6
Perspectives on the Spectral Theorem

6.1 The Difficulties with the Infinite-Dimensional Case

Suppose A is a self-adjoint $n \times n$ matrix, meaning that $A_{kj} = \overline{A_{jk}}$ for all $1 \leq j, k \leq n$. Then a standard result in linear algebra asserts that there exist an orthonormal basis $\{\mathbf{v}_j\}_{j=1}^n$ for $\mathbb{C}^n$ and real numbers $\lambda_1, \ldots, \lambda_n$ such that $A\mathbf{v}_j = \lambda_j \mathbf{v}_j$. (See Theorem 18 in Chap. 8 of [24] and Exercise 4 in Chap. 7.)

We may state the same result in basis-independent language as follows. Suppose $\mathbf{H}$ is a finite-dimensional Hilbert space and A is a self-adjoint linear operator on $\mathbf{H}$, meaning that $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\phi, \psi \in \mathbf{H}$. Then there exists an orthonormal basis of $\mathbf{H}$ consisting of eigenvectors for A with real eigenvalues.

Since there is a standard notion of orthonormal bases for general Hilbert spaces, we might hope that a similar result would hold for self-adjoint operators on infinite-dimensional Hilbert spaces. Simple examples, however, show that a self-adjoint operator may not have *any* eigenvectors. Consider, for example, $\mathbf{H} = L^2([0,1])$ and an operator A on $\mathbf{H}$ defined by

$$(A\psi)(x) = x\psi(x). \tag{6.1}$$

Then A satisfies $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\phi, \psi \in L^2([0,1])$, and yet A has no eigenvectors. After all, if $x\psi(x) = \lambda\psi(x)$, then ψ would have to be supported on the set where $x = \lambda$, which is a set of measure zero. Thus, only the zero element of $L^2([0,1])$ satisfies $A\psi = \lambda\psi$.

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Now, a physicist would say that the operator A in (6.1) *does* have eigenvectors, namely the distributions $\delta(x-\lambda)$. (See Appendix A.3.3.) These distributions indeed satisfy $x\delta(x-\lambda) = \lambda\delta(x-\lambda)$, but they do not belong to the Hilbert space $L^2([0,1])$. Such "eigenvectors," which belong to some larger space than $\mathbf{H}$, are known as *generalized eigenvectors*. Even though these generalized eigenvectors are not actually in the Hilbert space, we may hope that there is some sense in which they form something like a orthonormal basis. See Sect. 6.6 for an example of how such a "basis" might function.

Let us mention in passing that our simple expectation of a true orthonormal basis of eigenvectors *is* realized for compact self-adjoint operators, where an operator A on $\mathbf{H}$ is said to be compact if the image under A of every bounded set in $\mathbf{H}$ has compact closure; see Theorem VI.16 in Volume I of [34]. The operators of interest in quantum mechanics, however, are not compact. (Of course, even if a self-adjoint operator is not compact, it *might* still have an orthonormal basis of eigenvectors, as, e.g., in the case of the Hamiltonian operator for a harmonic oscillator. See Chap. 11.)

Meanwhile, there is another serious difficulty that arises with self-adjoint operators in the infinite-dimensional case. Most of the self-adjoint operators A of quantum mechanics are *unbounded* operators, meaning that there is no constant C such that $\|A\psi\| \leq C\|\psi\|$ for all ψ. Suppose, for example, that A is the position operator X on $L^2(\mathbb{R})$, given by $(X\psi)(x) = x\psi(x)$. If 1_E denotes the indicator function of E (the function that is 1 on E and 0 elsewhere), then it is apparent that

$$\left\|X 1_{[n,n+1]}\right\| \geq n \left\|1_{[n,n+1]}\right\|$$

for every positive integer n, and, thus, X cannot be bounded. Now, using the closed graph theorem and elementary results from Sect. 9.3, it can be shown that if A is defined on all of $\mathbf{H}$ and satisfies $\langle \phi, A\psi\rangle = \langle A\phi, \psi\rangle$ for all $\phi, \psi \in \mathbf{H}$, then A must be bounded. (See Corollary 9.9.) Thus, if A is unbounded and self-adjoint, *it cannot be defined on all of* $\mathbf{H}$.

We define, then, an "unbounded operator on $\mathbf{H}$ " to be a linear operator from a *dense subspace* of $\mathbf{H}$—known as the domain of A—to $\mathbf{H}$. The notion of self-adjointness for such operators is more complicated than in the bounded case. The obvious condition, that $\langle \phi, A\psi\rangle$ should equal $\langle A\phi, \psi\rangle$ for all ϕ and ψ in the domain of A, is not the "right" condition. Specifically, that condition is not sufficient to guarantee that the spectral theorem applies to A. Rather, for any unbounded operator A, we will define the adjoint A^* of A, which will be an unbounded operator with its own domain. An unbounded operator is then defined to be self-adjoint if the domains of A and A^* are the same *and* A and A^* agree on their common domain. That is to say, self-adjointness means not only that A and A^* agree whenever they are both defined, but also that the *domains* of A and A^* agree.

6.2 The Goals of Spectral Theory

Before getting into the details of the spectral theory, let us think for a moment about what it is we want the spectral theorem to do for us. In the first place, we would like the spectral theorem to allow us to apply various functions to an operator. We saw, for example, that the time-dependent Schrödinger equation can be "solved" by setting $\psi(t) = \exp\{-it\hat{H}/\hbar\}\psi_0$. Because the Hamiltonian operator $\hat{H}$ is unbounded, it is not convenient to use power series to define the exponential. If, however, $\hat{H}$ has a true orthonormal basis $\{e_k\}$ of eigenvectors with corresponding eigenvalues λ_n, then we can define $\exp\{-it\hat{H}/\hbar\}$ to be the unique bounded operator with the property that

$$e^{-it\hat{H}/\hbar}e_k = e^{-it\lambda_k/\hbar}e_k$$

for all k.

In cases where $\hat{H}$ does not have a true orthonormal basis of eigenvectors, we would like the spectral theorem to provide a "functional calculus" for $\hat{H}$, that is, a system for applying functions (including exponentials) to $\hat{H}$. This functional calculus should have properties similar to what we have in the case of a true orthonormal basis of eigenvectors.

In the second place, we would like the spectral theorem to provide a probability distribution for the result of measuring a self-adjoint operator A. Let us recall how measurement probabilities work in the case that A has a true orthonormal basis $\{e_j\}$ of eigenvectors with eigenvalues λ_j. Building on Example 3.12, we may compute the probabilities in such a case as follows. Given any Borel set E of $\mathbb{R}$, let V_E be the closed span of all the eigenvectors for A with eigenvalues in E, and let P_E be the orthogonal projection onto V_E. Then for any unit vector ψ, we have

$$\text{prob}_\psi(A \in E) = \langle \psi, P_E\psi \rangle \,. \tag{6.2}$$

In particular, if the eigenvalues are distinct and ψ decomposes as $\psi = \sum_j c_j e_j$, the probability of observing the value λ_j will be $|c_j|^2$ (as in Example 3.12), since $P_{\{\lambda_j\}}$ is just the projection onto e_j.

In cases where A does not have a true orthonormal basis of eigenvectors, we would like the spectral theorem to provide a family of projection operators P_E, one for each Borel subset $E \subset \mathbb{R}$, which will allow us to define probabilities as in (6.2). We will call these projection operators *spectral projections* and the associated subspaces V_E *spectral subspaces*. (Thus, P_E is the orthogonal projection onto V_E.) Intuitively, V_E may be thought of as the closed span of all the generalized eigenvectors with eigenvalues in E.

In the first version of the spectral theorem, both these goals will be achieved, with the spectral projections being provided by a *projection-valued measure* and the functional calculus being provided by integration with respect to this measure. Although having (generalized) eigenvectors for a self-adjoint operator is, from a practical standpoint, of secondary

importance, we provide a framework for understanding such eigenvectors, using the concept of a *direct integral*. The second version of the spectral theorem decomposes the Hilbert space $\mathbf{H}$ as a direct integral, with respect to a certain measure μ, of generalized eigenspaces for a self-adjoint operator A. The generalized eigenspace for a particular eigenvalue λ will not actually be a subspace of $\mathbf{H}$, unless $\mu(\{\lambda\}) > 0$. Thus, the notion of a direct integral gives a rigorous meaning to the notion of "eigenvectors" that are not actually in the Hilbert space.

6.3 A Guide to Reading

Although the portion of this book devoted to spectral theory is unavoidably technical in places, it has been designed so that the reader can take in as much or as little as desired. The reader who is willing to take things on faith can simply take in the examples of the position and momentum operators in Sects. 6.4 and 6.6 and accept these as prototypes of how the spectral theorem works. The reader who wants more details can find the statement of the spectral theorem for bounded operators, in two different forms, in Chap. 7, and can find the basics of unbounded self-adjoint operators in Chap. 9. Finally, the reader who wants a complete treatment of the subject can find full proofs of the spectral theorem in both forms, first for bounded operators in Chap. 8, and then for unbounded operators in Chap. 10.

6.4 The Position Operator

As our first example, let us consider the position operator X, given by $(X\psi)(x) = x\psi(x)$, acting on the Hilbert space $\mathbf{H} = L^2(\mathbb{R})$. As for the similar operator in Sect. 6.1, X has no true eigenvectors, that is, no eigenvectors that are actually in $\mathbf{H}$. If we think that the *generalized* eigenvectors for X are the distributions $\delta(x-\lambda)$, $\lambda \in \mathbb{R}$, then we may make an educated guess that the spectral subspace V_E should consist of those functions that "supported" on E, that is, those that are zero almost everywhere on the complement of E. (A superposition of the "functions" $\delta(x-\lambda)$, with $\lambda \in E$, should be a function supported on E.)

The spectral projection P_E is then the orthogonal projection onto V_E, which may be computed as

$$P_E\psi = 1_E\psi,$$

where 1_E is the indicator function of E. In that case, we have, following (6.2),

$$\text{prob}_\psi\,(X \in E) = \langle \psi, P_E\psi\rangle = \int_E |\psi(x)|^2 \; dx.$$

This formula is just what we would have expected from our discussion in Chap. 3, where we claimed that the probability distribution for the position of the particle is $|\psi(x)|^2$.

Meanwhile, let us consider the functional calculus for X. If $f(\lambda) = \lambda^m$, then $f(X)$ should be just the mth power of X, which is multiplication by x^m. It seems reasonable, then, to think that for any function f, we should define $f(X)$ to be simply multiplication by $f(x)$. In particular, the operator e^{iaX} should be simply multiplication by e^{iax}, which is a bounded operator on $L^2(\mathbb{R})$.

6.5 Multiplication Operators

Since the position operator acts simply as multiplication by the function x, it is straightforward to find the spectral subspaces and also to construct the functional calculus for X. We may consider multiplication operators in a more general setting. If $\mathbf{H} = L^2(X, \mu)$ and h is a real-valued measurable function on X, then we may define the multiplication operator M_h on $L^2(X, \mu)$ by

$$M_h \psi = h\psi.$$

We can then construct spectral subspaces as

$$V_E = \{\psi \,|\, \psi \text{ is supported on } h^{-1}(E)\}$$

and define a *functional calculus* by

$$f(A) = \text{multiplication by } f \circ h.$$

One form of spectral theorem may now be stated simply as follows: *A self-adjoint operator A on a separable Hilbert space is unitarily equivalent to a multiplication operator.* That is to say, there is some σ-finite measure space (X, μ) and some measurable function h on X such that A is unitarily equivalent to multiplication by h. (See Theorem 7.20.) Although this version of the spectral theorem is compellingly easy to state, there is slight modification of it, involving direct integrals, that is in some ways even better. See Sect. 7.3 for more information.

6.6 The Momentum Operator

Let us now see how the spectral theorem works out in the case of the momentum operator, $P = -i\hbar \, d/dx$ on $L^2(\mathbb{R})$. The "eigenvectors" for P are the functions e^{ikx}, $k \in \mathbb{R}$, with the corresponding eigenvalues being $\hbar k$. Although the functions e^{ikx} are not in $L^2(\mathbb{R})$, the Fourier transform shows that any function in $L^2(\mathbb{R})$ can be expanded as a *superposition*

(i.e., continuous version of a linear combination) of these functions. (See Appendix A.3.2.) Indeed, the Fourier transform is very much like the decomposition of a vector in an orthonormal basis, in that the Fourier coefficients $\hat{\psi}(k)$ can be expressed in terms of the "inner product" of a function ψ with e^{ikx}:

$$\hat{\psi}(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{-ikx} \psi(x) \, dx = (2\pi)^{-1/2} \left\langle e^{ikx}, \psi \right\rangle_{L^2(\mathbb{R})},$$

if we ignore the fact that e^{ikx} is not actually in L^2.

Indeed, physicists frequently understand the Fourier transform by asserting that the functions $e^{ikx}/\sqrt{2\pi}$ form an "orthonormal basis in the continuous sense" for $L^2(\mathbb{R})$. Orthonormality in the continuous sense is supposed to mean that one replaces the usual Kronecker delta in the definition of an orthonormal set by the Dirac *δ-function*

$$\left\langle \frac{e^{ikx}}{\sqrt{2\pi}}, \frac{e^{ilx}}{\sqrt{2\pi}} \right\rangle_{L^2(\mathbb{R})} = \delta(k-l), \tag{6.3}$$

where δ is supposed to satisfy

$$\int_{-\infty}^{\infty} f(k)\delta(k-l) \, dk = f(l)$$

for all continuous functions f. (Rigorously, $\delta(k-l)$ is a distribution; see Appendix A.3.3.)

To give some rigorous meaning to (6.3), note that although the inner product of e^{ikx} and e^{ilx} is not defined, we may approximate this inner product by the expression

$$\frac{1}{2\pi} \int_{-A}^{A} e^{-ikx} e^{ilx} \, dx = \frac{1}{2\pi} \frac{e^{-i(k-l)x}}{-i(k-l)} \Big|_{-A}^{A} = \frac{A}{\pi} \frac{\sin\left[A(k-l)\right]}{A(k-l)}.$$

It is possible to show that the above function, viewed as a function of k for fixed A and l, behaves like $\delta(k-l)$ in the limit as A tends to infinity. That is to say, for all sufficiently nice functions ψ, we have

$$\lim_{A\to\infty} \int_{-\infty}^{\infty} \psi(k) \frac{A}{\pi} \frac{\sin\left[A(k-l)\right]}{A(k-l)} dk = \psi(l). \tag{6.4}$$

Here is a heuristic argument for (6.4). By making the change of variable $k' = k - l$, we may reduce the general problem to the case $l = 0$. If we then make the change of variable $\kappa = Ak$, the desired result is equivalent to

$$\lim_{A\to+\infty} \int_{-\infty}^{\infty} \frac{1}{\pi} \frac{\sin\kappa}{\kappa} f\left(\frac{\kappa}{A}\right) \, d\kappa = f(0). \tag{6.5}$$

Now, *if* we can bring the limit inside the integral, $f(\kappa/A)$ will tend to $f(0)$ as A tends to infinity. Since the rest of the integrand on the right-hand side of (6.5) is already independent of A, the result would then follow if we could show that

$$\int_{-\infty}^{\infty} \frac{1}{\pi} \frac{\sin \kappa}{\kappa} \, d\kappa = 1. \tag{6.6}$$

Even though the integral in (6.6) is not absolutely convergent, it is a convergent improper integral. The value of the integral can be obtained by the method of contour integration (or the method of consulting a table of integrals), and indeed (6.6) holds. Since (6.3) is, in any case, only a heuristic way of thinking about the Fourier transform, we will not take the time to develop a rigorous version of the preceding argument.

It is possible to derive, at least formally, many of the standard properties of the Fourier transform by using (6.3), just as one can obtain properties of Fourier *series* by using the orthonormality of the functions $e^{2\pi inx}$ in $L^2([0,1])$. More importantly, the Fourier transform is precisely the unitary transformation that changes the momentum operator into a multiplication operator. To see this property of the Fourier transform more clearly, we introduce a simple rescaling of it.

Definition 6.1 *For any $\psi \in L^2(\mathbb{R})$, define $\tilde{\psi}$ by*

$$\tilde{\psi}(p) = \frac{1}{\sqrt{\hbar}} \hat{\psi}\left(\frac{p}{\hbar}\right),$$

so that

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) \, dx.$$

The function $\tilde{\psi}(p)$ is the ***momentum wave function*** *associated with ψ.*

By the Plancherel theorem (Theorem A.19) and a change of variable, if ψ is a unit vector, then so is $\hat{\psi}$ and also $\tilde{\psi}$. For any unit vector ψ, we interpret $|\tilde{\psi}(p)|^2$ as the probability density for the momentum of the particle, just as $|\psi(x)|^2$ is the probability distribution of the position of the particle. Using Proposition A.17, we may readily verify that for nice enough ψ, we have

$$\widetilde{P\psi}(p) = p\tilde{\psi}(p). \tag{6.7}$$

Equation (6.7) means that the unitary map $\psi \to \tilde{\psi}$ turns the momentum operator P into multiplication by p. That is to say, the spectral theorem, in its "multiplication operator" form, is accomplished in this case by the Fourier transform (scaled as in Definition 6.1).

In terms of the momentum wave function, we may define spectral projections and a functional calculus for P, just as in Sect. 6.5. For any Borel

set $E \subset \mathbb{R}$, we may define a projection P_E to be the orthogonal projection onto to the space of functions ψ for which $\tilde{\psi}(p)$ is zero almost everywhere outside of E. If f is any bounded measurable function on $\mathbb{R}$, we can define an operator $f(P)$ by defining $f(P)\psi$ to be the unique element of $L^2(\mathbb{R})$ for which

$$\widetilde{f(P)\psi}(p) = f(p)\tilde{\psi}(p).$$