10 Spectral theorem

An (orthogonal) projection $P = P^* = P$ has a closed $+1$-eigenspace (its range), and a complementary closed 0-eigenspace (its kernel). In quantum mechanics, it models a basic yes/no question asked of a normalized state $\psi \in \mathcal{H}$: "is $\psi \in \operatorname{Ran}(P)$"? According to the *Born rule*, the probability of "yes" is $\langle\psi|P\psi\rangle$.

An observable might have a discrete set of distinct real outcomes $\lambda_i \in \mathbb{R}$, $i = 1, 2 \ldots$, with the yes/no question for the i-th outcome being a projection P_i onto an eigenspace $\operatorname{Ran}(P_i) \subset \mathcal{H}$. The entire observable is then an orthogonal direct sum

$$T = \bigoplus_i \lambda_i P_i, . \tag{10.1}$$

and is self-adjoint on $\bigoplus_i \operatorname{Ran}(P_i)$.

However, an observable need not only have discrete and finitely many outcomes. Indeed, the discretization of measurement outcomes which are a priori $\mathbb{R}$-valued, is one of the most significant surprises of quantum mechanics. So we should not assume that observables are of the form (10.1). Instead, we should seek a general model of observables which include "continuous" versions of (10.1).

A basic example is the energy observable, or the Hamiltonian. The free Hamiltonian, $H = -\nabla^2$ has no eigenvalues at all! Rather, its spectrum is $\mathbb{R}_{\geq 0}$, with the plane waves $x \mapsto e^{\pm iEx}$ being "generalized eigenfunctions" for "eigenvalue E^2", for $E \in \sigma(H) = \mathbb{R}_{\geq 0}$. More generally, the Hamiltonian is $-\nabla^2 + V$ for some potential function, and the spectrum is a complicated mix of isolated eigenvalues and intervals.

The general question is not "does ψ have exactly energy E?", but "does ψ have energy within a given interval $[E_0, E_1]$?". The latter question corresponds to a *spectral projection* $P_{[E_0,E_1]}$ of the Hamiltonian. If we use a disjoint partition

$$\sqcup_i I_i = \mathbb{R}$$

by intervals I_i, we get projections $P_i = P_{I_i}$ for the yes/no question of having energy in I_i. These projections should give a corresponding "orthogonal partition" of the Hilbert space,

$$1_{\mathcal{H}} = \bigoplus_i \operatorname{Ran}(P_i).$$

Intuitively, as the partition gets finer and finer, the intervals become individual points, and we arrive at

$$\text{“}1_{\mathcal{H}} = \bigoplus_{E\in\sigma(H)} P_{\{E\}}\text{”}, \qquad \text{“}H = \bigoplus_{E\in\sigma(H)} \lambda P_{\{E\}}\text{”}. \tag{10.2}$$

Informally, the left expression is a “resolution of the identity” by the “eigenspaces” of H, while the right expression is its “eigen-decomposition”.

10.1 Integrals with respect to projection-valued measure

The following is a “quantum” version of the notion of probability measure.

Definition 31. A *projection-valued measure (PVM)* on a measurable space (X, Σ) is a projection-valued assignment

$$P : \Sigma \to \mathrm{Proj}(\mathcal{H}), \qquad E \mapsto P_E$$

satisfying

- $P_X = 1_{\mathcal{H}}$ and $P_\emptyset = 0$.
- If $E_i, i \in \mathbb{N}$ are disjoint, then

$$P_{\sqcup_{i\in\mathbb{N}} E_i} = \sum_{i\in\mathbb{N}} P_{E_i}, \qquad \text{SOT sense.} \tag{10.3}$$

The *support* of a PVM is

$$\mathrm{Supp}(P) := X \setminus \bigcup_{E\in\Sigma : P(E)=0} E.$$

Note: In (10.3), “SOT” means “strong operator topology”. It specifies the sense in which the infinite sum of projections is meant to converge,

$$P_{\sqcup_{i\in\mathbb{N}} E_i}\psi = \sum_{i\in\mathbb{N}} P_{E_i}\psi, \qquad \forall\psi \in \mathcal{H}.$$

That $\sum_{i\in\mathbb{N}} P_{E_i}$ is a projection can be deduced from the following exercise.

Exercise 10.1. Check the following statements.

- Let P_1, P_2 be orthogonal projections. Show that $P_1 + P_2$ is an orthogonal projection iff $P_1 P_2 = 0$.
- Let $P : \Sigma \to \mathrm{Proj}(\mathcal{H})$ be a PVM. Show that
  1. If $E, F \in \Sigma$ are disjoint, then $P_E P_F = 0$.
  2. $P_{E \cap F} = P_E P_F$ for all $E, F \in \Sigma$.

With some measure theory (omitted), we recover ordinary measures from a PVM P by taking inner products:

- Each pair $\varphi, \psi \in \mathcal{H}$ converts P into a complex measure,

$$P^{\varphi\psi} : \Sigma \to \mathbb{C}, \qquad E \mapsto \langle \varphi | P_E \psi \rangle. \tag{10.4}$$

- In particular, for $\varphi = \psi$, we have a finite measure,

$$P^{\psi} := P^{\psi\psi} : \Sigma \to \mathbb{R}_{\geq 0}, \qquad P^{\psi}(X) = \langle \psi | \underbrace{P_X}_{1_{\mathcal{H}}} \psi \rangle = ||\psi||^2.$$

Thus, each normalized $\psi \in \mathcal{H}$ converts P into an ordinary probability measure P^{ψ}. We may anticipate that P is associated to an observable taking possible values in X, and that P^{ψ} encodes the probabilities of measuring the various outcomes for the state ψ.

Remember that the purpose of ordinary measures μ on X is to integrate functions $f : X \to \mathbb{C}$, the result being a complex number built up from the values $f(x)$ weighted by $\mu(x)$. Likewise, we can integrate f with respect to a PVM, but the weights are now projection operators instead of numbers, so the result is a Hilbert space operator.

Definition 32. Let $P : \Sigma \to \mathrm{Proj}(\mathcal{H})$ be a PVM. For a measurable $f : X \to \mathbb{C}$, define $\int_X f\, dP$ to be the operator specified by

$$\mathrm{Dom}\left(\int_X f\, dP\right) := \{\psi \in \mathcal{H} \,:\, f \in L^2(X; dP^{\psi})\}, \tag{10.5}$$

$$\left\langle \varphi \middle| \left(\int_X f\, dP\right) \psi \right\rangle := \int_X f\, dP^{\varphi\psi}, \qquad \forall \psi \in \mathrm{Dom}\left(\int_X f\, dP\right), \varphi \in \mathcal{H}. \tag{10.6}$$

Eq. (10.6) is a somewhat indirect characterization of the operator $\int_X f\,dP$, so let us discuss its construction more concretely. (Details can be found in, e.g., Chapter 9 of Moretti's book, or Chapter 4 of Schmüdgen's Unbounded self-adjoint operators on Hilbert space.)

- Write $B_b(X)$ for the *bounded* measurable functions with supremum norm. Some measure theory shows that the simple functions $s = \sum_{i=1}^n \alpha_i \chi_{E_i}$ are dense in the Banach space $B_b(X)$. For simple functions, we define

  $$\int_X s\,dP := \sum_{i=1}^n \alpha_i P_{E_i} \in \mathcal{B}(\mathcal{H}),$$

  and check that this is a continuous assignment. Extend by continuity (Exercise 6.2) to get

  $$\int_X (\cdot)\,dP : B_b(X) \to \mathcal{B}(\mathcal{H}). \tag{10.7}$$

  One checks that (10.7) is a $*$-homomorphism, i.e., respects sums, products, and adjoints. Note that (10.7) gives a *bounded* operator with domain being all of $\mathcal{H}$. It satisfies (10.6).

- For unbounded f, we define $\int_X f\,dP$ by specifying $\left(\int_X f\,dP\right)\psi$ for those $\psi \in \mathcal{H}$ such that $f \in L^2(X; dP^\psi)$,

  $$\left(\int_X f\,dP\right)\psi := \lim_{n\to\infty} \left(\int_X f_n\,dP\right)\psi. \tag{10.8}$$

  On the right side, $f_n \in B_b(X)$ is any sequence which approximates f in the $L^2(X; dP^\psi)$ sense. Concretely, one could take

  $$f_n(x) = \begin{cases} f(x), & |f(x)| \leq n, \\ 0, & \text{otherwise.} \end{cases}$$

  One checks that this definition of $\int_X f\,dP$ still satisfies (10.6), and is the unique operator with that property.

10.1.1 Important properties of $\int_X (\cdot)\, dP$.

For proofs of the following properties, see Theorem 4.16 of Schmüdgen, or Theorem 9.4 of Moretti.

- We have
$$\int_X \overline{f}\, dP = \left(\int_X f dP\right)^*. \tag{10.9}$$
In particular, $\int_X f\, dP$ is a closed operator, and self-adjoint if f is real-valued.

- The assignment $f \mapsto \int_X f$ is a homomorphism, up to domain considerations,
$$\begin{aligned} \int_X f\, dP + \alpha \int_X g\, dP \ &\subset \ \int_X f + \alpha g\, dP, \qquad\qquad \alpha \in \mathbb{C}, \\ \left(\int_X f\, dP\right)\left(\int_X g\, dP\right) \ &\subset \ \int_X fg\, dP, \end{aligned} \tag{10.10}$$

- $(\int_X f\, dP)^{-1} : \mathrm{Ran}(\int_X f\, dP) \to \mathrm{Dom}(\int_X f\, dP)$ exists iff f is P-a.e. nonzero. In that case,
$$\left(\int_X f\, dP\right)^{-1} = \left(\int_X f^{-1}\, dP\right). \tag{10.11}$$
The spectrum of $\int_X f\, dP$ coincides with the essential range of f,
$$\sigma\left(\int_X f\, dP\right) = \big\{\lambda \in \mathbb{C} \,:\, P_{f^{-1}(\lambda-\epsilon,\lambda+\epsilon)} \neq 0 \quad \forall \epsilon > 0\big\}. \tag{10.12}$$

- $\lambda \in \mathbb{C}$ is an eigenvalue of $\int_X f\, dP$ iff $P_{f^{-1}(\lambda)}$ is nonzero. In that case, $P_{f^{-1}(\lambda)}$ is the eigenspace projection,
$$\mathrm{Range}\big(P_{f^{-1}(\lambda)}\big) = \ker\left(\int_X f\, dP\, - \lambda\right). \tag{10.13}$$

- Let $\eta : X \to X'$, then we can push-forward P to a PVM P' on (X', Σ'),
$$\begin{aligned} \Sigma' &:= \{E' \subset X' \,:\, \eta^{-1}(E') \in \Sigma\}, \\ P'_{E'} &:= P_{\eta^{-1}(E')}, \qquad E' \in \Sigma'. \end{aligned}$$

Then for measurable $f' : X' \to \mathbb{C}$,

$$\int_{X'} f' \, dP' = \int_X (f' \circ \eta) \, dP. \tag{10.14}$$

We are mostly concerned with the case where $X = \mathbb{R}$ and $\Sigma = \mathrm{Bor}(\mathbb{R})$ is the Borel σ-algebra. Then property (10.9) says that

$$\int_{\mathbb{R}} \lambda \, dP(\lambda) \tag{10.15}$$

is a self-adjoint operator, since the map

$$X = \mathbb{R} \to \mathbb{C}, \qquad \lambda \mapsto \lambda$$

is real-valued. Intuitively, we are assembling a bunch of "eigenprojections" $P_{\{\lambda\}}$ weighted by the real "eigenvalues" λ, obtaining a "diagonal" self-adjoint operator, see (10.2). The spectral theorem is the statement that any self-adjoint operator is constructed this way, as formalized by a PVM integral, (10.15).

10.2 Spectral theorem for bounded self-adjoint operators

Theorem 10.1. *Let H be a bounded self-adjoint operator on $\mathcal{H}$. Let I be a compact interval containing $\sigma(H)$. There exists a unique PVM, $P : \mathrm{Borel}(I) \to \mathrm{Proj}(\mathcal{H})$, such that*

$$H = \int_I \lambda \, dP(\lambda). \tag{10.16}$$

Proof. (Optional.) When a polynomial p is considered as a function on the non-empty compact set $I \supset \sigma(H)$ (recall Prop. 6.2, 6.11), its supremum norm $||p||_\infty$ makes sense. It is not hard to check that $||p(H)||_{\mathrm{op}} \le ||p||_\infty$. Now, for each $\varphi, \psi \in \mathcal{H}$,

$$|\langle\varphi|p(H)\psi\rangle| \le ||\varphi|| \, ||\psi|| \underbrace{||p(H)||_{\mathrm{op}}}_{\le ||p||_\infty},$$

so $F^{\varphi,\psi} : p \mapsto \langle\varphi|p(H)\psi\rangle$ defines a continuous linear functional on the polynomials, with

$$||F^{\varphi,\psi}|| \le ||\varphi|| \, ||\psi||.$$

By the *Stone–Weierstrass* theorem[19] and the *Riesz–Markov* representation theorem, there is a unique (regular, complex) Borel measure $\mu^{\varphi\psi}$ on I which represents the functional $F^{\varphi\psi}$, in the sense that

$$\langle\varphi|p(H)\psi\rangle = \int_I p\, d\mu^{\varphi\psi}$$

holds for all polynomials p. Furthermore, $|\mu^{\varphi\psi}(E)| \leq ||F^{\varphi,\psi}|| \leq ||\varphi||\,||\psi||$ holds for each $E \in \text{Borel}(I)$. Thus, for each E, we have a bounded sesquilinear form $\mu^{\varphi\psi}(E)$, which by Lemma 6.6, defines a bounded operator which we call P_E,

$$\mu^{\varphi,\psi}(E) = \langle\varphi|P_E\psi\rangle, \qquad \varphi,\psi \in \mathcal{H},\ E \in \text{Borel}(I).$$

The next algebraic step is to show that the P_E are projections (Omitted). Together with the fact that $E \mapsto \langle\psi|P_E\psi\rangle$ is an ordinary measure for each $\psi \in \mathcal{H}$, we deduce that $E \mapsto P_E$ satisfies the properties of a PVM on Borel(I).

Since $H = p(H)$ for the identity polynomial $p : \lambda \mapsto \lambda$, the above constructions give

$$\langle\varphi|H\psi\rangle = \int_I \lambda\, d\mu^{\varphi\psi}(\lambda), \qquad \varphi,\psi \in \mathcal{H}.$$

By definition of integrating against a PVM (see (10.6)),

$$\int_I \lambda\, d\mu^{\varphi\psi}(\lambda) = \left\langle\varphi\middle| \left(\int_I \lambda\, dP(\lambda)\right)\psi\right\rangle, \qquad \varphi,\psi \in \mathcal{H}.$$

So $H = \int_I \lambda\, dP(\lambda)$.

The uniqueness proof is also omitted. □

10.2.1 Positive square root

Our first application of the spectral theorem is in the construction of positive square roots.

Definition 33. An operator $L : \text{Dom}(L) \to \mathcal{H}$ is *positive* if

$$\langle\psi|L\psi\rangle \geq 0, \qquad \forall\, \psi \in \text{Dom}(L). \tag{10.17}$$

Exercise 10.2. Let L be a bounded positive operator. Show that L is self-adjoint, and has non-negative spectrum.

---

[19] Polynomials are dense in $C(I)$ in sup-norm.

Proposition 10.2. *A bounded* positive *operator L admits a unique positive square root $\sqrt{L}$, satisfying $(\sqrt{L})^2 = L$. We may approximate $\sqrt{L}$ in operator norm by a sequence $p_n(L)$ where p_n are polynomials.*

Proof. Let $I = [0, a]$ be an interval containing $\sigma(L)$. By Exercise 10.2, the positive square root function $\sqrt{(\cdot)} : C(I) \to [0, \infty)$ is well-defined. Integrate it against the PVM P of L (Theorem 10.1),

$$\sqrt{L} := \int_I \sqrt{\lambda}\, dP(\lambda).$$

This results in a positive operator, because for all $\psi \in \mathcal{H}$,

$$\left\langle \psi \middle| \left(\int_I \sqrt{\lambda}\, dP(\lambda) \right) \psi \right\rangle = \int_I \underbrace{\sqrt{\lambda}}_{\geq 0}\, dP^\psi \geq 0,$$

as P^ψ is an ordinary positive measure.

For a general $f \in B_b(I)$, the operator norm of $\int_I f\, dP$ is bounded by $||f||_\infty$. This is first checked for simple functions, then continues to hold for general f due to the construction of $\int_I f\, dP$ by continuity. This norm-decreasing property implies

$$||p_n(L) - \sqrt{L}||_{\text{op}} \to 0$$

for any sequence of polynomials p_n uniformly convergent to $\sqrt{(\cdot)}$ over I. Such a sequence exists by Stone–Weierstrass.

For the uniqueness part, suppose A is another positive operator such that $A^2 = L$. Then $AL = A^3 = LA$, thus $Ap_n(L) = p_n(L)A$ for the polynomial p_n as well, and by continuity, $A\sqrt{L} = \sqrt{L}A$. Then we have

$$0 = \langle \varphi | (A^2 - (\sqrt{L})^2)\psi \rangle = \langle \varphi | (A + \sqrt{L})(A - \sqrt{L})\psi \rangle, \qquad \forall\, \varphi, \psi \in \mathcal{H}.$$

In particular, setting $\varphi = (A - \sqrt{L})\psi$, we get

$$\begin{aligned} 0 = \langle \varphi | (A + \sqrt{L})\varphi \rangle &= \langle \varphi | A\varphi \rangle + \langle \varphi | \sqrt{L}\varphi \rangle \geq 0 \\ &\Rightarrow \langle \varphi | A\varphi \rangle = 0 = \langle \varphi | \sqrt{L}\varphi \rangle, \ \ \forall\, \varphi = (A - \sqrt{L})\psi \,:\, \psi \in \mathcal{H}. \end{aligned}$$

Now, since A is positive, we can consider $\sqrt{A}$, and use the Cauchy–Schwarz inequality to get

$$\begin{aligned} |\langle \xi | A\varphi \rangle|^2 = |\langle \sqrt{A}\xi | \sqrt{A}\varphi \rangle|^2 &\leq \langle \sqrt{A}\xi | \sqrt{A}\xi \rangle \langle \sqrt{A}\varphi | \sqrt{A}\varphi \rangle \\ &= \langle \xi | A\xi \rangle \underbrace{\langle \varphi | A\varphi \rangle}_{=0}, \qquad \forall \xi \in \mathcal{H}. \end{aligned}$$

This shows that $A\varphi = 0$; similarly, $\sqrt{L}\varphi = 0$. Thus

$$0 = \langle\psi|(A-\sqrt{L})\varphi\rangle = \langle\psi|(A-\sqrt{L})^2\psi\rangle = ||(A-\sqrt{L})\psi||^2, \qquad \forall\,\psi\in\mathcal{H},$$

showing that $A-\sqrt{L}=0$. ☐

10.3 Bounded transform

The bounded transform of a self-adjoint operator is a way to "regularize" it, such that its spectrum is converted from a subset of $\mathbb{R}$ to a subset of $[-1,1]$. The idea is the following transformation,

$$\mathbb{R}\ni\lambda=\sinh\theta\mapsto\tanh\theta=\frac{\sinh\theta}{\cosh\theta}=\frac{\sinh\theta}{\sqrt{1+\sinh^2\theta}}=\frac{\lambda}{\sqrt{1+\lambda^2}}\in(-1,1),$$

with inverse map

$$(-1,1)\ni\lambda=\tanh\theta\mapsto\sinh\theta=\frac{\tanh\theta}{\operatorname{sech}\theta}=\frac{\tanh\theta}{\sqrt{1-\tanh^2\theta}}=\frac{\lambda}{\sqrt{1-\lambda^2}}\in\mathbb{R}. \tag{10.18}$$

Accordingly, the bounded version of H should be $H\sqrt{(1+H^2)^{-1}}$. Let us make this precise.

Lemma 10.3. *Let H be a self-adjoint operator on $\mathcal{H}$. Then*

$$(1+H^2)^{-1}:\mathcal{H}\to\mathrm{Dom}(H^2)$$

exists, and it is a bounded positive operator.

Proof. Recall (7.3): With $U:(\psi,\tilde{\psi})\mapsto(-\tilde{\psi},\psi)$ the unitary "swap" on $\mathcal{H}\oplus\mathcal{H}$, we have

$$\Gamma_H=\Gamma_{H^*}=\big(U(\Gamma_H)\big)^\perp\ \Rightarrow\ \mathcal{H}\oplus\mathcal{H}\cong\Gamma_H\oplus U(\Gamma_H).$$

So for any $\psi\in\mathcal{H}$, we can find $\varphi,\eta\in\mathrm{Dom}(H)$ such that

$$\begin{aligned}(0,\psi)=(\eta,H\eta)+U(\varphi,H\varphi)&=(\overbrace{\eta-H\varphi}^{0},H\eta+\varphi)\\&=(0,H^2\varphi+\varphi).\end{aligned}$$

Thus $\psi \in \mathcal{H}$ can be written as $(1+H^2)\varphi$ for some $\varphi \in \mathrm{Dom}(H^2)$, i.e., $1+H^2$ is surjective. Injectivity, thus invertibility, follows from it being bounded below,

$$\begin{aligned} ||(1+H^2)\varphi||^2 &= \langle \varphi + H^2\varphi | \varphi + H^2\varphi \rangle \\ &= ||\varphi||^2 + ||H^2\varphi||^2 + 2||H\varphi||^2, \qquad \forall\, \varphi \in \mathrm{Dom}(H^2). \end{aligned} \tag{10.19}$$

Eq. (10.19) also yields

$$||(1+H^2)^{-1}\psi|| = ||\varphi|| \leq ||(1+H^2)\varphi|| = ||\psi||, \qquad \psi = (1+H^2)\varphi \in \mathcal{H}.$$

This shows that the operator norm of $(1+H^2)^{-1}$ is at most 1. Furthermore,

$$\langle \psi | (1+H^2)^{-1}\psi \rangle = \langle (1+H^2)\varphi | \varphi \rangle = ||\varphi||^2 + ||H\varphi||^2 \geq 0, \qquad \forall \psi \in \mathcal{H},$$

so $(1+H^2)^{-1}$ is positive. □

Due to Lemma 10.3 and Prop. 10.2, the operator $\sqrt{(1+H^2)^{-1}}$ makes sense, and we use it for the following definition.

Definition 34. Let H be a self-adjoint operator operator on $\mathcal{H}$. Its *bounded transform* is the operator

$$\check{H} := H\sqrt{(1+H^2)^{-1}}.$$

Proposition 10.4. *For any self-adjoint operator H, its bounded transform $\check{H}$ is a bounded self-adjoint operator with spectrum in $[-1,1]$. Furthermore,*

$$(1+H^2)^{-1} = 1 - \check{H}^2. \tag{10.20}$$

Proof. Let us write $L := (1+H^2)^{-1} : \mathcal{H} \to \mathrm{Dom}(H^2)$, so $\check{H} = H\sqrt{L}$.

First, for any $\psi \in \mathcal{H}$,

$$\begin{aligned} ||\check{H}\sqrt{L}\psi||^2 &\equiv ||HL\psi||^2 \\ &= \langle HL\psi | HL\psi \rangle \\ &= \langle H^2 L\psi | L\psi \rangle \qquad (\mathcal{H} \xrightarrow{L} \mathrm{Dom}(H^2) \xrightarrow{H} \mathrm{Dom}(H = H^*)) \\ &\leq \langle (1+H^2)L\psi | L\psi \rangle \\ &= \langle \psi | L\psi \rangle = ||\sqrt{L}\psi||^2. \end{aligned}$$

We rephrase the above as

$$||\check{H}\varphi|| \leq ||\varphi||, \qquad \forall\, \varphi \in \mathrm{Ran}\sqrt{L}. \tag{10.21}$$

Next, the density of $\mathrm{Ran}\sqrt{L}$ follows from the injectivity of L,

$$\ker L = 0 \;\Rightarrow\; \ker \underbrace{\sqrt{L}}_{\text{self-adjoint}} = 0 \;\Rightarrow \overline{\mathrm{Ran}\sqrt{L}} = \mathcal{H}.$$

So any given $\varphi_\infty \in \mathcal{H}$ can be approximated by a sequence $\varphi_n \in \mathrm{Ran}\sqrt{L}$. Due to (10.21), we know that $\check{H}\varphi_n$ converges. But $\check{H} = H\sqrt{L}$ is closed (Exercise 7.1), so actually $\varphi_\infty \in \mathrm{Dom}(\check{H})$. As φ_∞ was arbitrary, this means that $\mathrm{Dom}(\check{H}) = \mathcal{H}$, i.e., $\check{H}$ is actually an everywhere-defined operator, with norm bounded by at 1 (Eq. (10.21)).

By its construction, we have $L : \mathcal{H} \to \mathrm{Dom}(H^2) \subset \mathrm{Dom}(H)$, so we can restrict it to a map $L : \mathrm{Dom}(H) \to \mathrm{Dom}(H)$. We can do the same for any polynomial function of L,

$$p(L) : \mathrm{Dom}(H) \to \mathrm{Dom}(H).$$

Now, H commutes with L when acting on $\eta \in \mathrm{Dom}(H)$,

$$\begin{aligned} LH\eta &= LH(1+H^2)(1+H^2)^{-1}\eta \\ &= L(1+H^2)H(1+H^2)^{-1}\eta \\ &= HL\eta. \end{aligned}$$

so inductively,

$$Hp_n(L)\eta = p_n(L)H\eta, \qquad \eta \in \mathrm{Dom}(H), \tag{10.22}$$

for any polynomial p.

By Prop. 10.2, there is a sequence of polynomials such that

$$p_n(L) \to \sqrt{L} \;\text{ in operator norm.}$$

The left side of (10.22) converges to $H\sqrt{L}\eta$ (the closed property of H is needed for $\sqrt{L}\eta \in \mathrm{Dom}(H)$). The right side converges to $\sqrt{L}H\eta$. The two limits coincide,

$$H\sqrt{L}\eta = \sqrt{L}H\eta, \qquad \eta \in \mathrm{Dom}(H).$$

It follows that

$$\begin{aligned}\langle\eta|\check{H}\eta\rangle &= \langle\eta|H\sqrt{L}\eta\rangle = \langle\eta|\sqrt{L}H\eta\rangle\\ &= \langle\sqrt{L}\eta|H\eta\rangle = \langle H\sqrt{L}\eta|\eta\rangle = \langle\check{H}\eta|\eta\rangle, \quad \eta\in\mathrm{Dom}(H).\end{aligned}$$

By continuity (recall $\check{H}$ is bounded), this shows that $\langle\eta|\check{H}\eta\rangle\in\mathbb{R}$ for all $\eta\in\mathcal{H}$, so by Prop. 6.9, $\check{H}$ is self-adjoint. We'd previously seen that $||\check{H}||\leq 1$, so its spectrum lies within $[-1,1]$, by Prop. 6.11.

Finally, for the identity (10.20) it suffices to check it on the dense subspace $\mathrm{Ran}\sqrt{L}$. Using $\check{H}^* = (H\sqrt{L})^* \supset \sqrt{L}H$ (Exercise 7.2),

$$\begin{aligned}(1-\check{H}^2)\sqrt{L} = (1-\check{H}^*\check{H})\sqrt{L} &\supset \sqrt{L}-\sqrt{L}H^2L\\ &= \sqrt{L}-\sqrt{L}(1+H^2)L + L^{3/2}\\ &= \sqrt{L}-\sqrt{L}L^{-1}L + L^{3/2} = L\sqrt{L}.\end{aligned}$$

Thus $(1-\check{H}^2) = L = (1+H^2)^{-1}$. □

10.4 Spectral theorem for unbounded self-adjoint operators

Theorem 10.5. *Let H be a self-adjoint operator on $\mathcal{H}$. There exists a unique PVM, $P:\mathrm{Bor}(\mathbb{R})\to\mathrm{Proj}(\mathcal{H})$, such that*

$$H = \int_{\mathbb{R}} \lambda\, dP(\lambda). \tag{10.23}$$

Proof. As before, write $L = (1+H^2)^{-1}$, and $\check{H} = H\sqrt{L}$ for the bounded transform. According to Prop. 10.4, we have $\sigma(\check{H})\subset[-1,1]$, and the identity

$$L = 1-\check{H}^2. \tag{10.24}$$

The bounded Spectral Theorem 10.1 gives

$$\check{H} = \int_{[-1,1]} \lambda\, d\check{P}(\lambda)$$

for the PVM $\check{P}$ of $\check{H}$. We expect to recover H by integrating the inverse bounded transform map $\tau:\lambda\mapsto\frac{\lambda}{\sqrt{1-\lambda^2}}$ of Eq. (10.18) against the PVM of $\check{H}$,

$$H \overset{?}{=} \int_{[-1,1]} \lambda(\sqrt{1-\lambda^2})^{-1}\, d\check{P}(\lambda).$$

Let us examine what operator on the right side actually is.

First, by the identity (10.24) and the uniqueness of positive square roots, Prop. 10.2, we have

$$\sqrt{L} = \int_{[-1,1]} \sqrt{1-\lambda^2}\, d\check{P}(\lambda).$$

By properties (10.11) and (10.13), existence of $\sqrt{L}^{-1} : \mathrm{Ran}(\sqrt{L}) \to \mathcal{H}$ follows from triviality of

$$\check{P}_{\{-1,+1\}} = \ker(\check{H}+1) \oplus \ker(\check{H}-1) \subset \ker(1-\check{H}^2) = \ker((1+H^2)^{-1}) = \{0\}.$$

Then from property (10.10) of PVM integrals,

$$\int_{[-1,1]} \lambda(\sqrt{1-\lambda^2})^{-1}\, d\check{P} \supset \left(\int_{[-1,1]} \lambda\, d\check{P}\right)\left(\int_{[-1,1]} \sqrt{1-\lambda^2}^{-1}\, d\check{P}\right) = \check{H}\sqrt{L}^{-1}.$$

The right side has domain $\mathrm{Ran}\sqrt{L}$, which is dense (proof of Prop. 10.4). Since $\check{H} = H\sqrt{L}$ is everywhere-defined, we have $\mathrm{Ran}\sqrt{L} \subset \mathrm{Dom}(H)$. Thus

$$\int_{[-1,1]} \lambda(\sqrt{1-\lambda^2})^{-1}\, d\check{P} = \check{H}\sqrt{L}^{-1} = H\sqrt{L}\sqrt{L}^{-1} = H \qquad \text{on } \mathrm{Ran}\sqrt{L} \subset \mathrm{Dom}(H),$$

which we rewrite as

$$\int_{[-1,1]} \tau\, d\check{P} \subset H.$$

But both sides are self-adjoint, so they are actually equal. Finally, Property (10.14) says that we can use the function τ to pushforward $\check{P}$ to the PVM $P = \check{P} \circ \tau^{-1}$, satisfying

$$\int_{\mathbb{R}} \lambda\, dP = \int_{[-1,1]} \tau\, d\check{P} = H.$$

The uniqueness part is omitted. □

Remark 3. Because of property (10.12), the PVM of a self-adjoint H is actually supported on its spectrum $\sigma(H) \subset \mathbb{R}$.

Example 10.1. If H is self-adjoint on a finite-dimensional Hilbert space, then its PVM is supported on the set of eigenvalues λ_i, with each $P_{\{\lambda_i\}}$ being the corresponding eigenspace projection. In general, the spectrum can include continuous intervals $[a, b]$, and usually $P_{\{\lambda\}} = 0$ for $\lambda \in [a, b]$, unless λ is an eigenvalue embedded inside $[a, b]$.

10.5 Functional calculus

For any operator T, it makes sense to apply a polynomial p to it, with the domain of $p(T)$ dictated by the rules of Definition 21. For self-adjoint $T = H = H^*$, it is not obvious that, $H^2, H^3 + H$ etc., remain self-adjoint.

Nevertheless, by Theorem 10.5, we know that H has a PVM P, so we may consider $\int_{\mathbb{R}} p\, dP$. By chasing through the definitions, one verifies that

$$p(H) = p\left(\int_{\mathbb{R}} \lambda\, dP(\lambda)\right) = \int_{\mathbb{R}} p(\lambda)\, dP(\lambda), \tag{10.25}$$

so we can take the right side of (10.25) as the definition of $p(H)$. The reason for such a redefinition, is that we often have occasion to apply more general functions to H, for example, continuous functions, or even Borel functions $f : \mathbb{R} \to \mathbb{C}$.

Definition 35. For a self-adjoint operator H and a measurable $f : \mathbb{R} \to \mathbb{C}$, we write

$$f(H) := \int_{\mathbb{R}} f\, dP. \tag{10.26}$$

where P is the unique PVM of H coming from Theorem 10.5.

The assignment $f \mapsto f(H)$ is called the *functional calculus* of H. The properties (10.9),(10.10) say that the assignment $f \mapsto f(H)$ respects sums, products, and adjoints (up to domain issues in case f is unbounded).

Example 10.2. With the functional calculus of a self-adjoint H, we can directly and unambiguously write its bounded transform in a simpler way, as

$$\check{H} = \int_{\mathbb{R}} \frac{\lambda}{\sqrt{1+\lambda^2}}\, dP(\lambda) \ \in\ \mathcal{B}(\mathcal{H}).$$

We could also use some other increasing continuous function $f : (-\infty, \infty) \to (-1, 1)$, with $\lim_{\lambda\to\pm\infty} f(\lambda) = \pm 1$, sometimes called a *switch function*, to get a modified bounded transform

$$f(H) = \int_{\mathbb{R}} f(\lambda)\, dP(\lambda) \ \in\ \mathcal{B}(\mathcal{H}).$$

Pushing this idea further, we can compose such an f with the exponential map

$$\exp(\pi i(\cdot)) : [-1, 1] \to \mathrm{U}(1) \subset \mathbb{C},$$

to obtain a unitary (why?) operator $\exp(\pi i f(H))$. A standard example is the *Cayley transform* of H,

$$U(H) := \frac{H-i}{H+i} \tag{10.27}$$

which may be shown to give a one-to-one correspondence between self-adjoint operators and unitary operators.

10.5.1 Borel functional calculus

If we restrict $f \mapsto f(H)$ to the *bounded* Borel functions f, then we get a $*$-homomorphism $B_b(\mathbb{R}) \to \mathcal{B}(\mathcal{H})$, which is continuous, with respect to the sup-norm on $B_b(\mathbb{R})$ and the operator norm on $\mathcal{B}(\mathcal{H})$. This is called the *Borel functional calculus* of H. It actually enjoys a further continuity property.

Proposition 10.6. *If $f_n \in B_b(\mathbb{R})$ is a bounded sequence converging pointwise to f, then $f_n(H)$ converges to $f(H)$ in strong operator topology.*

Proof. Note that $f \in B_b(\mathbb{R})$. For each $\psi \in \mathcal{H}$, we have

$$\begin{aligned} ||f_n(H)\psi - f(H)\psi||^2 &= \langle (f_n(H) - f(H))\psi | (f_n(H) - f(H))\psi \rangle \\ &= \langle \psi | ((f_n - f)(H))^* ((f_n - f)(H))\psi \rangle \\ &= \langle \psi | (|f_n - f|^2(H))\psi \rangle \\ &= \int_{\mathbb{R}} |f_n - f|^2 \, dP^\psi, \end{aligned}$$

where P is the PVM of H. As the f_n are sup-norm bounded, dominated convergence applies to the right side, which therefore goes to zero as $n \to \infty$. This says that $f_n(H) \to f(H)$ strongly. □

For any Borel subset $E \subset \mathbb{R}$, the characteristic function χ_E satisfies $\chi_E = \chi_E^2 = \overline{\chi_E}$. Using the Borel functional calculus, we therefore obtain a *spectral projection* $\chi_E(H)$. In applications to quantum mechanics, H is a self-adjoint Hamiltonian, and E is a subset of energies of interest. Then $\chi_E(H)$ projects onto the Hilbert subspace of "states with energies in E".