Spectral Theorem for Bounded Self-Adjoint Operators

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We introduce the concepts of functional calculus and spectral measure for bounded linear operators on a Hilbert space. We state the spectral theorem for bounded self-adjoint operators in the cyclic case. We also compute the spectrum and the spectral measure in two concrete examples: a self-adjoint linear operator on a finite dimensional Hilbert space, and the discrete Laplacian operator on $\ell^2(\mathbb{Z})$.

1 Introduction

Diagonalization is one of the most important topics one learns in an elementary linear algebra course. Unfortunately, it only works on finite dimensional vector spaces, where linear operators can be represented by finite matrices.

Later, one encounters infinite dimensional vector spaces (spaces of sequences, for example), where linear operators can be thought of as "infinite matrices"[1]. Extending the idea of diagonalization to these operators requires some new machinery. We present it below for the (relatively simple) case of bounded self-adjoint operators.

It is important to note that this generalization is not merely a heuristic desire: infinite dimensions are inescapable. Indeed, mathematical physics is necessarily done in an infinite dimensional setting. Moreover, quantum theory requires the careful study of functions of operators on these spaces – the functional calculus.

This may seem awfully abstract at first, but an example of a function of operators is known to anyone familiar with systems of linear ODEs. Given a system of ordinary linear differential equation of the form

$$x'(t) = Ax(t)$$

where A is a constant matrix, the solution is given by

$$x(t) = \exp(tA)x(0) .$$

This is an instance of the matrix exponential, an operation that is well defined for finite dimensions.

Yet, quantum mechanics demands that we are able to define objects like this for any operator. In particular, the time evolution of a quantum mechanical state, ρ is expressed by conjugating the state by $\exp(itH)$ where H is the Hamiltonian of the system. This motivates the development of a functional calculus which allows us to define operator-valued equivalents of real functions.

But enough motivation, let us get on with the theory!

2 Operators & Spectrum

2.1 Self-adjoint operators

Let $\mathscr{H}$ be a Hilbert space and $A \in \mathscr{B}(\mathscr{H})$, the set of bounded linear operators on $\mathscr{H}$. In particular, in this exposition, we will focus on self-adjoint operators. In finite dimensions, an operator A is called self-ajoint if, as a matrix, $A = A^*$, where A^* denotes the conjugate transpose of A, i.e. $A^* = \overline{A}^T$.

Of course, in infinite dimensional space, this definition does not apply directly. We first need the notion of an adjoint operator in a Hilbert space. We begin by stating a result that we will use several times in this exposition.

Let $T \in \mathscr{B}(\mathscr{H})$, for $y \in \mathscr{H}$, the map

$$x \overset{\phi}{\longmapsto} \langle y \,|\, Tx \rangle$$

defines a bounded linear operator. Riesz's representation theorem for Hilbert spaces then tells us that $\exists\,!\, z \in \mathscr{H}$, such that

$$\phi(x) = \langle y \,|\, Tx \rangle = \langle z \,|\, x \rangle$$

We can now write $T^*(y) = z$ and *define* the adjoint T^* this way.

Definition. An operator $A \in \mathscr{B}(\mathscr{H})$ is said to be self-adjoint if

$$\langle Ax \,|\, y \rangle = \langle x \,|\, Ay \rangle$$

for all $x, y \in \mathscr{H}$, that is if $A = A^*$ with respect to our definition of the adjoint above.

Definition. λ is an eigenvalue of A if there exists $v \neq 0$, $v \in \mathscr{H}$ such that $Av = \lambda v$.

Equivalently, λ is an eigenvalue if and only if $(A - \lambda I)$ is not injective.

Several important properties of self-adjoint operators follow directly from our definition. First, the eigenvalues of a self-adjoint operator, A, are real. Indeed, let

$$Av = \lambda v$$

then,

$$\lambda \langle v \,|\, v \rangle = \langle Av \,|\, v \rangle = \langle v \,|\, Av \rangle = \overline{\lambda} \langle v \,|\, v \rangle$$

so $\lambda = \overline{\lambda}$. Moreover, if

$$Av = \lambda v, \quad Au = \mu u$$

then

$$\lambda \langle v \,|\, u \rangle = \langle Av \,|\, u \rangle = \langle v \,|\, Au \rangle = \overline{\mu} \langle v \,|\, u \rangle$$

Since $\lambda \neq \mu = \overline{\mu}$, we conclude that $\langle v \,|\, u \rangle = 0$, Which tells us that the eigenspaces of A corresponding to different eigenvalues are orthogonal.

[1] Matrices with *lots* of dots!

These two simple facts are not only reassuring, but crucial for the study of quantum mechanical systems. In fact, for a quantum system, the Hamiltonian is a self-adjoint operator whose eigenvalues correspond to the energy levels of the bound states of the system. We can sleep well at night knowing that these energy levels are real values.

2.2 Spectrum

The spectrum of an infinite dimensional operator is an entirely different beast than just the sets of eigenvalues we are used to. To describe it, it is best to introduce some new terminology. We define this for a general operator T:

Definition. The resolvent set of T, $\rho(T)$ is the set of all complex numbers λ such that

$$R_\lambda(T) := (\lambda I - T)^{-1}$$

is a bijection with a bounded inverse. The spectrum of T, $\sigma(T)$ is then given by $\mathbb{C} \setminus \rho(T)$.

In general, the spectrum of a linear operator T is comprised of two disjoint components:

1. The set of eigenvalues is now called the *point spectrum*.
2. The remaining part is called the *continuous spectrum*.

Before we discuss some examples of continuous spectra, let us prove a simple result about $\sigma(T)$ that will be necessary later in the development of the functional calculus.

Lemma 1. The spectrum of a bounded linear operator is a closed and bounded subset of $\mathbb{C}$. In fact,

$$\sigma(T) \subseteq \{z \in \mathbb{C} : |z| \leq \|T\|\}$$

Proof. Recall that $\sigma(T) = \mathbb{C} \setminus \rho(T)$.

Closed Enough to show that $\rho(T)$ is open. Indeed, remark that by the convergence of the Neumann series, namely if $\|S\| < 1$ then $(I - S)$ is invertible and its inverse is given by

$$(I - S)^{-1} = \sum_{n=0}^{\infty} S^n.$$

Let $\lambda \in \rho(T)$. For any $\mu \in \mathbb{C}$,

$$\mu I - T = (\lambda I - T)^{-1} \left[(\mu - \lambda)(\lambda I - T)^{-1} - I\right]$$

exists if $|\mu - \lambda| \left\|(\lambda I - T)^{-1}\right\| < 1$.

Bounded Now, let $\lambda \in \mathbb{C}$ be such that $|\lambda| > \|T\|$. Then, $\exists \delta \in \mathbb{R}$,

$$|\lambda| > \delta > \|T\|$$

This means that $\forall x \in \mathscr{H}$,

$$\|Tx\| \leq \|T\| < \|\delta x\| < \|\lambda x\|$$

And thus, $\forall x$,

$$0 < \left\|(\lambda I - T)^{-1} x\right\| < \left\|(\delta I - T)^{-1} x\right\| < \infty$$

so that $\lambda \in \rho(T)$. □

2.3 Examples of continuous spectra

The phenomenon of a purely continuous spectrum is uniquely found in infinite dimensional spaces, so for those who might never have ventured into these spaces before, this may seem a bit bizarre at first glance.

To offer a simple example, we consider the space $C([0,1])$ of continuous functions defined on $[0,1]$ and the operator A defined by

$$Ax(t) = tx(t).$$

Then $(A - \lambda I)x(t) = (t - \lambda)x(t)$ so

$$(A - \lambda I)^{-1} x(t) = \frac{1}{(t - \lambda)} x(t)$$

We cannot have that $tx(t) = \lambda x(t)$ so this operator has no eigenvalues. However, the spectrum is any value λ for which $t - \lambda$ vanished. Thus, the whole interval $[0,1]$ is in the spectrum of A. Hence A has purely continuous specturm.

Consider now a much more realistic example that will arise later in our treatment. We let $\mathscr{H} = l^2(\mathbb{Z})$, the Hilbert space of doubly infinite, square summable sequences and we let $A = \Delta$, the discrete Laplacian. If $x = (x_n)$,

$$(Ax)(n) = x_{n+1} + x_{n-1} - 2x_n \; .$$

Then A is self-adjoint and has no eigenvalues. We will later see that its continuous spectrum is the entire interval $[0,4]$.

3 Functional Calculus

3.1 Operator-valued functions

In finite dimenional case, there is a natural way to write down the formula of a linear operator with solely the knowledge of its eigenvalues (i.e. spectrum) and eigenvectors. In fact, if $M \in M_n(\mathbb{C})$ with eigenvalues $\{\lambda_k\}$ and associated eigenvectors $\{v_k\}$, then

$$M = \sum_{k=1}^{K} \lambda_k P_k$$

where P_k is the orthogonal projection on v_k.

We can view this linear combination as an operator-valued function defined on the spectrum of M:

$$\sigma(M) \to M_n(\mathbb{C}), \qquad \lambda_k \mapsto \lambda_k P_k$$

We can use this idea to define functions of operators. Indeed, if $f : \sigma(M) \to \mathbb{C}$ we can set

$$f(M) := \sum_{k=1}^{K} f(\lambda_k) P_k$$

Note that as the spectrum consists of finitely many points, this construction allows us to define $f(M)$ for *any* complex-valued f defined on the spectrum. For instance, in the case of the matrix exponential, mentioned in the introduction, we obtain

$$\exp(M) = \sum_{n=0}^{\infty} \frac{M^n}{n!} = \sum_{k=1}^{K} \mathrm{e}^{\lambda_k} P_k.$$

We can think of this definition as a mapping associating an operator-valued equivalent to functions on $\sigma(M)$:

$$f(z) \overset{\phi}{\longmapsto} f(M)$$

However, as we pointed out above, in infinite dimensional case, the spectrum need not be pure point. Hence, we need to extend this idea to a larger class of functions.

For this section, our goal is to extend the mapping ϕ above to *all* continuous functions defined on the spectrum of a bounded self-adjoint operator A. Before we begin, let us introduce the notion of an algebra-morphism.

Definition. An *algebra-morphism* is a map

$$\phi : X \to Y$$

preserving scalar multiplication, addition and multiplication in the spaces X and Y. In other words, $\forall x \in X,\ y \in Y$ and all scalars α,

1. $\phi(\alpha x) = \alpha \phi(x)$
2. $\phi(x+y) = \phi(x) + \phi(y)$
3. $\phi(xy) = \phi(x)\phi(y)$

Note that these properties simply reflect our notions of pointwise addition and multiplication of functions. Indeed, we want the operator-valued equivalents defined by ϕ to obey these notions, and so, requiring ϕ to be an algebra-morphism is a natural constraint.

3.2 Continuous functional calculus

For this section, we let A be a bounded, self-adjoint operator. Let P be a polynomial, with

$$P(x) = \sum_{k=0}^{n} \alpha_k x^k$$

then we define

$$P(A) := \sum_{k=0}^{n} \alpha_k A^k$$

We thus have a map $\varphi : \mathbb{C}[x] \longrightarrow \mathscr{B}(\mathscr{H})$ with

$$P \overset{\varphi}{\longmapsto} P(A)$$

This φ is an algebra-morphism and satisfies $\varphi(\overline{P}) = \varphi(P)^*$. Moreover, if λ is an eigenvalue of A then $P(\lambda)$ is an eigenvalue of $P(A)$. This fact can be reformulated as the following

Lemma 2 (Spectral Mapping Theorem).

$$\sigma\big(P(A)\big) = \{P(\lambda) : \lambda \in \sigma(A)\}$$

Proof. Let $\lambda \in \sigma(A)$ and consider $Q(x) = P(x) - P(\lambda)$ then λ is a root of $Q(x)$ and so there is a polynomial $R \in \mathbb{C}[x]$ such that $Q(x) = (x-\lambda)R(x)$. Thus

$$P(A) - P(\lambda) = (A - \lambda I)R(A) = R(A)(A - \lambda I)$$

Since $(A - \lambda I)$ is not invertible for $\lambda \in \sigma(A)$, $P(A) - P(\lambda)$ is not invertible, so $P(\lambda) \in \sigma\big(P(A)\big)$. Conversely, let $\mu \in \sigma\big(P(A)\big)$ then, by factoring we obtain that

$$P(x) - \mu = \alpha(x - \lambda_1)\cdots(x - \lambda_n)$$

and

$$P(A) - \mu = \alpha(A - \lambda_1)\cdots(A - \lambda_n)$$

Since $\mu \in \sigma\big(P(A)\big)$, $P(A) - \mu$ is not invertible and so there is some $i \in \{1, \dots, n\}$ such that $A - \lambda_i$ is not invertible. This $\lambda_i \in \sigma(A)$ but $P(\lambda_i) = \mu$ by the first part of this discussion. □

Before developing a continuous functional calculus, we require one more simple technical claim.

Lemma 3.

$$\|P(A)\| = \sup\{|P(\lambda)| : \lambda \in \sigma(A)\}$$

Proof.

$$\begin{aligned} \|P(A)\|^2 &= \|P(A)^* P(A)\| = \|\overline{P}P(A)\| = \\ &= r\big(\overline{P}P(A)\big) \end{aligned}$$

Now, by the above lemma we have that

$$\begin{aligned} r\big(\overline{P}P(A)\big) &= \sup\{|\mu| : \mu \in \sigma\big(\overline{P}P(A)\big)\} \\ &= \sup\{|\overline{P}P(\lambda)| : \lambda \in \sigma(A)\} \\ &= \sup\{|P^2(\lambda)| : \lambda \in \sigma(A)\} \end{aligned}$$ □

This brings us to the main result of this section:

Theorem 4 (Continuous Functional Calculus). Let $C\big(\sigma(A)\big)$ be the continuous functions defined on the spectrum of A. There exists a unique map $\varphi : C\big(\sigma(A)\big) \longrightarrow \mathscr{B}(\mathscr{H})$,

$$\varphi(f) = f(A)$$

such that

1. φ is an algebra-morphism.
2. $f(A)^* = \overline{f(A)}$.

3. If $f(x) = x$ then $f(A) = A$.
4. $\|f(A)\| = \|f\|_\infty$.
5. $\sigma\big(f(A)\big) = \{f(\lambda) : \lambda \in \sigma(A)\}$ and if λ is an eigenvalue of A then $f(\lambda)$ is and eigenvalue of $f(A)$.

Proof. Due to 1 and 3, φ must coincide with our previously defined map on the polynomials. We only need to extend it uniquely to $C\big(\sigma(A)\big)$, the space of continuous functions

$$\sigma(A) \to \mathbb{C}$$

Recall the Stone-Weierstrass theorem:

> If X is compact, the set of polynimials over X is dense in $C(X)$.

By lemma 1, $\sigma(A)$ is closed and bounded in $\mathbb{C}$, and hence, compact by Heine-Borel theorem. Thus, the map φ is densely defined on $C\big(\sigma(A)\big)$ and can be extended by continuity. The uniqueness of such an extension is guaranteed by the isometry from lemma 3.

Finally, taking limits in lemmas 2 and 3 proves the properties 5 and 4 respectively. □

So far, this has been a natural extension, but what follows is a miracle.

4 Spectral measures & Borel functional calculus

We let A be as before and, given any $\psi \in \mathscr{H}$, we define

$$L : C\big(\sigma(A)\big) \longrightarrow \mathbb{C}$$

$$f \overset{L}{\longmapsto} \langle \psi \,|\, f(A)\psi \rangle$$

L is a continuous linear functional with

$$|\langle \psi \,|\, f(A)\psi \rangle|^2 \leq \|f(A)\|\|\psi\|^2 \leq \|f\|_\infty \|\psi\|^2$$

Moreover, L is positive. Indeed, if $f \geq 0$, by theorem 4(5),

$$\sigma\big(f(A)\big) = f\big(\sigma(A)\big) \subseteq (0, \infty)$$

Also, by continuity of f, $\sigma\big(f(A)\big)$ is compact. Recall the Riesz-Markov theorem for a locally compact Hausdorff space X:

> For any positive linear functional Φ on $C_c(X)$, there exists a unique Borel measure μ on X such that $\forall f \in C_c(X)$,
>
> $$\Phi(f) = \int_X f \, \mathrm{d}\mu$$

As we have seen before, $\sigma(A)$ is compact, so every continuous function on it is compactly supported, i.e. $C_c\big(\sigma(A)\big) = C\big(\sigma(A)\big)$.

Thus, by the Riesz-Markov theorem, there is a positive Borel measure μ_ψ such that for all $f \in C\big(\sigma(A)\big)$,

$$L(f) = \langle \psi \,|\, f(A)\psi \rangle = \int f d\mu_\psi$$

Something interesting has just happened here. The right hand side makes sense even if f is not continuous, just measurable. So we can extend our definition of L to an arbitrary measurable g by setting

$$\langle \psi \,|\, g(A)\psi \rangle := \int g d\mu_\psi$$

We can push our luck a bit further. Using the polarization identity, we define for all φ, $\psi \in \mathscr{H}$

$$\begin{aligned}\langle \varphi \,|\, g(A)\psi \rangle := \frac{1}{4}\big[&\langle \varphi + \psi \,|\, g(A)\varphi + \psi \rangle - \\ &- \langle \varphi - \psi \,|\, g(A)\varphi - \psi \rangle + \\ &+ i \langle \varphi + i\psi \,|\, g(A)\varphi + i\psi \rangle - \\ &- i \langle \varphi - i\psi \,|\, g(A)\varphi - i\psi \rangle \big]\end{aligned}$$

Given g and ψ, $\varphi \longmapsto \langle \varphi \,|\, g(A)\psi \rangle$ is linear and continuous. We can (yet again!) apply Riesz's representation theorem. It states that for such a bounded linear functional, there is a unique $h_{g,\psi} \in \mathscr{H}$ such that

$$\langle \varphi \,|\, g(A)\psi \rangle = \big\langle \varphi \,\big|\, h_{g,\psi} \big\rangle$$

for all $\varphi \in \mathscr{H}$.

Remark. Be careful to note that the left-hand side is merely notation for our extended definition of the inner product, while the right-hand side is the true inner product of our Hilbert space.

We should also note that the above is sheer magic. It is a good day when we can unite both forms of the Riesz representation theorem in one proof.

We now let $g(A) : \mathscr{H} \longrightarrow \mathscr{H}$ with $\psi \longmapsto h_{g,\psi}$.

Theorem 5. All the properties of $g(A)$ that hold for a continuous g also hold for a measurable g.

The proof is left as exercise for the reader.

Special Case. If $g(x) = \chi_A(x)$, then $g(A)$ is an orthogonal projection.

Proof. By the algebra property, $g(A)^2 = g^2(A)$, and as $\chi_A^2 = \chi_A$, we get that $g(A)^2 = g(A)$. Hence, $g(A)$ is a projection.

$$g(A)^* = \overline{g(A)} = g(A)$$

Thus, $g(A)$ is an orthogonal projection. □

Definition. $\psi \in \mathscr{H}$ is called a cyclic vector of A if

$$\{P(A)\psi : P \in \mathbb{C}[x]\}$$

is dense in $\mathscr{H}$.

Theorem 6 (Spectral theorem for self-adjoint operators). Let A be a self-adjoint operators on a Hilbert space $\mathscr{H}$ and suppose that ψ is a cyclic vector of A. Then there is a measurable function $f : \sigma(A) \longrightarrow \mathbb{R}$ and a unitary map

$$U : \mathscr{H} \longrightarrow L^2(\sigma(A), \mu_\psi)$$

so that

$$(UAU^{-1} f)(\lambda) = \lambda f(\lambda) \; .$$

Remark. In finite dimensions, a unitary matrix is a change of basis matrix from one orthonormal basis to another. Thus, the unitary operator U can be though of as a change of basis operator. In fact, diagonalization of finite matrices produces a similar result:

$$D = PAP^{-1}$$

where P is the matrix changing standard basis to the eigenbasis of A.

Now, if A does not admit of a cyclic vector on the entire space, we are not entirely out of luck.The decomposition theorem for Hilbert spaces (see [2]) comes to our aid. It assures us that we may decompose our Hilbert space into orthogonal subspaces $\mathscr{H}_n$ and our operator into corresponding components A_n, such that A_n has a cyclic vector on $\mathscr{H}_n$. The proof of this theorem as well as the proof of the general case of the spectral theorem will be ommitted here.

5 Examples

5.1 Finite dimensional case

Let $\mathscr{H} = \mathbb{C}^n$, and, as in section 3, set

$$A = \sum_{j=1}^{k} \lambda_j P_j \qquad f(A) = \sum_{j=1}^{k} f(\lambda_j) P_j .$$

This can always be done, as any self-adjoint operator on a finite dimensional vector space is necessarily diagonalizable. Fix $\psi \in \mathbb{C}^n$, then

$$\begin{aligned} \int f \, \mathrm{d}\mu_\psi &= \langle \psi \, | \, f(A)\psi \rangle \\ &= \sum_{j=1}^{k} f(\lambda_j) \left\langle \psi \, \middle| \, P_j \psi \right\rangle \\ &= \sum_{j=1}^{k} f(\lambda_j) \left\| P_j \psi \right\|^2 . \end{aligned}$$

$$\Longrightarrow \forall f, \; \int f \, \mathrm{d}\mu_\psi = \sum_{j=1}^{k} f(\lambda_j) \left\| P_j \psi \right\|^2$$

Thus, using the second equation in theorem 6, we can conclude that

$$\mu_\psi = \sum_{j=1}^{k} \left\| P_j \psi \right\|^2 \delta(\lambda - \lambda_j).$$

That is, the spectral measure is a counting measure, where each λ_j is weighted according to the norm of the corresponding $P_j \psi$ vector.

$\longrightarrow$ *When does A admit a cyclic vector?*

By definition above, ψ is cyclic if

$$\{P(A)\psi : P \in \mathbb{C}[x]\} = \mathbb{C}^n \iff$$

$$\iff \overbrace{\{\sum_{j=1}^{k} P(\lambda_j) P_j \psi}^{\dim k} : P \in \mathbb{C}[x]\} = \mathbb{C}^n \leftarrow \dim n$$

Hence, ψ is cyclic if $k = n$, i.e. there are n distinct (simple) eigenvalues.

$$\psi \text{ is cyclic} \iff \text{spectrum is simple.}$$

5.2 Discrete Laplacian

Let Δ be the discrete Laplacian on $\ell^2(\mathbb{Z})$. For $\psi \in \ell^2(\mathbb{Z})$, Δ acts as

$$(\Delta\psi)(n) = \psi_{n+1} + \psi_{n-1} - 2\psi_n$$

Given $\psi \in \ell^2(\mathbb{Z})$ we can define $\hat{\psi} \in L^2\big([0, 2\pi)\big)$ by

$$\hat{\psi}(\xi) = \sum_{n \in \mathbb{Z}} e^{in\xi} \psi_n$$

with

$$\psi_n = \frac{1}{2\pi} \int_0^{2\pi} e^{in\xi} d\xi$$

then the map

$$U : \ell^2(\mathbb{Z}) \longrightarrow L^2([0, 2\pi), \frac{d\xi}{2\pi})$$

$$\psi \stackrel{U}{\longmapsto} \hat{\psi}$$

is unitary. We wish to investigate the behaviour of Δ under this map, that is what does $U\Delta U^{-1}$ give us. Take $f(\xi) \in L^2\big([0, 2\pi)\big)$ then $(\Delta U^{-1} f)(n) =$

$$\begin{aligned} &= \frac{1}{2\pi} \int_0^{2\pi} \left[\mathrm{e}^{-i(n+1)\xi} + \mathrm{e}^{-i(n-1)\xi} + \mathrm{e}^{-in\xi} \right] f(\xi) d\xi \\ &= \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{-in\xi} (\mathrm{e}^{-i\xi} + \mathrm{e}^{i\xi} - 2) f(\xi) d\xi . \end{aligned}$$

Hence $(U\Delta U^{-1})(\xi) = (2\cos\xi - 2) f(\xi)$.

Remark (about analysis, the universe and life in general[2]). Note that the unitary map U defined above is the discrete Fourier transform on $\ell^2(\mathbb{Z})$. Thus, this provides us with an example of the Fourier transform mapping a complicated looking operator on a sequence space, to a *multiplication* operator on the familiar space $L^2([0, 2\pi), \frac{d\xi}{2\pi})$. Fairy tales really do come true!

[2] Many thanks to Prof. Jakobson.

Spectrum Now that we have the form of our operator in Fourier space, we are equipped to determine what its spectrum is. We look at the resolvent set

$$\begin{aligned}\rho(\Delta) &= \{\lambda : (\lambda-\Delta) \text{ is invertible}\}\\ &= \{\lambda : \lambda - 2\cos\xi + 2 \neq 0\ \forall \xi \in [0,2\pi)\}\\ &= \mathbb{C}\setminus[-4,0]\end{aligned}$$

Hence $\sigma(\Delta) = [-4,0]$.

Spectral measure Lastly, for $f \in C([-4,0])$, in Fourier space $f(\Delta)$ is just multiplication by $f(2\cos\xi - 2)$. Fix $\psi \in l^2(\mathbb{Z})$ and let $\hat{\psi}$ be the corresponding function in $L^2\big([0,2\pi)\big)$. Then

$$\begin{aligned}\int f(\Delta)\,\mathrm{d}\mu_\psi &= \langle \psi \,|\, f(\Delta)\psi\rangle_{\ell^2}\\ &= \left\langle U^{-1}U\psi \,\middle|\, f(\Delta)U^{-1}U\psi\right\rangle_{\ell^2}\\ &= \left\langle U\psi \,\middle|\, \left(Uf(\Delta)U^{-1}\right)U\psi\right\rangle_{L^2}\\ &= \langle \hat{\psi} \,|\, f(2\cos\xi-2)\hat{\psi}\rangle_{L^2}\\ &= \frac{1}{2\pi}\int_0^{2\pi} \overline{\hat{\psi}} f(2\cos\xi - 2)\hat{\psi}\,\mathrm{d}\xi\\ &= \frac{1}{2\pi}\int_0^{2\pi} f(2\cos\xi-2)\,|\hat{\psi}(\xi)|^2\,\mathrm{d}\xi.\end{aligned}$$

Now splitting the region of integration into two equal parts and applying the change of variables

$$\lambda = 2\cos\xi - 2$$

yields

$$\begin{aligned}\int f\,\mathrm{d}\mu_\psi = \int_{-4}^{0} f(\lambda)\Bigg[\left|\hat{\psi}\left(\arccos(\frac{\lambda+2}{2})\right)\right|^2 + \\ + \left|\hat{\psi}\left(-\arccos(\frac{\lambda+2}{2}+2\pi)\right)\right|^2\Bigg]\frac{\mathrm{d}\lambda}{\sqrt{-\lambda^2-4\lambda}}\end{aligned}$$

Thus,

$$\mathrm{d}\mu_\psi = [\ldots]\frac{\mathrm{d}\lambda}{\sqrt{-\lambda^2-4\lambda}}$$

6 Conclusion

We conclude this article with an interesting result. We recall Lebesgue's decomposition theorem that states that any measure μ on $\mathbb{R}$ has a unique decomposition into

$$\mu = \mu_{pp} + \mu_{ac} + \mu_{sing},$$

the pure-point, absolutely continuous and singularly continuous parts. Moreover, these three measures are mutually singular.

Given a self-adjoint operator, $A \in \mathscr{B}(\mathscr{H})$, we define

$$\mathscr{H}_{pp} = \{\psi | \mu_\psi \text{ is pure point}\}$$

and similarly for $\mathscr{H}_{ac}$ and $\mathscr{H}_{sing}$. We then have that

$$\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sing}$$

where each subspace is invariant under A. We can now define $\sigma_{pp}(A)$ to be the spectrum of A restricted to $\mathscr{H}_{pp}$ and we further have that

$$\sigma(A) = \sigma_{pp}(A) \cup \sigma_{ac}(A) \cup \sigma_{sing}(A)$$

where this union might not be disjoint. In quantum mechanics, in particular, self-adjoint operators represent physical observables of a given system and their spectra correspond to the outcomes of measurements. Roughly speaking, the absolutely continuous spectrum corresponds to free states while the pure point corresponds to bound states.

However, the observables are not necessarily bounded (take the momentum and position operators, say). Hence, in order to fully appreciate and apply spectral theory in a quantum mechanical setting, one must turn to spectral theory for unbounded operators.

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