert space $\mathbf{H}$), it is best to define the *spectrum* of the operator as

$$\sigma(T) = \{\lambda \in \mathbb{C} : T - \lambda I \text{ is not invertible}\}$$

It is easy to see that this definition coincides with the usual definition in

finite dimensions, but in an infinite dimensional Hilbert space, things might be more complicated.

The problem lies in the fact that there are more ways to fail invertibility in infinite dimensions than just having nontrivial kernel. There are three general ways to fail invertibility in a Hilbert space, and each failure will lead to a different subclassification of the spectrum. The subclassifications of the spectrum will be called the spectral partitions of $\sigma(T)$.

The spectral partitions are as follows ([7, p. 115]):

1. $T - \lambda I$ has nontrivial kernel (the *point spectrum*).
2. $T - \lambda I$ is not bounded below (the *approximate point spectrum*).
3. $T - \lambda I$ does not have dense range (the *compression spectrum*).

Let's consider each of these cases individually.

3.1.1 The Point Spectrum

The *point spectrum* is all λ such that $T - \lambda I$ has a nontrivial kernel. More succinctly, $\lambda \in \sigma_P(T)$ if and only if there exists some vector $x \in \mathbf{H}$ such that $(T - \lambda I)x = 0$, or $Tx = \lambda x$. This is the familiar eigenvalue equation seen in an introductory linear algebra course, and leads to the conclusion that for any linear operator on a finite dimensional Hilbert space (like $\mathbb{C}^n$), the spectrum of the operator is entirely a point spectrum.

Example 3.1.1. Consider the matrix

$$M = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \lambda_n \end{bmatrix}$$

This has eigenvalues λ_n, and thus its spectrum is

$$\sigma(M) = \sigma_P(M) = \{\lambda_n\}$$

3.1.2 The Approximate Point Spectrum

The point spectrum is actually a subset of the larger *approximate point spectrum* , which consists of all λ such that the operator $T - \lambda I$ is not bounded below. That is, $\lambda \in \sigma_{AP}(T)$ if and only if there exists some sequence of unit vectors $\{h_n : h_n \in \mathbf{H}\}$ for which

$$||(T - \lambda I)h_n|| \to 0.$$

The vectors h_n are commonly referred to as "approximate eigenvectors".

It is easy to see that if $\lambda \in \sigma_P(T)$, then $\lambda \in \sigma_{AP}(T)$, since one can take for h_n the constant sequence of the eigenvector corresponding to λ. Then, $||(T - \lambda I)h_n|| = 0$ and $\lambda \in \sigma_{AP}(T)$.

Because of this, it is convenient to define the *strict approximate point spectrum* σ_{SAP} to be $\sigma_{AP} \setminus \sigma_P$.

3.1.3 The Compression Spectrum

If $T - \lambda I$ fails to have dense range, λ is said to be part of the *compression spectrum* of T. This part of the spectrum will not be explored further: the following theorem will motivate why.

Theorem 3.1.1. *For a normal operator T, the spectrum of T is entirely approximate point spectrum.*

Proof. Let λ be in $\sigma(T)$ for a normal operator T, and consider the ways in which $T - \lambda I$ can fail to be invertible.

If the kernel of $T-\lambda I$ is nontrivial, then $\lambda \in \sigma_P(T)$, and thus $\lambda \in \sigma_{AP}(T)$.

Consider, then, the case where the kernel of $T - \lambda I = \{0\}$. Now, since $||Ax|| = ||A^*x||$ for any normal operator (see [7, prop. 2.14]), $||(T-\lambda I)x|| = ||(T^* - \overline{\lambda} I)x|| \neq 0$, so the kernel of $T^* - \overline{\lambda} I$ is trivial as well. By the Fredholm alternative ([8, p. 350]),

$$\overline{\mathrm{Ran}(T - \lambda I)} = \mathrm{Ker}(T^* - \overline{\lambda} I)^{\perp} = \{0\}^{\perp} = \mathbf{H}$$

And thus the range of $T - \lambda I$ is dense, and λ is not in the compression spectrum of T. $\square$

All that being said, there are easy examples of operators with a compression spectrum.

Example 3.1.2. Consider the Hilbert space $l^2(\mathbb{R})$, the space of square-summable sequences. Sequences in this space are commonly represented as "infinite tuples" of the form $(a_1, a_2, \ldots)$. The right shift operator U, defined as

$$U((a_1, a_2, \ldots)) = (0, a_1, a_2, \ldots)$$

is a bounded linear operator on $l^2(\mathbb{R})$. Furthermore, the operator $U - 0I = U$ does not have dense range: it misses the entire dimension spanned by $(1, 0, 0, \ldots)$. Thus, $0 \in \sigma_C(U)$.

For more examples of operators and their spectra, see [5, Ch. 6.5].

4 The Spectral Theorem

Normal operators are quite special. We've already seen that a normal operator will only have an approximate point spectrum, but a far more important result–the spectral theorem–will better characterize the spectrum of a normal operator. The spectral theorem will also give a very useful way of understanding and computing with normal operators by expressing them as multiplication operators. In this section, different formulations of the spectral theorem will be explored, with the goal of understanding more concretely the relationship between a normal operator and its spectrum.

4.1 Spectral Theorem: The Finite Case

The computational technique of matrix diagonalization is a very powerful tool for working with matrices, since a diagonal matrix is much easier to compute with. Diagonal matrices commute with each other, since multiplication of diagonal matrices corresponds to entrywise multiplication. Furthermore, the matrix exponential e^D corresponds to exponentiation of each entry. Unfortunately, not every matrix is diagonalizable.

Normal matrices are somewhat unique: the additional condition of normality gives a somewhat surprising characterization of their diagonalization. This characterization is stated in the *spectral theorem* for normal matrices.

Theorem 4.1.1 (The Spectral Theorem in Finite Dimensions)**.** *Every normal matrix $A \in \mathbb{C}^{n\times n}$ is unitarily equivalent to a diagonal matrix. That is,*

$$A = UDU*$$

for a unitary matrix U and a diagonal matrix D. Furthermore, the columns of U are the eigenvectors of A, and the components of D are the corresponding eigenvalues.

Proofs of this theorem are standard in any introductory linear algebra text, and the generalized proof for *compact* operators can be found in [6, Ch. 17.3] or [7, p. 91].

Recall that a unitary matrix U is an invertible matrix that satisfies $U^*U = UU^* = I$. Unitary matrices are precisely the invertible matrices that preserve inner products ([7, p. 39-40]).

Theorem 4.1.2. *Let $U : T \to V$ be a unitary transformation. Then, $\langle Ux, Uy\rangle = \langle x, y\rangle$.*

Thus, unitary matrices are isometric isomorphisms, which are the isomorphisms in the category of inner product spaces. In finite dimensions, a unitary matrix corresponds to an orthonormal change of basis, where the columns of the unitary matrix are the new basis vectors.

In light of this understanding of unitary matrices, another way of stating the spectral theorem is as follows: any normal matrix A has a set of eigenvectors that form an orthonormal basis for the space it operates on.

Since the matrix A corresponds to multiplication by an eigenvalue on the corresponding eigenspace, the spectral theorem can again be restated:

Theorem 4.1.3 (The Spectral Theorem in Finite Dimensions: Projection Version)**.** *Every normal matrix $A \in \mathbb{C}^{n\times n}$ is expressible as*

$$A(x) = \sum_{i=1}^{n} \lambda_i \langle x, e_i\rangle e_i$$

where λ_i is an eigenvalue, and e_i is the associated eigenvector. Furthermore, the collection $\{e_i\}$ forms an orthonormal set.

If $\lambda_i\langle x, e_i\rangle e_i$ is interpreted as a projection onto the subspace spanned by e_i, the spectral theorem looks like

$$A = \sum_{i=1}^{n} \lambda_i P_i$$

Where P_i is projection onto the subspace spanned by the eigenvectors associated with λ_i. In particular, the projections are all orthogonal to each other: $P_i \circ P_j = 0$ if $i \neq j$.

Note that in the case where an eigenvalue is repeated ($\lambda_i = \lambda_j$ for some $i \neq j$), the eigenspace is multidimensional, and one can apply Grahm-Schmidt

orthonormalization to obtain an orthonormal basis of eigenvectors $\{e_i\}$ for that eigenvalue. Taking this into consideration, the spectral theorem still works with repeated eigenvalues.

The spectral theorem for matrices can be interpreted in two ways. First, it says that a normal matrix is isometrically isomorphic to a diagonal matrix. That is, normal matrices correspond to multiplication on some isomorphic space to the space they operate on. This makes some amount of sense; normality is a condition based on commutativity, and scalar multiplication is inherently commutative.

Second, a normal matrix can be expressed as a linear combination of mutually orthogonal projection operators. This formulation respects the invariance of the eigenspaces of A. In particular, if A is applied to a vector already in an eigenspace, the vector stays in that eigenspace. The projections that make up A characterize the invariant subspaces of A, and the spectral theorem says that A on each of these subspaces is just multiplication by a (possibly different) scalar.

4.2 Spectral Theorem: Extending to the Infinite Case

As is the theme of Hilbert spaces, extending familiar results to infinite dimensions will cause problems. It's somewhat surprising, then, that the spectral theorem even holds at all in infinite dimensions. One of the biggest differences between finite and infinite dimensional Hilbert spaces is one we've already seen. The spectrum of a finite operator is always a collection of disjoint points, whereas the spectrum of an infinite operator may have infinitely many points, and could even be continuous!

Following the pattern from the finite dimensional spectral theorem statements, there are two equivalent ways of stating the spectral theorem in general. One version creates a Hilbert space for a normal operator where the operator is isomorphic to multiplication, and the other version will express a normal operator as an integral of projections.

4.2.1 Projection-valued Measures and the Projection-valued Integral

The projection-valued measure approach to the spectral theorem utilizes a bit of measure theory in building a certain type of integral. Measure theory is the cornerstone of Lebesgue integration, and gives a rigorous way to construct integrals on more arbitrary spaces.

A *measure* μ on a space X is a function from certain subsets of X to the positive real numbers (and possibly infinity) that satisfies

- $\mu(\emptyset) = 0$
- $\mu(\bigcup_i = 1^{infty} A_i) = \sum_{i=1}^{\infty}$ for mutually disjoint sets A_i

Intuitively, a measure assigns to subsets their "weight". Thus, the weight of the empty set is zero, and the weight of a countable union of disjoint sets is the sum of their individual weights.

Integration on a measure space is first defined for characteristic functions $\chi_S(x)$ defined as

$$\chi_S(x) = \begin{cases} 1, & \text{if } x \in S \\ 0 & \text{else} \end{cases}$$

The *Lebesgue integral* on a measure space X is defined as the integral for which

$$\int_X \chi_S d\mu = \mu(S)$$

Then, functions on X are approximated by sums of characteristic functions, and with appropriate limits taken, a full integral can be defined.

Example 4.2.1. $X = \mathbb{R}$, and $d\mu = dx$ leads to the standard measure on the real number line: $\mu([a, b]) = b - a$. Here, the integral is the standard integral

$$\int_{\mathbb{R}} f(x)dx$$

Example 4.2.2. $X = \mathbb{N}$, and $d\mu$ is the counting (δ) measure $\mu(S) = |S|$ leads to the integral

$$\int_{\mathbb{N}} f(n)d\mu = \sum_{i=1}^{\infty} f(n)$$

which is just familiar summation of sequences.

Further study of measure theory can be found in any graduate analysis text, such as [6].

This idea of measures can be extended. In the spectral theorem, associated with each point in the spectrum was a projection onto a subspace of the Hilbert space; that is, there was a function from subsets of the spectrum to projection operators on the Hilbert space. This observation leads to the definition of a *projection-valued measure* ([7, Ch. 6.2]).

Definition 4.2.1. A *projection-valued measure* E on a space X is a function from subsets of X to the set of orthogonal projections on a Hilbert space $\mathbf{H}$ such that

- $E(\emptyset) = 0$ and $E(X) = I$
- For disjoint subsets A and B, $E(A)(\mathbf{H}) \perp E(B)(\mathbf{H})$
- For a sequence $\{S_i\}_{i=1}^{\infty}$ of disjoint subsets, $\sum_{i=1}^{n} E(S_i)h \to E(\cup_i S_i)h$ for each $h \in \mathbf{H}$.

Using this definition of a measure, a projection-valued integral can be constructed. In a similar way to regular Lebesgue integration, the integral is defined first on characteristic functions

$$\int_X \chi_S dE = E(S)$$

and then is extended to more arbitrary functions via limits. With this definition of a projection-valued integral, we are ready to explore the first restatement of the spectral theorem.

Theorem 4.2.1 (The Spectral Theorem: Projection-Valued Integral)**.** *Let A be a normal operator on a Hilbert space $\boldsymbol{H}$, and let $\sigma(A)$ denote the spectrum of A. Then, there exists a unique projection-valued measure on $\sigma(A)$ such that*

$$A = \int_{\sigma(A)} z dE(z)$$

For a proof of this, see [7, Ch. 6].

Of course, the difficulty will come in constructing the projection-valued measure, but one is always guaranteed to exist.

To better understand this result, consider the case where $\mathbf{H}$ is finite-dimensional.

Example 4.2.3. Let $M = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \lambda_n \end{bmatrix}$

Then, the spectral measure $E(S)$ is the δ-measure on $\sigma(M)$ with $E(\lambda_i) = P_{\lambda_i}$, and the spectral theorem states that

$$M = \int_{\sigma(M)=\{\lambda_i\}} z dE(z) = \sum_{i=1}^{n} \lambda_i P_{\lambda_i}$$

which is a restatement of the familiar spectral theorem.

For discrete points in a point spectrum, the projection-valued measure just assigns each eigenvalue a projection onto its eigenspace. In a similar way to how the counting measure worked on $\mathbb{N}$, the counting measure on $\sigma_P(M)$ converted the integral into a familiar sum. This correspondence is what motivates the projection-valued measure approach to the spectral theorem. The simplest way to take a sum over a continuous interval is by converting it to an integral.

Let's consider a more difficult example.

Example 4.2.4. Let M_x be the familiar multiplication operator on $L^2([0,1], dx)$. It is easy to show that $\sigma(M_x) = \sigma_{AP}(M_x) = [0,1]$. If λ is not in $[0,1]$, then the operator of multiplication by $\frac{1}{x-\lambda}$ inverts $(M_x - \lambda I)$, and thus λ is not in $\sigma(M_x)$.

The spectral measure $E(S)$ for an interval S is given as M_{χ_S} for χ_S the characteristic function on S. That is, a projection in this space is multiplication by a characteristic function.

See [7, Ex. 6.11] for more details on the construction of this spectral measure.

4.2.2 The Direct Integral

Recall the alternative definition of the spectral theorem, which stated that every normal matrix is isometrically isomorphic to a multiplication operator. Here, the infinite-dimensional pathologies will come into play in defining the space on which a normal operator is isometrically isomorphic to multiplication.

To begin with, we define an additional structure on a collection of Hilbert spaces. For a measure space (X, μ), let $\{\mathbf{H}_\lambda\}_{\lambda \in X}$ be a collection of Hilbert spaces, one for each point λ in X. Define a *section* of the collection to be a function s from X to the collection of Hilbert spaces such that $s(\lambda) \in \mathbf{H}_\lambda$. In essence, s picks out one vector from each $\mathbf{H}_\lambda$. Furthermore, we can give the set of all such sections an inner product structure by defining

$$\langle s_1, s_2 \rangle = \int_X \langle s_1(\lambda), s_2(\lambda) \rangle d\mu(\lambda)$$

Finally, we define the *direct integral* of a collection of Hilbert spaces $\{\mathbf{H}_\lambda\}$ to be the inner product space of (equivalence classes of) sections on $\{\mathbf{H}_\lambda\}$, denoted

$$\int_X^\oplus H_\lambda d\mu(\lambda)$$

It is easily shown ([3, Ch. 7.3]) that this new space is complete, and thus is a Hilbert space.

Example 4.2.5. Let X be a measure space, and let $H_\lambda = \mathbb{C}$ for all $\lambda \in X$. Then,

$$\int_X^\oplus H_\lambda d\mu(\lambda) = L^2(X)$$

Example 4.2.6. Let $X = \{a_1, a_2, \ldots, a_n\}$ with the counting measure. Then

$$\int_X^\oplus H_{a_i} d\mu(a_i) = \oplus_{i=1}^n H_{a_i}.$$

That is, the counting measure again reduces integration to a familiar sum

The spectral theorem can now be stated.

Theorem 4.2.2 (The Spectral Theorem: Direct Integral)**.** *Given a normal operator A on a Hilbert space, there exists a measure μ on the spectrum $\sigma(A)$ of A, and Hilbert spaces H_λ for $\lambda \in \sigma(A)$ such that A is unitarily equivalent to multiplication on the direct integral*

$$\int_{\sigma(M)}^{\oplus} H_\lambda d\mu(\lambda).$$

That is, $(UAU^*)s(\lambda) = \lambda s(\lambda)$ for s in the direct integral.

The spaces H_λ in general will not be subspaces of the original Hilbert space, but instead will represent more generalized eigenspaces of the operator A. However, in the case of finite dimensions, each H_λ is a subspace, and the original spectral theorem is recovered.

Example 4.2.7. Let M be a normal matrix with distinct eigenvalues. Then, let μ be the counting measure on $\sigma(A)$, and let H_λ be the one-dimensional eigenspace associated with the eigenvalue λ. Then, the direct integral becomes

$$\int_{\sigma(M)}^{\oplus} H_\lambda d\mu(\lambda) = \oplus_{i=1}^{n} H_{\lambda_i}$$

and the spectral theorem states that M is unitarily equivalent to multiplication on each subspace. In other words, M is unitarily equivalent to a diagonal matrix.

5 Quantum Revisited

With the new tools of the spectral theorem, we can now better understand the more subtle intricacies of quantum mechanics. Recall that one of the rules of quantum mechanics gives a way of computing a probability distribution for an observable from its spectrum. Specifically, a consequence of rule 3 is that the possible values an observable can take coincide with the spectrum of the observable. Furthermore, the relative probabilities of each value are given by the length of the projections of a state onto the "eigenspace" of that value. However, it was clear in the finite square well example that some parts of the spectrum may not have actual eigenspaces. The spectral theorem gives a way to better understand what the general projections and invariant spaces look like for these more complicated operators.

5.1 The Finite Square Well Revisited

Let's reconsider the finite square well potential in quantum mechanics. Recall that the relevant Hilbert space for this problem is $L^2(\mathbb{R})$, and the Hamiltonian operator is of the form

$$\hat{H}(x) = \begin{cases} \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} - V_0 & \text{if } x \in [-a, a] \\ \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} & \text{else} \end{cases}$$

The Hamiltonian can be shown to have a spectrum that looks like

$$\sigma(\hat{H}) = \{E_1, E_2, \ldots, E_n\} \cup (0, \infty)$$

Explicit, square-integrable functions could be found that lie in the kernel of $\hat{H} - EI$ for $E < 0$, which are of the form

$$\psi(x) = \begin{cases} C_1 e^{\sqrt{\epsilon}x} & \text{if } x \in (-\infty, -a] \\ C_2 \cos(\sqrt{v - \epsilon}) & \text{if } x \in [-a, a] \\ C_3 e^{-\sqrt{\epsilon}x} & \text{if } x \in [a, \infty) \end{cases}$$

where $\epsilon = -\frac{2mE}{\hbar^2}$ and $v = \frac{2mV_0}{\hbar^2}$, and C_1, C_2, and C_3 were constants set to normalize ψ. Since such eigenfunctions exist, the points E_n where $E_n < 0$ are part of the point spectrum $\sigma_P(\hat{H})$.

Showing that $(0, \infty)$ is in the spectrum of $\hat{H}$ requires a bit more work. In our first attempt at finding the eigenfunctions for $E > 0$, we saw that the only solutions for the eigenvalue equation $\hat{H}\psi = E\psi$ were complex exponentials of the form $e^{\pm ikx}$ for $k = \frac{\sqrt{2mE}}{\hbar}$. Since these solutions are not in $L^2(\mathbb{R})$, they do not lie in the kernel of $\hat{H} - EI$, and are not sufficient to show that E is a part of the spectrum of $\hat{H}$. However, the point spectrum is not the only spectral partition available to us. It may be the case that E is in the approximate point spectrum of $\hat{H}$ without being in the point spectrum. As it turns out, this is the case.

Theorem 5.1.1. *For all $E > 0$, $E \in \sigma_{SAP}(\hat{H})$, where $\hat{H}$ is the Hamiltonian for the finite square well acting on the Hilbert space $L^2(\mathbb{R})$.*

Proof. Fix $E > 0$, and let f_n be a C^∞ function on $\mathbb{R}$ such that

$$f_n(x) = \begin{cases} 1 & x \in (-n, n) \\ 0 & x \notin (-(n+1), n+1) \end{cases}$$

For the intervals $(-(n+1), -n)$ and $(n, n+1)$, f will smoothly increase/decrease in such a way that the entire function is C^∞. The existence of such smooth functions with compact support can be found in [6, p.299-300]. Then, let $\psi_n(x) = \frac{e^{ikx} f_n(x)}{||e^{ikx} f_n(x)||}$ for $k = \frac{\sqrt{2mE}}{\hbar}$. This defines a sequence of unit length states for which it can be shown that

$$||(\hat{H} - EI)\psi_n(x)|| \to 0$$

Thus, the operator $\hat{H} - EI$ is not bounded below, and $E \in \sigma_{AP}(\hat{H})$. Since $E \notin \sigma_P(\hat{H})$, this implies that $E \in \sigma_{SAP}(\hat{H})$ as desired. □

We find that the spectrum of $\hat{H}$ is made up of finitely many isolated points E_n below zero (the point spectrum of $\hat{H}$, and the entire positive real number line (the approximate point spectrum of $\hat{H}$).

Constructing the projection-valued measure for this operator is fairly straightforward, using the results of the previous analysis. For simplicity, E will represent an energy (an element of the spectrum of $\hat{H}$), and F will be the projection-valued measure.

For the point spectrum,

$$dF(E) = F(E) = P_E$$

where P_E is the orthogonal projection onto the one dimensional subspace of the state with energy E.

For the strict approximate point spectrum, one can interpret $dF(E)$ to be a projection onto the two dimensional subspace spanned by the "states"

$$\psi_E(x) = e^{-ikx}$$
$$\psi_E(x) = e^{ikx}$$

Thus, the spectral theorem states that

$$\begin{aligned}\hat{H} &= \int_{\sigma(\hat{H})} z dF(z) \\ &= \sum_n E_n P_{E_n} + \int_0^\infty E dF(E)\end{aligned}$$

Now, the problem with interpreting the complex exponentials as eigenstates is much clearer. Each E_n yielded a true eigenstate, which allowed for their projection-valued measure to be the "point mass" measure. That is, the discrete points had weight on their own. However, in the continuum $(0, \infty)$, the measure is more akin to the Lebesgue measure on the reals. Single points have no weight, but instead it takes a whole interval of points to integrate over to have positive mass. Here, a single $E > 0$ does not yield a projection, but an interval of energies will yield a projection onto a subspace in L^2.

Now, let's construct the direct integral for this operator. Similar to the projection-valued measure approach, each part of the spectrum will be taken separately.

The measure on the point spectrum is the counting measure, so that part of the integral becomes

$$\int_{\sigma_P(\hat{H})}^{\oplus} \mathbf{H}_{E_n} d\mu(E) = \oplus_{i=1}^n \mathbf{H}_{E_n}$$

where $\mathbf{H}_{E_n}$ is the one dimensional subspace of the state with energy E_n.

The measure on the approximate point spectrum will be similar to the Lebesgue measure, and the integrand $\mathbf{H}_E$ can be shown to be the two-dimensional subspace of complex exponentials e^{ikx} and e^{-ikx} for $k = \frac{\sqrt{2mE}}{\hbar}$.

Thus, the Hilbert space for which $\hat{H}$ acts as multiplication is

$$\oplus_{i=1}^{n} \mathbf{H}_{E_n} \oplus \int_{\sigma_{AP}(\hat{H})}^{\oplus} H_E d\mu(E)$$

Again, we see that the problem with treating the complex exponentials as eigenstates has to do with their measure. In this formulation, the distinction is even more clear, as $\mu(E) = 0$ for a single $E > 0$. Thus, while the complex exponentials do form a sort of "invariant subspace" in the sense that they are part of the direct integral, their measure being zero hints at the fact that they are not part of the original Hilbert space. Rather, a positive-measure interval of these invariant subspaces is needed to properly fit them in L^2.

Note that in each case, the point spectrum of the operator behaved well and led to the familiar theory of eigenvalue decomposition, while the approximate point spectrum led to pathologies that had to be resolved. The point spectrum was a set of isolated points, and the approximate point spectrum ended up being a continuum.

This observation yields a more general result:

Theorem 5.1.2. *Isolated points in the spectrum of a normal operator are part of the point spectrum.*

The proof for this statement is most easily stated using the functional calculus (see [7, p. 140-143]).

Proof. Let λ be an isolated point in the spectrum of an operator T with a projection-valued measure E. Then, consider the function $f : \sigma(T) \to \sigma(T)$

defined as $f(z) = z - \lambda$, and let $S = \{\lambda\}$. Then

$$\begin{aligned}\left(\int f(z)dE(z)\right) E(S) &= \int_S f(z)dE(z) \\ (T - \lambda I)E(\{\lambda\}) &= \int_{\{\lambda\}} (z - \lambda)dE(z) \\ &= 0\end{aligned}$$

Thus, the subspace $E(S)((H))$ is in the kernel of $T - \lambda I$, and $\lambda \in \sigma_P(T)$. $\square$

That is to say, isolated energies of a quantum system always yield definite eigenstates. Furthermore, the contrapositive asserts that the approximate point spectrum will not have any isolated points.

6 Conclusion

Quantum mechanics relies heavily on functional analysis and Hilbert space mathematics, and without a good understanding of the intricacies of infinite-dimensional Hilbert spaces, apparent pathologies can easily confuse and mislead.

The spectrum of a quantum observable corresponds to the possible measurement results of that observable, so understanding the spectrum of observables is key in understanding a quantum system. The naive approach to understanding the spectrum is to solve the eigenvalue equation $\hat{f}x = \lambda x$ in a way analogous to finite-dimensional linear algebra. While this works in certain cases–like the Hamiltonian for the infinite square well–that have only point spectra, most observables will not be that simple. Trying to solve the eigenvalue equation in the finite square well setup yielded near-nonsensical results of "eigenstates" that were no longer in the Hilbert space of the system!

These pathologies can be resolved by exploring the spectral theorem for infinite-dimensional operators more closely. Two formulations of the spectral theorem provide key insight into the behavior of the spectrum of a normal (or self-adjoint) operator. Specifically, the projection-valued measure approach and the direct integral approach offer different but equivalent ways of interpreting the spectrum.

The projection-valued measure approach to the spectral theorem constructs a "differential projection", or a projection-valued measure, that takes into account the structure of the spectrum in constructing the projection operators onto the eigenspaces for a normal operator. For points in the spectrum that are isolated, this differential projection becomes an actual projection operator, but for intervals of points in the spectrum, the differential projection has to be integrated over to yield an actual projection. This reflects the apparent pathology encountered in the naive solution to the finite square well energies: for energies greater than zero, a single energy is not enough to generate a projection. However, when taking an interval of energies, an invariant subspace can be constructed that remains in the Hilbert space.

The direct integral approach constructs "generalized eigenspaces" for each

point in the spectrum, and assigns to the whole spectrum a measure that takes the structure of the spectrum into account. Here, the isolated points have a point mass measure, and their associated eigenspace is a true invariant subspace of the original Hilbert space. Again, for the continuous part of the spectrum, no single "generalized eigenspace" has positive measure, but an interval of them integrate to an actual invariant subspace.

Both formulations say the same thing: the point spectrum of an operator has true eigenvalues and eigenstates, whereas the strict approximate point spectrum of the operator will not have actual eigenstates for any particular eigenvalue. Rather, some positive-measure set of approximate spectrum points must be considered for the theory to work.

Any measurement device in the real world will have some uncertainty with it. That is, if one wishes to measure the energy of a certain system, the precision of the device is limited. However, if the energy values of a quantum system are isolated, a detector with good enough precision will be able to pick out which energy the system has. In the case of a continuum of energy, the detector cannot pick out any definite energy, and instead must return a range of energies that the particle has/might have. This corresponds well with the theory developed here, since a measurement of a quantum system corresponds to a projection onto the "eigenspace" associated with the measurement result. Stating that $dE(z) = 0$ for a point in the strict approximate point spectrum implies that there cannot be an infinitely precise measurement of the system for that variable.

7 Future Work

One of the clearest issues in this analysis is the fact that most quantum observables will be unbounded. While the spectral theorem still holds in the unbounded case, greater care must be taken to avoid the pathologies that unbounded operators bring with them. An introduction to unbounded operators can be found in [3, Ch. 9].

The idea of transforming the spectrum of an operator, as well as its implications to quantum mechanics, can be explored further. The functional calculus ([7, Ch. 5]) gives a way to transform a function on the spectrum of an operator to a function on the operator itself, which is a tool used in phase variable quantization methods. Furthermore, the Cayley transform ([3, Th. 10.28]) gives a way to transform the spectrum of an unbounded operator, which was not explored in this work.

While this work focused on the point spectrum/approximate point spectrum decomposition of the spectrum of an operator, there are other ways to partition the spectrum. [4] examines a finer partition of the spectrum, and it further exploration can be done on whether or not these finer partitions result in phenomenological differences in quantum mechanics.

Another aspect of quantum mechanics that was not touched on in this work is the quantization of more arbitrary phase variables. While [3, Ch. 13] examines different quantization schemes, the effect of these quantizations on the spectrum of their resultant observables should be examined further.

It was also hinted at in the direct integral approach that the measure assigned to the spectrum contained information regarding the multiplicity or degeneracy of points in the spectrum. Degeneracy is an important topic in quantum mechanics (see [2, Ch. 6.2]), and the spectrum measure from the direct integral may provide further insight into characterizing degeneracies.

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