9 Spectral theorem

The free Hamiltonian, $H = -\Delta$ has no eigenvalues at all. By Fourier transform and viewing as multiplication-by-$|p|^2$, we may deduce that $\sigma(-\Delta) = [0, \infty)$, with the plane waves $x \mapsto e^{\pm ip\cdot x}$ being "generalized eigenfunctions" for "eigenvalue $|p|^2$". More generally, the Hamiltonian is $H = -\nabla^2 + V$ for some potential function, and the spectrum is a complicated mix of isolated eigenvalues and intervals.

For a general $\psi \in L^2(\mathbb{R}^d)$, the general question is not "does ψ have exactly energy E?", but "For the quantum state ψ, what is the probability that the energy is found to lie in some interval $[E_0, E_1)$?". The latter yes/no question corresponds to a *spectral projection* $P_{[E_0,E_1)}$ of the Hamiltonian H. If we use a partition

$$\bigcup_i [E_i, E_{i+1}) = \mathbb{R}$$

we get projections $P_i = P_{[E_i,E_{i+1})}$ for the yes/no question of having energy in the i-th interval. These spectral projections of H should give a corresponding "orthogonal partition" of the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$,

$$1_{\mathcal{H}} = \bigoplus_i \mathrm{Ran}(P_i),$$

corresponding to probability 1 in total.

Intuitively, as the partition gets finer and finer, the intervals approach individual points. The spectrum $\sigma(H)$ is the set of all realizable energy outcomes, and we arrive at

$$\text{“}1_{\mathcal{H}} = \bigoplus_{E\in\sigma(H)} P_{\{E\}}\text{”}, \qquad \text{“}E = \bigoplus_{E\in\sigma(H)} \lambda P_{\{E\}}\text{”}. \tag{9.1}$$

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

When $\mathcal{H}$ is finite-dimensional and H is self-adjoint, (9.1) is precisely correct, and expresses the spectral theorem in that case. In infinite dimensions, the right side must be replaced by a certain integral against a "projection-valued measure P" on $\mathbb{R}$.

9.1 Integrals with respect to projection-valued measure

The following is an operator-theoretic version of the notion of probability measure.

Definition 24. Let $\mathcal{H}$ be a Hilbert space. 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

$$P_{\sqcup_{i\in\mathbb{N}} E_i} = \sum_{i\in\mathbb{N}} P_{E_i}, \qquad \text{SOT sense.} \tag{9.2}$$

Usually, X is a topological space and Σ is the Borel σ-algebra. In this case, the *support* of a PVM is

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

Remark. In (9.2), "SOT" means "strong operator topology". It means that for each $\psi \in \mathcal{H}$, the infinite sum applied to ψ converges in $\mathcal{H}$,

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

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

Exercise 9.1. 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 $E, F \in \Sigma$.

From a PVM P, we obtain ordinary measures by taking inner products:

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

$$P^{\varphi\psi} : \Sigma \to \mathbb{C}, \qquad E \mapsto \langle \varphi | P_E \psi \rangle. \tag{9.3}$$

- In particular, for each $\psi \in \mathcal{H}$, we have a non-negative measure,

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

which is a finite *probability* measure when ψ is normalized. (Some measure theory is needed to verify that (9.3) does define a measure on Σ. See, e.g, Moretti's textbook.)

Later, we will see that a self-adjoint operator ("observable") corresponds to a PVM on (the Borel σ-algebra of) $\mathbb{R}$. Then for any given state ψ, the probability measure P^ψ encodes the probabilities for the various real-valued observable outcomes to occur.

9.2 Generalities on integration against PVM

We can integrate functions $f : X \to \mathbb{C}$ with respect to a PVM, but instead of a number, we obtain an *operator* on $\mathcal{H}$.

Definition 25. Let $P : \Sigma \to \mathrm{Proj}(\mathcal{H})$ be a PVM. For measurable $f : X \to \mathbb{C}$, define $\int_X f\, dP$ to be the operator specified by

$$\mathrm{Dom}\left(\int_X f\, dP\right) := \{\psi \in \mathcal{H} \,:\, f \in L^2(X; dP^\psi)\}, \tag{9.4}$$

$$\left\langle \varphi \middle| \left(\int_X f\, dP\right) \psi \right\rangle := \int_X f\, dP^{\varphi\psi}, \qquad \forall \psi \in \mathrm{Dom}\left(\int_X f\, dP\right), \varphi \in \mathcal{H}. \tag{9.5}$$

One can check that Eq. (9.5) uniquely characterizes the operator $\int_X f\, dP$, but this is rather indirect, so let us sketch its concrete construction. (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.)

- The *bounded* measurable functions on X form a Banach space $B_b(X)$ with the supremum norm. Some measure theory shows that the simple functions $s = \sum_{i=1}^n \alpha_i \chi_{E_i}$ are dense in $B_b(X)$. 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 $s \mapsto \int_X s\, dP$ is continuous, then extend to an assignment

$$\int_X (\cdot)\, dP : B_b(X) \to \mathcal{B}(\mathcal{H}). \tag{9.6}$$

Check that (9.6) is a $*$-homomorphism, i.e., respects sums, products, and adjoints.

- For an unbounded measurable function f, we set, for each $\psi \in \mathcal{H}$ such that $f \in L^2(X; dP^\psi)$,

$$\left(\int_X f\, dP\right)\psi := \lim_{n\to\infty} \left(\int_X f_n\, dP\right)\psi, \qquad \psi \in, \tag{9.7}$$

where $f_n \in B_b(X)$ is a(ny) sequence which approximates f in the $L^2(X; dP^\psi)$ sense. For example, we could choose

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

Then check that the construction (9.7) satisfies (9.5).

9.2.1 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.

- $\int_X f\, dP$ is densely-defined, with adjoint

$$\left(\int_X f dP\right)^* = \int_X \overline{f}\, dP. \tag{9.8}$$

In particular, $\int_X f\, dP$ is a closed operator, and self-adjoint if f is real-valued.

- The assignment $f \mapsto \int_X f\,dP$ is a homomorphism, up to domain considerations,

$$\begin{aligned} \int_X f\,dP + \alpha \int_X g\,dP \;&\subset\; \int_X f + \alpha g\,dP, \qquad\qquad \alpha \in \mathbb{C}, \\ \left(\int_X f\,dP\right)\left(\int_X g\,dP\right) \;&\subset\; \int_X fg\,dP, \end{aligned} \tag{9.9}$$

- The resolvent $(\int_X f\,dP)^{-1}$ exists iff f is P-a.e. nonzero, in which case,

$$\left(\int_X f\,dP\right)^{-1} = \left(\int_X f^{-1}\,dP\right). \tag{9.10}$$

  The spectrum of $\int_X f\,dP$ coincides with the essential range of f,

$$\sigma\left(\int_X f\,dP\right) = \big\{\lambda \in \mathbb{C} \,:\, P_{f^{-1}(\lambda-\epsilon,\lambda+\epsilon)} \neq 0 \quad \forall\, \epsilon > 0\big\}. \tag{9.11}$$

- The operator $\int_X f\,dP$ has $\lambda \in \mathbb{C}$ as an eigenvalue iff $P_{f^{-1}(\lambda)} \neq 0$. In that case, the λ eigenspace is

$$\ker\left(\int_X f\,dP \,-\lambda\right) = \mathrm{Range}\big(P_{f^{-1}(\lambda)}\big). \tag{9.12}$$

- Let $\eta : X \to X'$ be measurable, 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 $f' : X' \to \mathbb{C}$,

$$\int_{X'} f'\,dP' = \int_X (f' \circ \eta)\,dP. \tag{9.13}$$

Specialize to $X = \mathbb{R}$ and $\Sigma = \mathrm{Bor}(\mathbb{R})$ the Borel σ-algebra. Given a PVM on $(\mathbb{R}, \mathrm{Bor}(\mathbb{R}))$, Property (9.8) says that

$$\int_{\mathbb{R}} \lambda\,dP(\lambda) \tag{9.14}$$

is a self-adjoint operator. (Compare Eq. (9.14) with the informal sum (9.1).) The Spectral Theorem 9.5 is the converse statement.

9.3 Spectral theorem for bounded self-adjoint operators (Sketched in lecture)

Theorem 9.1. *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*

$$H = \int_I \lambda \, dP(\lambda). \tag{9.15}$$

Proof. (Optional.) When a polynomial p is considered as a function on $I \supset \sigma(H)$, its supremum norm $||p||_\infty$ makes sense. It is not hard to check that $||p(H)||_{\mathrm{op}} \leq ||p||_\infty$. Now, for each pair $\varphi, \psi \in \mathcal{H}$,

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

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

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

By the *Stone–Weierstrass* theorem[16] and the *Riesz–Markov* representation theorem, there is a unique (regular, complex) Borel measure $\mu^{\varphi\psi}$ on I such 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 every $E \in \mathrm{Borel}(I)$. Thus, for each $E \in \mathrm{Borel}(I)$, we have a bounded sesquilinear form $\mu^{\varphi\psi}(E)$ on $\mathcal{H}$, which by Lemma 5.6, defines a bounded operator P_E on $\mathcal{H}$ via the equation

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

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

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

$$\langle \varphi | H \psi \rangle = \int_I \lambda \, d\mu^{\varphi\psi}(\lambda) \overset{(9.5)}{=} \left\langle \varphi \middle| \left(\int_I \lambda \, dP(\lambda) \right) \psi \right\rangle, \qquad \forall \, \varphi, \psi \in \mathcal{H}.$$

So $H = \int_I \lambda \, dP(\lambda)$. The uniqueness proof is omitted. □

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

9.3.1 Positive square root

The spectral theorem allows us to construct positive square roots of positive operators.

Definition 26. An operator $L : \mathrm{Dom}(L) \to \mathcal{H}$ is *positive* if

$$\langle \psi | L\psi \rangle \geq 0, \qquad \forall\, \psi \in \mathrm{Dom}(L). \tag{9.16}$$

Exercise 9.2. Let L be a bounded positive operator. Show that L is self-adjoint, and has non-negative spectrum.

Proposition 9.2. *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 $p_n(L)$ where p_n is a sequence of polynomials.*

Proof. There are three claims in this Proposition.

- Existence. By Exercise 9.2, there is an interval $I = [0, a]$ containing $\sigma(L)$, so the positive square root function $\sqrt{(\cdot)} : C(I) \to [0, \infty)$ is well-defined. Also, L has a PVM P (Spectral Theorem 9.1), so we get a (bounded) operator

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

  which is positive because

  $$\left\langle \psi \middle| \left(\int_I \sqrt{\lambda}\, dP(\lambda) \right) \psi \right\rangle = \int_I \sqrt{\lambda}\, dP^\psi \geq 0, \qquad \forall\, \psi \in \mathcal{H}.$$

  The homomorphism property (9.9) verifies the square root property,

  $$\sqrt{L}^2 = \Big(\int_I \sqrt{\lambda}\, dP(\lambda) \Big) \Big(\int_I \sqrt{\lambda}\, dP(\lambda) \Big) = \int_I \lambda\, dP(\lambda) = L.$$

- Approximation. For 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 implies

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

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

- Uniqueness. 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

  $$\begin{aligned} 0 = \langle\varphi|(A + \sqrt{L})\varphi\rangle &= \langle\varphi|A\varphi\rangle + \langle\varphi|\sqrt{L}\varphi\rangle \geq 0 \\ &\Rightarrow \langle\varphi|A\varphi\rangle = 0 = \langle\varphi|\sqrt{L}\varphi\rangle. \end{aligned}$$

  As A is positive, $\sqrt{A}$ exists, and the Cauchy–Schwarz inequality gives

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

  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 $A - \sqrt{L} = 0$.

□

9.4 Bounded transform

An unbounded self-adjoint operator can be "regularized" to become a bounded operator whose spectrum lies inside $[-1, 1]$. This "bounded transform" is basically the operator-theoretic version of the following homeomorphism $\mathbb{R} \to (-1, 1)$,

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

with inverse

$$(-1, 1) \ni \lambda = \tanh\theta \mapsto \sinh\theta = \frac{\lambda}{\sqrt{1 - \lambda^2}} \in \mathbb{R}. \tag{9.17}$$

The bounded transform of H is defined to be $H\sqrt{(1 + H^2)^{-1}}$, but we should first argue that this expression makes sense.

Lemma 9.3. *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 from (7.4) that Γ_{H^*} and the swapped version of Γ_{-H} are orthogonal complements in $\mathcal{H} \oplus \mathcal{H}$. So, for any $\psi \in \mathcal{H}$, we can find $\varphi, \eta \in \mathrm{Dom}(H)$ such that

$$(0,\psi) = (\eta, \underbrace{H}_{=H^*}\eta) + (-H\varphi, \varphi) = (\overbrace{\eta - H\varphi}^{0}, H\eta + \varphi) = (0, (H^2+1)\varphi).$$

This shows that $1+H^2$ is surjective. Injectivity of $1+H^2$ follows from it being bounded below,

$$\begin{aligned} ||(1+H^2)\varphi||^2 &= \langle \varphi + H^2\varphi | \varphi + H^2\varphi \rangle \\ &= ||\varphi||^2 + ||H^2\varphi||^2 + 2||H\varphi||^2, \qquad \forall\, \varphi \in \mathrm{Dom}(H^2). \end{aligned} \tag{9.18}$$

Eq. (9.18) also shows that $(1+H^2)^{-1}$ is bounded (or use closed graph theorem). 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. □

Lemma 9.3 and Prop. 9.2 imply that $\sqrt{(1+H^2)^{-1}}$ exists, so the following definition makes sense.

Definition 27. Let H be a self-adjoint operator operator on $\mathcal{H}$. Its *bounded transform* is the operator

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

Proposition 9.4. *For any self-adjoint operator H, its bounded transform $\check{H}$ is a bounded self-adjoint operator with spectrum a subset of $[-1,1]$. Furthermore,*

$$(1+H^2)^{-1} = 1 - \check{H}^2. \tag{9.19}$$

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

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

We rephrase the above as

$$||\check{H}\varphi|| \leq ||\varphi||, \qquad \forall\, \varphi \in \mathrm{Ran}\sqrt{L}. \tag{9.20}$$

Next, $\mathrm{Ran}\sqrt{L}$ is dense because

$$\ker L = 0 \;\Rightarrow\; \ker \underbrace{\sqrt{L}}_{\text{self-adjoint}} = 0.$$

So any given $\varphi_\infty \in \mathcal{H}$ can be approximated by a sequence $\varphi_n \in \mathrm{Ran}\sqrt{L}$. Due to (9.20), 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 ≤ 1 (Eq. (9.20)).

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 $L : \mathrm{Dom}(H) \to \mathrm{Dom}(H)$. Now, H commutes with L when acting on $\mathrm{Dom}(H)$,

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

For any polynomial p, it makes sense to also consider $p(L) : \mathrm{Dom}(H) \to \mathrm{Dom}(H)$, and inductively,

$$Hp(L)\eta = p(L)H\eta, \qquad \eta \in \mathrm{Dom}(H), \tag{9.21}$$

as well. Apply (9.21) to the sequence of polynomials $p_n \to_{\mathrm{norm}} \sqrt{L}$ from Prop. 9.2. The left side of (9.21) converges to $H\sqrt{L}\eta$, while the right side converges to $\sqrt{L}H\eta$. The two limits coincide,

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

It follows that

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

By continuity ($\check{H}$ is bounded), this shows that $\langle \eta | \check{H}\eta \rangle \in \mathbb{R}$ for all $\eta \in \mathcal{H}$, so by Prop. 6.8, $\check{H}$ is self-adjoint. We had previously seen that $||\check{H}|| \leq 1$, so its spectrum lies within $[-1, 1]$, by Prop. 6.10.

Finally, for the identity (9.19) 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), the following identity holds when applied to any $\psi \in \mathcal{H}$,

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

Thus $(1 - \check{H}^2) = L \equiv (1 + H^2)^{-1}$ holds on $\mathrm{Ran}\sqrt{L}$, thus on $\mathcal{H}$. □

9.5 Spectral theorem for unbounded self-adjoint operators

Theorem 9.5. *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*

$$H = \int_{\mathbb{R}} \lambda \, dP(\lambda). \tag{9.22}$$

Proof. According to Prop. 9.4, we have $\sigma(\check{H}) \subset [-1, 1]$, and the identity

$$L = 1 - \check{H}^2. \tag{9.23}$$

The bounded self-adjoint Spectral Theorem 9.1 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. (9.17) against the PVM of $\check{H}$,

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

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

First, by the identity (9.23) and the uniqueness of positive square roots, Prop. 9.2, we have

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

By properties (9.10) and (9.12), 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 (9.9) 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. 9.4). 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 (9.13) 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 (9.11), the PVM of a self-adjoint H is supported on its spectrum $\sigma(H) \subset \mathbb{R}$.

Example 9.1. 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 $[a,b]$. For $\lambda \in [a,b]$, unless λ is an eigenvalue embedded inside $[a,b]$, we would have $P_{\{\lambda\}} = 0$.

9.6 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 13. For self-adjoint $T = H = H^*$, it is not obvious that $H^2, H^3 + H$ etc., remain self-adjoint.

Nevertheless, by Theorem 9.5, 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

$$p(H) = p\left(\int_{\mathbb{R}} \lambda\, dP(\lambda)\right) = \int_{\mathbb{R}} p(\lambda)\, dP(\lambda), \tag{9.24}$$

so we can take the right side of (9.24) as the *definition* of $p(H)$. The right side continues to make sense for more general functions, such as continuous functions, or even Borel functions $f : \mathbb{R} \to \mathbb{C}$.

Definition 28. For a self-adjoint operator H and a measurable $f : \mathbb{R} \to \mathbb{C}$, we write

$$f(H) := \int_{\mathbb{R}} f\, dP. \tag{9.25}$$

where P is the unique PVM of H coming from Theorem 9.5.

The assignment $f \mapsto f(H)$ is called the *functional calculus* of H. The properties (9.8),(9.9) say that the assignment $f \mapsto f(H)$ respects sums, products, and adjoints (up to domain issues in case f is unbounded).

Example 9.2. 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,

$$U(H) := \frac{i - H}{i + H} \tag{9.26}$$

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

9.6.1 Borel functional calculus and spectral projections

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 9.6. *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* $\chi_E(H)$.

10 Stone's theorem

10.1 Time-evolution

Recall the fundamental (abstract) Schrödinger equation of motion,

$$i\hbar\frac{\partial}{\partial t}\psi_t = H\psi_t.$$

The formal solution,

$$\psi_t = U_t\psi_0, \qquad U_t = e^{-iHt/\hbar},$$

only makes sense if $t \mapsto U_t$ is differentiable in a suitable sense, and this is equivalent to the self-adjointness of H, as we will see.

We write $\mathcal{U}(\mathcal{H})$ for the group of unitary operators on a Hilbert space $\mathcal{H}$.

Definition 29. A *strongly-continuous one-parameter unitary group* is a group homomorphism $U : \mathbb{R} \to \mathcal{U}(\mathcal{H})$, such that

$$\lim_{s\to 0} U_{s+t}\psi = U_t\psi, \qquad \forall\, \psi \in \mathcal{H},\, t \in \mathbb{R}. \tag{10.1}$$

At $t = 0$, (10.1) is the statement

$$\lim_{s\to 0} U_s\psi = \psi = 1_{\mathcal{H}}\psi, \qquad \forall\, \psi \in \mathcal{H}. \tag{10.2}$$

In other words, $U_s \to 1_{\mathcal{H}}$ in strong operator topology (SOT), as $s \to 0$. Applying (10.2) to $U_t\psi$ shows that (10.1) holds at any t as well.

Proposition 10.1. *If H is a self-adjoint operator on $\mathcal{H}$, then the map $U : t \mapsto e^{-iHt}$ is a strongly-continuous one-parameter unitary group. Furthermore,*

$$\mathrm{Dom}(H) = \{\psi \in \mathcal{H} \,:\, \lim_{s\to 0} \frac{1}{s}(U_s\psi - \psi) \text{ exists}\}. \tag{10.3}$$

Furthermore,

$$\lim_{s\to 0} \frac{1}{s}(U_{t+s}\psi - U_t\psi) = -iHU_t\psi, \qquad \psi \in \mathrm{Dom}(H),\, t \in \mathbb{R}. \tag{10.4}$$

Proof. That $t \mapsto U_t = e^{-iHt}$ is a group homomorphism follows from the functional calculus of H.

For each $\psi \in \mathcal{H}$, consider

$$||e^{-isH}\psi - \psi||^2 = \left\langle \psi \middle| \left(\int_{\mathbb{R}} |e^{-is\lambda} - 1|^2 \, dP(\lambda) \right) \psi \right\rangle$$
$$= \int_{\mathbb{R}} |e^{-is\lambda} - 1|^2 \, dP^{\psi}(\lambda), \tag{10.5}$$

where P is the PVM of H. The map $\lambda \mapsto |e^{-i\lambda s} - 1|^2$ tends pointwise to 0 as $s \to 0$, and is dominated by the constant function 2. So Lebesgue's dominated convergence theorem applies to the right side of (10.5), and we deduce that the left side converges to 0. As $\psi \in \mathcal{H}$ was arbitrary, this shows (10.2) (thus (10.1) holds).

Next, we show the inclusion $\subset$ in (10.3). Observe that for any $\lambda \in \mathbb{R}$,

$$\frac{1}{s}(e^{-is\lambda} - 1) \underset{s \to 0}{\longrightarrow} -i\lambda.$$

Check that the left side is bounded by $|\lambda|$. Then the same kind of dominated convergence argument works to establish

$$\left\langle \varphi \middle| \lim_{s \to \infty} \frac{1}{s}(U_s\psi - \psi) \right\rangle = \int_{\mathbb{R}} -i\lambda \, dP^{\varphi\psi} = \langle \varphi | -iH\psi \rangle, \qquad \forall\, \psi \in \mathrm{Dom}(H),\ \varphi \in \mathcal{H}.$$

(Recall the Spectral Theorem 9.5 and (9.4)). So $\lim_{s\to\infty} \frac{1}{s}(U_s\psi - \psi)$ exists, and equals $-iH\psi$.

We may extend the last calculation, and define the following extension $\tilde{H}$ of H,

$$\mathrm{Dom}(\tilde{H}) = \{\psi \in \mathcal{H} \,:\, \lim_{s \to 0} \frac{1}{s}(U_s\psi - \psi) \text{ exists}\}$$
$$\tilde{H}\psi = i \lim_{s \to 0} \frac{1}{s}(U_s\psi - \psi).$$

It is easily checked that $\tilde{H}$ is symmetric (use continuity of inner product). But H is already self-adjoint, so $\tilde{H} = H$, with the same domain, thus (10.3) holds.

Finally, we derive the formula (10.4) for the "infinitesimal generator" of U_t. Note that for any $t \in \mathbb{R}$, the limit

$$\lim_{s \to 0} \left(\frac{U_{t+s} - U_t}{s} \psi \right) = \lim_{s \to 0} U_t \frac{1}{s}((U_s - 1)\psi) = U_t \big(\lim_{s \to 0} \frac{1}{s}(U_s - 1)\psi \big).$$

exists iff it does for $t = 0$, iff $\psi \in \mathrm{Dom}(H)$, in which case

$$\lim_{s\to 0}\left(\frac{U_{t+s}-U_t}{s}\psi\right) = \lim_{s\to 0}\left(\frac{U_s - 1}{s}U_t\psi\right) = -iHU_t\psi.$$

□

Following Prop. 10.1, we say that for a self-adjoint operator H, the 1-parameter unitary group $t \mapsto e^{-iHt}$ is *differentiable* on $\mathrm{Dom}(H)$, with derivative, or *infinitesimal generator*, being the operator $-iH$. Conversely:

Theorem 10.2 (Stone's theorem)**.** *A strongly-continuous one-parameter unitary group $t \mapsto U_t$ has a unique self-adjoint* infinitesimal generator *H, in the sense that $U_t = e^{-iHt}, t \in \mathbb{R}$.*

Proof. We will construct a domain $\mathrm{Dom}(A) \subset \mathcal{H}$ canonically associated to U_t. A symmetric operator A with this domain will then be constructed, and essential self-adjointness proven, then the required H will be $\overline{A}$.

- For each $\psi \in \mathcal{H}$, and each $f \in C_c^\infty(\mathbb{R})$, define

  $$\psi_f := \int_{\mathbb{R}} f(t)U_t\psi\, dt,$$

  viewed as a $\mathcal{H}$-valued Riemann integral ($t \mapsto U_t\psi$ is continuous). Let $\mathrm{Dom}(A)$ be the linear span of such ψ_f.

- Next, we use a fundamental result that smooth, compactly-supported bump functions exist over $\mathbb{R}$, e.g., take

  $$x \mapsto \begin{cases} e^{-\frac{1}{1-x^2}}, & |x| \le 1, \\ 0, & |x| \ge 1. \end{cases}$$

  Let η be the above bump function, normalized to have integral 1 over $\mathbb{R}$. For $\epsilon > 0$, define $\eta_\epsilon(\cdot) = \frac{1}{\epsilon}\eta((\cdot)/\epsilon)$, which also has integral 1 but has modified support $[-\epsilon, \epsilon]$.

- Now consider

  $$\begin{aligned} ||\psi_{\eta_\epsilon} - \psi|| &= \left|\left| \int_{\mathbb{R}} \eta_\epsilon(t)U_t\psi - \eta_\epsilon(t)\psi\, dt \right|\right| \\ &\le \left(\int_{\mathbb{R}} \eta_\epsilon\right) \cdot 2\epsilon \cdot \sup_t ||(U_t - 1)\psi||. \end{aligned}$$

  This shows that any $\psi \in \mathcal{H}$ can be norm-approximated by elements of $\mathrm{Dom}(A)$, i.e., $\mathrm{Dom}(A)$ is dense in $\mathcal{H}$.

- For $\psi_f \in \mathrm{Dom}(A)$, and $s \in \mathbb{R}$,

$$\begin{aligned}\frac{1}{s}(U_s - 1)\psi_f &\equiv \frac{1}{s}U_s \int_{\mathbb{R}} f(t)U_t\psi \, dt - \frac{1}{s}\int_{\mathbb{R}} f(t)U_t\psi \, dt \\ &= \int_{\mathbb{R}} f(t)\frac{U_{t+s} - U_t}{s}\psi \, dt \\ &= \int_{\mathbb{R}} \frac{f(\tau - s) - f(\tau)}{s}U_\tau\psi \, d\tau \qquad (s + t =: \tau)\end{aligned}$$

Since f is smooth and compactly-supported,

$$\lim_{s\to 0}\left(\frac{1}{s}(U_s - 1)\psi_f\right) = -\int_{\mathbb{R}} f'(\tau)U_\tau\psi \, d\tau \equiv -\psi_{f'}. \tag{10.6}$$

We may thus define the linear map (with (10.4) in mind),

$$\begin{aligned}A : \mathrm{Dom}(A) &\to \mathrm{Dom}(A) \\ \psi &\mapsto i\lim_{s\to 0}\left(\frac{U_s - 1}{s}\psi\right), \\ \psi_f &\overset{(10.6)}{\mapsto} -i\psi_{f'}.\end{aligned} \tag{10.7}$$

Notice that U_t also takes $\mathrm{Dom}(A)$ to $\mathrm{Dom}(A)$, since

$$\begin{aligned}U_t\psi_f = U_t\int_{\mathbb{R}} f(\tau)U_\tau\psi \, d\tau &= \int_{\mathbb{R}} f(\tau)U_{t+\tau}\psi \, d\tau \\ &= \int_{\mathbb{R}} f(s - t)U_s\psi \, ds = \psi_{f((\cdot)-t)}.\end{aligned}$$

Together with (10.7), we have

$$\frac{d}{dt}(U_t\psi) = -\psi_{f'((\cdot)-t)} = -iA\psi_{f((\cdot)-t)} = -iAU_t\psi, \qquad \psi \in \mathrm{Dom}(A),\ t \in \mathbb{R}. \tag{10.8}$$

- For $\psi_f, \psi_g \in \mathrm{Dom}(A)$, Eq. (10.7) allows us to deduce

$$\begin{aligned}\langle A\psi_f|\psi_g\rangle = \langle i\psi_{f'}|\psi_g\rangle &= \left\langle i\lim_{s\to 0}\frac{1}{s}(U_s - 1)\psi_f \middle| \psi_g\right\rangle \\ &= \left\langle \psi_f \middle| -i\lim_{s\to 0}\frac{1}{s}(U_{-s} - 1)\psi_g\right\rangle \\ &= \langle\psi_f|A\psi_g\rangle, \qquad (\text{Eq. (10.7)})\end{aligned}$$

so A is symmetric.

- We check that A is essentially self-adjoint, using the criterion in Prop. 8.4, that $\ker(A^* \mp i) = 0$. Suppose otherwise, that $\xi \in \mathrm{Dom}(A^*)$ satisfies $(A^* \mp i)\xi = 0$. Let $\psi \in \mathrm{Dom}(A)$. We have

$$\begin{aligned} \frac{d}{dt}\langle \xi | U_t \psi \rangle &= \langle \xi | - iAU_t\psi \rangle \qquad\qquad \text{(Eq. (10.8))} \\ &= \langle iA^*\xi | U_t \psi \rangle \\ &= \mp \langle \xi | U_t \psi \rangle. \end{aligned}$$

  Consider the function $F \equiv F_\psi : t \mapsto \langle \xi | U_t \psi \rangle$. The above calculation says that $F'(t) = \mp F(t)$, i.e., $F(t) = F(0)e^{\mp t}$. But U_t has norm 1, so $F(t)$ must be bounded, for every $t \in \mathbb{R}$. Thus $\langle \xi | \psi \rangle = F(0)$ must vanish. As $\psi \in \mathrm{Dom}(A)$ was arbitrary, we must have $\xi = 0$.

- Since $H := \overline{A}$ is self-adjoint, Prop. 10.1 gives the strongly-continuous one-parameter unitary group $V_t := e^{-iHt}$. For $\psi \in \mathrm{Dom}(A)$, write

$$\varphi(t) := (U_t - V_t)\psi.$$

  We have, by (10.8) and Prop. 10.1,

$$\frac{d}{dt}\varphi(t) = -iAU_t\psi + iHV_t\psi = -iH\varphi(t) \ \in \mathrm{Dom}(A) \subset \mathrm{Dom}(H),$$

  and so

$$\begin{aligned} \frac{d}{dt}||\varphi(t)||^2 &= \big\langle \varphi(t) \big| \frac{d}{dt}\varphi(t) \big\rangle + \big\langle \frac{d}{dt}\varphi(t) \big| \varphi(t) \big\rangle \\ &= 2\mathrm{Re}\langle \varphi(t) | - iH\varphi(t) \rangle = -2\mathrm{Re}(i\langle \varphi(t) | H\varphi(t) \rangle) = 0. \end{aligned}$$

  Since $\varphi(0) = 0$, we have

$$(U_t - V_t)\psi = \varphi(t) = 0, \qquad\qquad \forall\, t \in \mathbb{R},\ \psi \in \mathrm{Dom}(A).$$

  As $\mathrm{Dom}(A)$ is dense, this shows that $U_t = V_t \equiv e^{-iHt}$, for all $t \in \mathbb{R}$.

- Suppose $U_t = e^{iH't}$ holds for some other self-adjoint H'. We would deduce, in a similar way, that A is a restriction of H'. But we know that A is essentially self-adjoint, so H' must coincide with $H = \overline{A}$.

□

Corollary 10.3. *Let $t \mapsto U_t$ be a strongly-continuous 1-parameter unitary group. Suppose* Dom *is a dense domain such that $U_t : \mathrm{Dom} \to \mathrm{Dom}, t \in \mathbb{R}$, and that $t \mapsto U_t$ is differentiable on* Dom*. Then*

$$\lim_{s\to 0}\left(\frac{U_s\psi - \psi}{s}\right) = -iA\psi, \qquad \psi \in \mathrm{Dom}$$

with A essentially self-adjoint on Dom*, and $\overline{A}$ is the self-adjoint generator of $t \mapsto U_t$.*

Proof. These follow from the proof of Theorem 10.2. □

Example 10.1. On the Hilbert space $L^2(\mathbb{R})$ (with Lebesgue measure on $\mathbb{R}$), consider the translation operators

$$U_t\psi(x) = \psi(x - t), \qquad \psi \in L^2(\mathbb{R}),\ t \in \mathbb{R}.$$

Exercise: show that $t \mapsto U_t$ is a strongly-continuous 1-parameter unitary group. Thus it has a self-adjoint generator. The dense domain $\mathcal{S}(\mathbb{R})$ of Schwartz functions is preserved by the unitary operators U_t, and the derivative on this domain is

$$\lim_{s\to 0}\left(\frac{U_s\psi - \psi}{s}\right) = -\frac{d}{dx}\psi = -i\left(-i\frac{d}{dx}\right)\psi, \qquad \psi \in \mathcal{S}(\mathbb{R}).$$

By Corollary 10.3, we see that the generator of the spatial translation group, $t \mapsto U_t$, is the closure of the above $-i\frac{d}{dx}$ operator, i.e., the self-adjoint momentum operator, $\hat{p} : \psi \mapsto -i\psi'$ (Definition 19).

Exercise 10.1. Suppose $t \mapsto U_t$ is a norm-continuous 1-parameter unitary group. What does this mean for its self-adjoint generator H?

10.2 Symmetries and conserved quantities

Stone's Theorem 10.2 is of fundamental importance in quantum theory. Recall that Hilbert space automorphisms are implemented by unitaries. If there is a certain 1-parameter (sub)group $t \mapsto g(t)$ of symmetries for the description of a quantum mechanical system, it should be unitarily implemented as a

strongly-continuous[17] 1-parameter unitary group[18] $t \mapsto U_t$. By Stone's theorem, there is therefore an associated self-adjoint generator H. The generator H is a quantum mechanical observable which is "conserved". (In classical mechanics, the relationship between continuous symmetries and conserved quantities is due to E. Noether.)

Example 10.2. The time line is affine — it has no preferred origin. The self-adjoint Hamiltonian/energy operator $H = H^*$ is the infinitesimal generator for the 1-parameter unitary group of *time translation operators*, $t \mapsto e^{-iHt/\hbar}$.

Suppose, at time 0, that $\psi_0 \in \mathrm{Dom}(H)$ is an eigenvector of H with energy eigenvalue E. For the time-translated $\psi_t = e^{-iHt/\hbar}\psi_0$, we have

$$H\psi_t = He^{-iHt/\hbar}\psi_0 = e^{-iHt/\hbar}H\psi_0 = e^{-iHt/\hbar}E\psi_0 = Ee^{-iHt/\hbar}\psi_0 = E\psi_t,$$

so ψ_t still has energy E. This is the quantum mechanical notion of "conservation of energy".

Example 10.3. The affine Euclidean line has no preferred origin. Example 10.1 says that the unitary group $a \mapsto V_a$ of spatial translations on $L^2(\mathbb{R})$ is generated by the momentum operator $\hat{p} = -i\hbar\frac{d}{dx}$ (more precisely, the weak derivative),

$$V_a = e^{-ia\hat{p}/\hbar}.$$

One says that momentum is the conserved quantity associated to spatial-translation symmetry. For $p \in \mathbb{R}$, the plane-wave $\psi_p : x \mapsto e^{ixp}$ is a "generalized eigenvector" of $\hat{p}$ with "eigenvalue" $\hbar p$. If we spatially translate ψ_p by any $a \in \mathbb{R}$,

$$V_a\psi_p(x) = \psi_p(x-a) = \psi_p(x)e^{-iap},$$

then $V_a\psi_p$ remains a "generalized eigenvector" of $\hat{p}$ with eigenvalue $\hbar p$.

Example 10.4. On $\psi \in L^2(S^1)$, there is a 1-parameter unitary group $\theta \mapsto R_\theta$ acting by rotations,

$$R_\theta\psi(z) = \psi(e^{-i\theta}z), \qquad \theta \in \mathbb{R}, \tag{10.9}$$

[17] A remarkable result by von Neumann says that strong continuity of $t \mapsto U_t$ is already implied by weak measurability in the sense that $t \mapsto \langle\varphi|U_t\psi\rangle$ is measurable for all $\varphi, \psi \in \mathcal{H}$. See Reed–Simon Theorem VIII.9 for a proof.

[18] More precisely, because only $|\langle\varphi|\psi\rangle|$ matters, symmetries can also be implemented projectively (up to a U(1)-phase ambiguity), and/or antiunitarily; this is *Wigner's Theorem*.

which is strongly-continuous (exercise). Consider the orthonormal basis elements (Fourier series)

$$\psi_n(z) = \frac{1}{\sqrt{2\pi}} z^n, \qquad n \in \mathbb{Z}.$$

Note that $R_\theta \psi_n = e^{-in\theta}\psi_n$. We have

$$\frac{R_\theta \psi_n(z) - \psi_n(z)}{\theta} = \underbrace{\frac{(e^{-in\theta}-1)}{\theta}}_{\stackrel{\theta\to 0}{\longrightarrow} -in} \underbrace{\frac{1}{\sqrt{2\pi}} z^n}_{\psi_n(z)},$$

and deduce that

$$\lim_{\theta\to 0} \left(\frac{(R_\theta - 1)\psi_n}{\theta} \right) = -in\psi_n. \qquad (\text{in } L^2(S^1))$$

By Corollary 10.3, the operator

$$L\psi = i\hbar \sum_n -in a_n \psi_n = -i\hbar \frac{d}{d\theta}\psi, \qquad \psi = \sum_n a_n \psi_n \in \operatorname{span}\{\psi_n : n \in \mathbb{Z}\},$$

is essentially self-adjoint, and its closure $\overline{L}$ is the self-adjoint generator of

$$\theta \mapsto R_\theta = e^{-i\theta \overline{L}/\hbar}.$$

The self-adjoint operator $\overline{L} = -i\hbar \frac{d}{d\theta}$ (weak derivative) is the *orbital angular momentum* operator. Its eigenvalues are quantized to integer multiplies of $\hbar$, with respective eigenfunctions ψ_n.

Let x_1, x_2, x_3 be the Cartesian coordinates of $\mathbb{R}^3$, and X_1, X_2, X_3 be the respective operators of multiplication by the x_1, x_2, x_3 coordinates. Eq. (10.9) can be viewed as a unitary action on $L^2(\mathbb{R}^3)$, implementing rotation about the x_3-axis. On the Schwartz functions,

$$L_3\psi = -i\hbar \left(X_1 \frac{\partial}{\partial x_2} - X_2 \frac{\partial}{\partial x_1} \right) \psi, \qquad \psi \in \mathcal{S}(\mathbb{R}^3).$$

Similarly, for rotations about the x_1 and x_2-axes, we have the operators on $\mathcal{S}(\mathbb{R}^3)$,

$$L_2\psi = -i\hbar \left(X_3 \frac{\partial}{\partial x_1} - X_1 \frac{\partial}{\partial x_3} \right),$$
$$L_1\psi = -i\hbar \left(X_2 \frac{\partial}{\partial x_3} - X_3 \frac{\partial}{\partial x_2} \right).$$

It may be shown that the L_i are essentially self-adjoint (Moretti Section 10.2.3). The closure $\overline{L_i}$ is the orbital angular momentum operator, generating the unitary group of rotations about the i-th coordinate axis.

In terms of representation theory, the non-abelian group SO(3) is being represented on $L^2(\mathbb{R}^3)$ by pullback of wavefunctions. This is a strongly-continuous unitary representation. Inside SO(3), there are some one-parameter subgroups, e.g., corresponding to rotations around an axis. Such a subgroup gives rise to a strongly-continuous 1-parameter unitary group in $\mathcal{U}(L^2(\mathbb{R}^3))$. At the "infinitesimal" level, the Lie algebra $\mathfrak{so}(3)$ (a 3-dimensional real vector space, studied in later lectures) is being represented as the infinitesimal generators L_i. The Lie bracket becomes the operator commutator, and the noncommutativity of the L_i reflects the non-trivial Lie bracket.

Remark. There is another kind of angular momentum, called *spin* angular momentum, which is due to symmetry under local (spin) frame rotations, and is quantized in units of $\frac{\hbar}{2}$. We will discuss this in the spin geometry part of the lectures.

Dynamical symmetries Suppose the Hamiltonian operator H "commutes" with the self-adjoint generator A of some 1-parameter unitary group $V_s = e^{-isA/\hbar}$. Let $\psi_0 \in \mathrm{Dom}(A)$ be an eigenvector of A, with eigenvalue λ. Then, formally,

$$A\psi_t = Ae^{-iHt/\hbar}\psi_0 \stackrel{?}{=} e^{-iHt/\hbar}A\psi_0 = \lambda e^{-iHt/\hbar}\psi_0 = \lambda\psi_t, \tag{10.10}$$

so ψ_t continues to have definite eigenvalue λ for the A, at any time t. Thus the quantity λ is *dynamically unchanged* (time-independent). Indeed, in a quantum dynamical setting, one often uses the word "symmetry" to mean (a group of) unitary operators which "commute with the Hamiltonian".

For example, the free Hamiltonian $-\frac{\hbar^2}{2m}\nabla^2 = \frac{1}{2m}\hat{p}^2$ is translation invariant, and commutes with the spatial translation generator $\hat{p}$, leading to "conservation of momentum". Similarly, on $\mathbb{R}^3$, the free Hamitonian $-\frac{\hbar^2}{2m}\nabla^2$ is rotationally invariant, and commutes with $\overline{L}_i$, leading to "conservation of angular momenta". Schrödinger operators $H = -\frac{\hbar^2}{2m}\nabla^2 + V$ with *central potential* V (meaning V depends only on the radial coordinate) are also rotationally invariant, the Coulomb Hamiltonian being the basic example.

However, can we really commute A past $e^{-iHt/\hbar}$ in (10.10)? For unbounded H (and/or A), what does "H commutes with A" really mean?

We emphasize that commutativity of unbounded operators A, B is a very delicate issue. Even if A, B are essentially self-adjoint on the same Dom, and $A, B : \mathrm{Dom} \to \mathrm{Dom}$, it is not true that the naïve commutativity

$$AB\psi = BA\psi, \ \forall \psi \in \mathrm{Dom}$$

implies commutativity of $\overline{A}, \overline{B}$ in the following sense:

Definition 30. Two self-adjoint operators A, B are said to *commute*, if all the projections in their associated PVMs commute.

Proposition 10.4. *Self-adjoint operators A, B commute iff*

$$e^{itA}e^{isB} = e^{isB}e^{itA}, \qquad \forall\, s, t \in \mathbb{R}.$$

Proof. Omitted. A proof can be found in Reed–Simon VIII.13. □

Example 10.5 (Nelson's (counter)example). Let M be a 2-sheeted Riemann surface, and the Hilbert space $L^2(M)$. The formal differential operators $-i\partial_x, -i\partial_y$ can be shown to be essentially self-adjoint on the smooth functions with compact support away from a branch cut, and they commute when applied to such functions. Their self-adjoint closures, denoted $\hat{p}_x, \hat{p}_y$, generate the translations in the coordinates x and y respectively. However, these translation groups do not commute, due to the global monodromy. In view of Prop. 10.4, $\hat{p}_x, \hat{p}_y$ do not commute.

Returning to the situation where H commutes with A, now understood in the sense of Definition 30. By Prop. 10.4, when $\psi_0 \in \mathrm{Dom}(A)$ has eigenvalue λ, we deduce that

$$\begin{aligned} A\psi_t = AU_t\psi_0 &= \lim_{s\to 0}(s^{-1}(V_s - 1)(U_t\psi_0)) \\ &= U_t \lim_{s\to 0}(s^{-1}(V_s - 1)\psi_0) = U_tA\psi_0 = U_t\lambda\psi_0 = \lambda U_t\psi_0 = \lambda\psi_t, \end{aligned}$$

so the time-evolved state ψ_t remains an eigenvector of A with the same eigenvalue λ.

10.3 Canonical commutation relations

Let A be self-adjoint. It is tempting to expand the unitaries e^{-itA} as power series,

$$e^{-itA} = \text{“}\, 1 + \sum_{k=1}^{\infty} \frac{(-itA)^k}{k!} \,\text{”}, \tag{10.11}$$

When A is unbounded, this series does not make sense. (Although it might make sense when applied to certain Hilbert space vectors; recall Definition 22.)

Definition 31. Let $t \mapsto U_t$ and $s \mapsto V_s$ be strongly-continuous 1-parameter unitary groups. They are said to satisfy the *Weyl commutation relation* if

$$U_t V_s = e^{its} V_s U_t, \qquad s, t \in \mathbb{R}. \tag{10.12}$$

To see a commonly encountered pitfall when applying the "power series" (10.11), consider

$$U_t = e^{-it\hat{p}}, \qquad V_s = e^{-is\hat{x}}.$$

In the "expansion" of the Weyl commutation relation, the terms of order st would give

$$[\hat{x}, \hat{p}] = i.$$

This "infinitesimal" form of (10.12) is true, at least on $\mathrm{Dom}(\hat{x}\hat{p}) \cap \mathrm{Dom}(\hat{p}\hat{x})$. Indeed, it is called the "canonical commutation relation" (CCR).

However, suppose that conversely, $A, B : \mathrm{Dom} \to \mathrm{Dom}$ are essentially self-adjoint operators such that $[A, B] = i$ holds on Dom. This does *not* imply that the 1-parameter unitary groups $e^{-it\overline{A}}$ and $e^{-is\overline{B}}$ satisfy the Weyl commutation relation. For example, one could consider

$$A = x - i\partial_y, \qquad B = -i\partial_x.$$

So the "infinitesimal" CCR is not really "canonical".

Example 10.6. On $L^2(\mathbb{R})$, let $t \mapsto U_t = e^{-it\hat{p}}$ be the translation group (Example 10.1), and $s \mapsto V_s = e^{-is\hat{x}}$ be the group of multiplication operators,

$$V_s \psi(x) = e^{-isx} \psi(x), \qquad \psi \in L^2(\mathbb{R}).$$

We check that

$$\begin{aligned} U_t V_s \psi(x) &= V_s \psi(x - t) = e^{-is(x-t)} \psi(x - t), \\ V_s U_t \psi(x) &= e^{-isx} U_t \psi(x) = e^{-isx} \psi(x - t), \qquad \psi \in L^2(\mathbb{R}) \end{aligned}$$

so the Weyl commutation relation (10.12) is satisfied.

Indeed, a theorem of von Neumann says that the above U_t, V_s uniquely realize the Weyl commutation relation, up to unitary equivalence and multiplicity.

Exercise 10.2. On the Hilbert space $L^2(S^1)$, let U_t be the rotation operators,

$$U_t\psi(z) = \psi(e^{-it}z), \qquad t \in \mathbb{R},$$

and V_s be the multiplication operators,

$$V_s\psi(e^{i\theta}) = e^{is\theta}\psi(e^{i\theta}), \qquad e^{i\theta} \in S^1, s \in \mathbb{R}.$$

Discuss whether U_t, V_s satisfy the Weyl commutation relations.