Chapter 3

The spectral theorem

The time evolution of a quantum mechanical system is governed by the Schrödinger equation

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\psi(t). \tag{3.1}$$

If $\mathfrak{H} = \mathbb{C}^n$ and H is hence a matrix, this system of ordinary differential equations is solved by the matrix exponential

$$\psi(t) = \exp(-\mathrm{i}tH)\psi(0). \tag{3.2}$$

This matrix exponential can be defined by a convergent power series

$$\exp(-\mathrm{i}tH) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i}t)^n}{n!} H^n. \tag{3.3}$$

For this approach the boundedness of H is crucial, which might not be the case for a quantum system. However, the best way to compute the matrix exponential and to understand the underlying dynamics is to diagonalize H. But how do we diagonalize a self-adjoint operator? The answer is known as the spectral theorem.

3.1. The spectral theorem

In this section we want to address the problem of defining functions of a self-adjoint operator A in a natural way, that is, such that

$$(f+g)(A) = f(A)+g(A), \quad (fg)(A) = f(A)g(A), \quad (f^*)(A) = f(A)^*. \tag{3.4}$$

As long as f and g are polynomials, no problems arise. If we want to extend this definition to a larger class of functions, we will need to perform some limiting procedure. Hence we could consider convergent power series or equip the space of polynomials on the spectrum with the sup norm. In both cases this only works if the operator A is bounded. To overcome this limitation, we will use characteristic functions $\chi_\Omega(A)$ instead of powers A^j. Since $\chi_\Omega(\lambda)^2 = \chi_\Omega(\lambda)$, the corresponding operators should be orthogonal projections. Moreover, we should also have $\chi_{\mathbb{R}}(A) = \mathbb{I}$ and $\chi_\Omega(A) = \sum_{j=1}^n \chi_{\Omega_j}(A)$ for any finite union $\Omega = \bigcup_{j=1}^n \Omega_j$ of disjoint sets. The only remaining problem is of course the definition of $\chi_\Omega(A)$. However, we will defer this problem and begin by developing a functional calculus for a family of characteristic functions $\chi_\Omega(A)$.

Denote the Borel sigma algebra of $\mathbb{R}$ by $\mathfrak{B}$. A **projection-valued measure** is a map

$$P : \mathfrak{B} \to \mathfrak{L}(\mathfrak{H}), \qquad \Omega \mapsto P(\Omega), \tag{3.5}$$

from the Borel sets to the set of orthogonal projections, that is, $P(\Omega)^* = P(\Omega)$ and $P(\Omega)^2 = P(\Omega)$, such that the following two conditions hold:

(i) $P(\mathbb{R}) = \mathbb{I}$.

(ii) If $\Omega = \bigcup_n \Omega_n$ with $\Omega_n \cap \Omega_m = \emptyset$ for $n \neq m$, then $\sum_n P(\Omega_n)\psi = P(\Omega)\psi$ for every $\psi \in \mathfrak{H}$ (strong σ-additivity).

Note that we require strong convergence, $\sum_n P(\Omega_n)\psi = P(\Omega)\psi$, rather than norm convergence, $\sum_n P(\Omega_n) = P(\Omega)$. In fact, norm convergence does not even hold in the simplest case where $\mathfrak{H} = L^2(I)$ and $P(\Omega) = \chi_\Omega$ (multiplication operator), since for a multiplication operator the norm is just the sup norm of the function. Furthermore, it even suffices to require weak convergence, since $\text{w-lim}\, P_n = P$ for some orthogonal projections implies $\text{s-lim}\, P_n = P$ by $\langle\psi, P_n\psi\rangle = \langle\psi, P_n^2\psi\rangle = \langle P_n\psi, P_n\psi\rangle = \|P_n\psi\|^2$ together with Lemma 1.12 (iv).

Example. Let $\mathfrak{H} = \mathbb{C}^n$ and let $A \in \mathrm{GL}(n)$ be some symmetric matrix. Let $\lambda_1, \dots, \lambda_m$ be its (distinct) eigenvalues and let P_j be the projections onto the corresponding eigenspaces. Then

$$P_A(\Omega) = \sum_{\{j | \lambda_j \in \Omega\}} P_j \tag{3.6}$$

is a projection-valued measure. ⋄

Example. Let $\mathfrak{H} = L^2(\mathbb{R})$ and let f be a real-valued measurable function. Then

$$P(\Omega) = \chi_{f^{-1}(\Omega)} \tag{3.7}$$

is a projection-valued measure (Problem 3.3). ⋄

It is straightforward to verify that any projection-valued measure satisfies

$$P(\emptyset) = 0, \qquad P(\mathbb{R}\backslash\Omega) = \mathbb{I} - P(\Omega), \tag{3.8}$$

and

$$P(\Omega_1 \cup \Omega_2) + P(\Omega_1 \cap \Omega_2) = P(\Omega_1) + P(\Omega_2). \tag{3.9}$$

Moreover, we also have

$$P(\Omega_1)P(\Omega_2) = P(\Omega_1 \cap \Omega_2). \tag{3.10}$$

Indeed, first suppose $\Omega_1 \cap \Omega_2 = \emptyset$. Then, taking the square of (3.9), we infer

$$P(\Omega_1)P(\Omega_2) + P(\Omega_2)P(\Omega_1) = 0. \tag{3.11}$$

Multiplying this equation from the right by $P(\Omega_2)$ shows that $P(\Omega_1)P(\Omega_2) = -P(\Omega_2)P(\Omega_1)P(\Omega_2)$ is self-adjoint and thus $P(\Omega_1)P(\Omega_2) = P(\Omega_2)P(\Omega_1) = 0$. For the general case $\Omega_1 \cap \Omega_2 \neq \emptyset$ we now have

$$\begin{aligned} P(\Omega_1)P(\Omega_2) &= (P(\Omega_1 - \Omega_2) + P(\Omega_1 \cap \Omega_2))(P(\Omega_2 - \Omega_1) + P(\Omega_1 \cap \Omega_2)) \\ &= P(\Omega_1 \cap \Omega_2) \end{aligned} \tag{3.12}$$

as stated.

Moreover, a projection-valued measure is monotone, that is,

$$\Omega_1 \subseteq \Omega_2 \quad \Rightarrow \quad P(\Omega_1) \le P(\Omega_2), \tag{3.13}$$

in the sense that $\langle \psi, P(\Omega_1)\psi \rangle \le \langle \psi, P(\Omega_2)\psi \rangle$ or equivalently $\mathrm{Ran}(P(\Omega_1)) \subseteq \mathrm{Ran}(P(\Omega_2))$ (cf. Problem 1.7). As a useful consequence note that $P(\Omega_2) = 0$ implies $P(\Omega_1) = 0$ for every subset $\Omega_1 \subseteq \Omega_2$.

To every projection-valued measure there corresponds a **resolution of the identity**

$$P(\lambda) = P((-\infty, \lambda]) \tag{3.14}$$

which has the properties (Problem 3.4):

(i) $P(\lambda)$ is an orthogonal projection.

(ii) $P(\lambda_1) \le P(\lambda_2)$ for $\lambda_1 \le \lambda_2$.

(iii) $\text{s-lim}_{\lambda_n \downarrow \lambda} P(\lambda_n) = P(\lambda)$ (strong right continuity).

(iv) $\text{s-lim}_{\lambda \to -\infty} P(\lambda) = 0$ and $\text{s-lim}_{\lambda \to +\infty} P(\lambda) = \mathbb{I}$.

As before, strong right continuity is equivalent to weak right continuity.

Picking $\psi \in \mathfrak{H}$, we obtain a finite Borel measure $\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle = \|P(\Omega)\psi\|^2$ with $\mu_\psi(\mathbb{R}) = \|\psi\|^2 < \infty$. The corresponding distribution function is given by $\mu_\psi(\lambda) = \langle \psi, P(\lambda)\psi \rangle$ and since for every distribution function there is a unique Borel measure (Theorem A.2), for every resolution of the identity there is a unique projection-valued measure.

Using the polarization identity (2.16), we also have the complex Borel measures

$$\mu_{\varphi,\psi}(\Omega) = \langle \varphi, P(\Omega)\psi \rangle = \frac{1}{4}(\mu_{\varphi+\psi}(\Omega) - \mu_{\varphi-\psi}(\Omega) + \mathrm{i}\mu_{\varphi-\mathrm{i}\psi}(\Omega) - \mathrm{i}\mu_{\varphi+\mathrm{i}\psi}(\Omega)). \tag{3.15}$$

Note also that, by Cauchy–Schwarz, $|\mu_{\varphi,\psi}(\Omega)| \le \|\varphi\| \, \|\psi\|$.

Now let us turn to integration with respect to our projection-valued measure. For any simple function $f = \sum_{j=1}^n \alpha_j \chi_{\Omega_j}$ (where $\Omega_j = f^{-1}(\alpha_j)$) we set

$$P(f) \equiv \int_{\mathbb{R}} f(\lambda) dP(\lambda) = \sum_{j=1}^n \alpha_j P(\Omega_j). \tag{3.16}$$

In particular, $P(\chi_\Omega) = P(\Omega)$. Then $\langle \varphi, P(f)\psi \rangle = \sum_j \alpha_j \mu_{\varphi,\psi}(\Omega_j)$ shows

$$\langle \varphi, P(f)\psi \rangle = \int_{\mathbb{R}} f(\lambda) d\mu_{\varphi,\psi}(\lambda) \tag{3.17}$$

and, by linearity of the integral, the operator P is a linear map from the set of simple functions into the set of bounded linear operators on $\mathfrak{H}$. Moreover, $\|P(f)\psi\|^2 = \sum_j |\alpha_j|^2 \mu_\psi(\Omega_j)$ (the sets Ω_j are disjoint) shows

$$\|P(f)\psi\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi(\lambda). \tag{3.18}$$

Equipping the set of simple functions with the sup norm, we infer

$$\|P(f)\psi\| \le \|f\|_\infty \|\psi\|, \tag{3.19}$$

which implies that P has norm one. Since the simple functions are dense in the Banach space of bounded Borel functions $B(\mathbb{R})$, there is a unique extension of P to a bounded linear operator $P : B(\mathbb{R}) \to \mathfrak{L}(\mathfrak{H})$ (whose norm is one) from the bounded Borel functions on $\mathbb{R}$ (with sup norm) to the set of bounded linear operators on $\mathfrak{H}$. In particular, (3.17) and (3.18) remain true.

There is some additional structure behind this extension. Recall that the set $\mathfrak{L}(\mathfrak{H})$ of all bounded linear mappings on $\mathfrak{H}$ forms a C^* algebra. A C^* algebra homomorphism ϕ is a linear map between two C^* algebras which respects both the multiplication and the adjoint; that is, $\phi(ab) = \phi(a)\phi(b)$ and $\phi(a^*) = \phi(a)^*$.

Theorem 3.1. *Let $P(\Omega)$ be a projection-valued measure on $\mathfrak{H}$. Then the operator*

$$\begin{array}{rccc} P: & B(\mathbb{R}) & \to & \mathfrak{L}(\mathfrak{H}) \\ & f & \mapsto & \int_{\mathbb{R}} f(\lambda) dP(\lambda) \end{array} \tag{3.20}$$

is a C^* algebra homomorphism with norm one such that

$$\langle P(g)\varphi, P(f)\psi \rangle = \int_{\mathbb{R}} g^*(\lambda) f(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{3.21}$$

In addition, if $f_n(x) \to f(x)$ pointwise and if the sequence $\sup_{\lambda\in\mathbb{R}} |f_n(\lambda)|$ is bounded, then $P(f_n) \stackrel{s}{\to} P(f)$ strongly.

Proof. The properties $P(1) = \mathbb{I}$, $P(f^*) = P(f)^*$, and $P(fg) = P(f)P(g)$ are straightforward for simple functions f. For general f they follow from continuity. Hence P is a C^* algebra homomorphism.

Equation (3.21) is a consequence of $\langle P(g)\varphi, P(f)\psi\rangle = \langle \varphi, P(g^*f)\psi\rangle$.

The last claim follows from the dominated convergence theorem and (3.18). □

As a consequence of (3.21), observe

$$\mu_{P(g)\varphi,P(f)\psi}(\Omega) = \langle P(g)\varphi, P(\Omega)P(f)\psi\rangle = \int_\Omega g^*(\lambda)f(\lambda)d\mu_{\varphi,\psi}(\lambda), \quad (3.22)$$

which implies

$$d\mu_{P(g)\varphi,P(f)\psi} = g^* f d\mu_{\varphi,\psi}. \quad (3.23)$$

Example. Let $\mathfrak{H} = \mathbb{C}^n$ and $A = A^* \in \mathrm{GL}(n)$, respectively, P_A, as in the previous example. Then

$$P_A(f) = \sum_{j=1}^m f(\lambda_j)P_j. \quad (3.24)$$

In particular, $P_A(f) = A$ for $f(\lambda) = \lambda$. ⋄

Next we want to define this operator for unbounded Borel functions. Since we expect the resulting operator to be unbounded, we need a suitable domain first. Motivated by (3.18), we set

$$\mathfrak{D}_f = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi(\lambda) < \infty\}. \quad (3.25)$$

This is clearly a linear subspace of $\mathfrak{H}$ since $\mu_{\alpha\psi}(\Omega) = |\alpha|^2\mu_\psi(\Omega)$ and since $\mu_{\varphi+\psi}(\Omega) = \|P(\Omega)(\varphi+\psi)\|^2 \le 2(\|P(\Omega)\varphi\|^2 + \|P(\Omega)\psi\|^2) = 2(\mu_\varphi(\Omega)+\mu_\psi(\Omega))$ (by the triangle inequality).

For every $\psi \in \mathfrak{D}_f$, the sequence of bounded Borel functions

$$f_n = \chi_{\Omega_n} f, \qquad \Omega_n = \{\lambda | \, |f(\lambda)| \le n\}, \quad (3.26)$$

is a Cauchy sequence converging to f in the sense of $L^2(\mathbb{R}, d\mu_\psi)$. Hence, by virtue of (3.18), the vectors $\psi_n = P(f_n)\psi$ form a Cauchy sequence in $\mathfrak{H}$ and we can define

$$P(f)\psi = \lim_{n\to\infty} P(f_n)\psi, \qquad \psi \in \mathfrak{D}_f. \quad (3.27)$$

By construction, $P(f)$ is a linear operator such that (3.18) holds. Since $f \in L^1(\mathbb{R}, d\mu_\psi)$ (μ_ψ is finite), (3.17) also remains true at least for $\varphi = \psi$.

In addition, $\mathfrak{D}_f$ is dense. Indeed, let Ω_n be defined as in (3.26) and abbreviate $\psi_n = P(\Omega_n)\psi$. Now observe that $d\mu_{\psi_n} = \chi_{\Omega_n} d\mu_\psi$ and hence $\psi_n \in \mathfrak{D}_f$. Moreover, $\psi_n \to \psi$ by (3.18) since $\chi_{\Omega_n} \to 1$ in $L^2(\mathbb{R}, d\mu_\psi)$.

The operator $P(f)$ has some additional properties. One calls an unbounded operator A **normal** if $\mathfrak{D}(A) = \mathfrak{D}(A^*)$ and $\|A\psi\| = \|A^*\psi\|$ for all $\psi \in \mathfrak{D}(A)$. Note that normal operators are closed since the graph norms on $\mathfrak{D}(A) = \mathfrak{D}(A^*)$ are identical.

Theorem 3.2. *For any Borel function f, the operator*

$$P(f) \equiv \int_{\mathbb{R}} f(\lambda) dP(\lambda), \qquad \mathfrak{D}(P(f)) = \mathfrak{D}_f, \tag{3.28}$$

is normal and satisfies

$$P(f)^* = P(f^*). \tag{3.29}$$

Proof. Let f be given and define f_n, Ω_n as above. Since (3.29) holds for f_n by our previous theorem, we get

$$\langle \varphi, P(f)\psi \rangle = \langle P(f^*)\varphi, \psi \rangle$$

for any $\varphi, \psi \in \mathfrak{D}_f = \mathfrak{D}_{f^*}$ by continuity. Thus it remains to show that $\mathfrak{D}(P(f)^*) \subseteq \mathfrak{D}_f$. If $\psi \in \mathfrak{D}(P(f)^*)$, we have $\langle \psi, P(f)\varphi \rangle = \langle \tilde{\psi}, \varphi \rangle$ for all $\varphi \in \mathfrak{D}_f$ by definition. By construction of $P(f)$ we have $P(f_n) = P(f)P(\Omega_n)$ and thus

$$\langle P(f_n^*)\psi, \varphi \rangle = \langle \psi, P(f_n)\varphi \rangle = \langle \psi, P(f)P(\Omega_n)\varphi \rangle = \langle P(\Omega_n)\tilde{\psi}, \varphi \rangle$$

for any $\varphi \in \mathfrak{H}$ shows $P(f_n^*)\psi = P(\Omega_n)\tilde{\psi}$. This proves existence of the limit

$$\lim_{n\to\infty} \int_{\mathbb{R}} |f_n|^2 d\mu_\psi = \lim_{n\to\infty} \|P(f_n^*)\psi\|^2 = \lim_{n\to\infty} \|P(\Omega_n)\tilde{\psi}\|^2 = \|\tilde{\psi}\|^2,$$

which by monotone convergence implies $f \in L^2(\mathbb{R}, d\mu_\psi)$; that is, $\psi \in \mathfrak{D}_f$.

That $P(f)$ is normal follows from (3.18), which implies $\|P(f)\psi\|^2 = \|P(f^*)\psi\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi$. □

Theorem 3.7 (Spectral theorem)**.** *To every self-adjoint operator A there corresponds a unique projection-valued measure P_A such that*

$$A = \int_{\mathbb{R}} \lambda dP_A(\lambda). \tag{3.49}$$

Finally, let us give a characterization of the spectrum of A in terms of the associated projectors.

Theorem 3.8. *The spectrum of A is given by*

$$\sigma(A) = \{\lambda \in \mathbb{R} | P_A((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \text{ for all } \varepsilon > 0\}. \tag{3.53}$$

Proof. Let $\Omega_n = (\lambda_0 - \frac{1}{n}, \lambda_0 + \frac{1}{n})$. Suppose $P_A(\Omega_n) \neq 0$. Then we can find a $\psi_n \in P_A(\Omega_n)\mathfrak{H}$ with $\|\psi_n\| = 1$. Since

$$\begin{aligned} \|(A - \lambda_0)\psi_n\|^2 &= \|(A - \lambda_0)P_A(\Omega_n)\psi_n\|^2 \\ &= \int_{\mathbb{R}} (\lambda - \lambda_0)^2 \chi_{\Omega_n}(\lambda) d\mu_{\psi_n}(\lambda) \leq \frac{1}{n^2}, \end{aligned}$$

we conclude $\lambda_0 \in \sigma(A)$ by Lemma 2.16.

Conversely, if $P_A((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)) = 0$, set

$$f_\varepsilon(\lambda) = \chi_{\mathbb{R}\backslash(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)}(\lambda)(\lambda - \lambda_0)^{-1}.$$

Then

$$(A - \lambda_0)P_A(f_\varepsilon) = P_A((\lambda - \lambda_0)f_\varepsilon(\lambda)) = P_A(\mathbb{R}\backslash(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)) = \mathbb{I}.$$

Similarly $P_A(f_\varepsilon)(A - \lambda_0) = \mathbb{I}|_{\mathfrak{D}(A)}$ and hence $\lambda_0 \in \rho(A)$. $\square$

In particular, $P_A((\lambda_1, \lambda_2)) = 0$ if and only if $(\lambda_1, \lambda_2) \subseteq \rho(A)$.

Corollary 3.9. *We have*

$$P_A(\sigma(A)) = \mathbb{I} \qquad \text{and} \qquad P_A(\mathbb{R} \cap \rho(A)) = 0. \tag{3.54}$$

Proof. For every $\lambda \in \mathbb{R} \cap \rho(A)$ there is some open interval I_λ with $P_A(I_\lambda) = 0$. These intervals form an open cover for $\mathbb{R} \cap \rho(A)$ and there is a countable subcover J_n. Setting $\Omega_n = J_n \backslash \bigcup_{m<n} J_m$, we have disjoint Borel sets which cover $\mathbb{R} \cap \rho(A)$ and satisfy $P_A(\Omega_n) = 0$. Finally, strong σ-additivity shows $P_A(\mathbb{R} \cap \rho(A))\psi = \sum_n P_A(\Omega_n)\psi = 0$. □

Consequently,

$$P_A(f) = P_A(\sigma(A))P_A(f) = P_A(\chi_{\sigma(A)} f). \tag{3.55}$$

In other words, $P_A(f)$ is not affected by the values of f on $\mathbb{R} \backslash \sigma(A)$!

It is clearly more intuitive to write $P_A(f) = f(A)$ and we will do so from now on. This notation is justified by the elementary observation

$$P_A(\sum_{j=0}^{n} \alpha_j \lambda^j) = \sum_{j=0}^{n} \alpha_j A^j. \tag{3.56}$$

Moreover, this also shows that if A is bounded and $f(A)$ can be defined via a convergent power series, then this agrees with our present definition by Theorem 3.1.

Problem 3.1. *Show that a self-adjoint operator P is a projection if and only if $\sigma(P) \subseteq \{0, 1\}$.*

Problem 3.2. *Consider the* **parity operator** $\Pi : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $\psi(x) \mapsto \psi(-x)$. *Show that Π is self-adjoint. Compute its spectrum $\sigma(\Pi)$ and the corresponding projection-valued measure P_Π.*

Problem 3.3. *Show that (3.7) is a projection-valued measure. What is the corresponding operator?*

Problem 3.4. *Show that $P(\lambda)$ defined in (3.14) satisfies properties* (i)–(iv) *stated there.*

Problem 3.5. *Show that for a self-adjoint operator A we have* $\|R_A(z)\| = \mathrm{dist}(z, \sigma(A))$.

Problem 3.9. *Let* λ_0 *be an eigenvalue and* ψ *a corresponding normalized eigenvector. Compute* μ_ψ.

Problem 3.10. *Show that* λ_0 *is an eigenvalue if and only if* $P(\{\lambda_0\}) \neq 0$. *Show that* $\mathrm{Ran}(P(\{\lambda_0\}))$ *is the corresponding eigenspace in this case.*

Chapter 5

Quantum dynamics

As in the finite dimensional case, the solution of the Schrödinger equation

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\psi(t) \tag{5.1}$$

is given by

$$\psi(t) = \exp(-\mathrm{i}tH)\psi(0). \tag{5.2}$$

A detailed investigation of this formula will be our first task. Moreover, in the finite dimensional case the dynamics is understood once the eigenvalues are known and the same is true in our case once we know the spectrum. Note that, like any Hamiltonian system from classical mechanics, our system is not hyperbolic (i.e., the spectrum is not away from the real axis) and hence simple results such as all solutions tend to the equilibrium position cannot be expected.

5.1. The time evolution and Stone's theorem

In this section we want to have a look at the initial value problem associated with the Schrödinger equation (2.12) in the Hilbert space $\mathfrak{H}$. If $\mathfrak{H}$ is one-dimensional (and hence A is a real number), the solution is given by

$$\psi(t) = \mathrm{e}^{-\mathrm{i}tA}\psi(0). \tag{5.3}$$

Our hope is that this formula also applies in the general case and that we can reconstruct a one-parameter unitary group $U(t)$ from its generator A (compare (2.11)) via $U(t) = \exp(-\mathrm{i}tA)$. We first investigate the family of operators $\exp(-\mathrm{i}tA)$.

Theorem 5.1. *Let A be self-adjoint and let $U(t) = \exp(-\mathrm{i}tA)$.*

(i) *$U(t)$ is a strongly continuous one-parameter unitary group.*

(ii) *The limit* $\lim_{t\to 0}\frac{1}{t}(U(t)\psi-\psi)$ *exists if and only if* $\psi\in\mathfrak{D}(A)$ *in which case* $\lim_{t\to 0}\frac{1}{t}(U(t)\psi-\psi)=-\mathrm{i}A\psi$.

(iii) $U(t)\mathfrak{D}(A)=\mathfrak{D}(A)$ *and* $AU(t)=U(t)A$.

Proof. The group property (i) follows directly from Theorem 3.1 and the corresponding statements for the function $\exp(-\mathrm{i}t\lambda)$. To prove strong continuity, observe that

$$\lim_{t\to t_0}\|\mathrm{e}^{-\mathrm{i}tA}\psi-\mathrm{e}^{-\mathrm{i}t_0A}\psi\|^2=\lim_{t\to t_0}\int_{\mathbb{R}}|\mathrm{e}^{-\mathrm{i}t\lambda}-\mathrm{e}^{-\mathrm{i}t_0\lambda}|^2 d\mu_\psi(\lambda)$$
$$=\int_{\mathbb{R}}\lim_{t\to t_0}|\mathrm{e}^{-\mathrm{i}t\lambda}-\mathrm{e}^{-\mathrm{i}t_0\lambda}|^2 d\mu_\psi(\lambda)=0$$

by the dominated convergence theorem.

Similarly, if $\psi\in\mathfrak{D}(A)$, we obtain

$$\lim_{t\to 0}\|\frac{1}{t}(\mathrm{e}^{-\mathrm{i}tA}\psi-\psi)+\mathrm{i}A\psi\|^2=\lim_{t\to 0}\int_{\mathbb{R}}|\frac{1}{t}(\mathrm{e}^{-\mathrm{i}t\lambda}-1)+\mathrm{i}\lambda|^2 d\mu_\psi(\lambda)=0$$

since $|\mathrm{e}^{\mathrm{i}t\lambda}-1|\le|t\lambda|$. Now let $\tilde{A}$ be the generator defined as in (2.11). Then $\tilde{A}$ is a symmetric extension of A since we have

$$\langle\varphi,\tilde{A}\psi\rangle=\lim_{t\to 0}\langle\varphi,\frac{\mathrm{i}}{t}(U(t)-1)\psi\rangle=\lim_{t\to 0}\langle\frac{\mathrm{i}}{-t}(U(-t)-1)\varphi,\psi\rangle=\langle\tilde{A}\varphi,\psi\rangle$$

and hence $\tilde{A}=A$ by Corollary 2.2. This settles (ii).

To see (iii), replace $\psi\to U(s)\psi$ in (ii). □

For our original problem this implies that formula (5.3) is indeed the solution to the initial value problem of the Schrödinger equation. Moreover,

$$\langle U(t)\psi,AU(t)\psi\rangle=\langle U(t)\psi,U(t)A\psi\rangle=\langle\psi,A\psi\rangle \tag{5.4}$$

shows that the expectations of A are time independent. This corresponds to conservation of energy.

On the other hand, the generator of the time evolution of a quantum mechanical system should always be a self-adjoint operator since it corresponds to an observable (energy). Moreover, there should be a one-to-one correspondence between the unitary group and its generator. This is ensured by Stone's theorem.

Theorem 5.2 (Stone)**.** *Let* $U(t)$ *be a weakly continuous one-parameter unitary group. Then its generator* A *is self-adjoint and* $U(t)=\exp(-\mathrm{i}tA)$.

Proof. First of all observe that weak continuity together with item (iv) of Lemma 1.12 shows that $U(t)$ is in fact strongly continuous.

Next we show that A is densely defined. Pick $\psi \in \mathfrak{H}$ and set

$$\psi_\tau = \int_0^\tau U(t)\psi dt$$

(the integral is defined as in Section 4.1) implying $\lim_{\tau\to 0} \tau^{-1}\psi_\tau = \psi$. Moreover,

$$\begin{aligned}\frac{1}{t}(U(t)\psi_\tau - \psi_\tau) &= \frac{1}{t}\int_t^{t+\tau} U(s)\psi ds - \frac{1}{t}\int_0^\tau U(s)\psi ds \\ &= \frac{1}{t}\int_\tau^{\tau+t} U(s)\psi ds - \frac{1}{t}\int_0^t U(s)\psi ds \\ &= \frac{1}{t}U(\tau)\int_0^t U(s)\psi ds - \frac{1}{t}\int_0^t U(s)\psi ds \to U(\tau)\psi - \psi\end{aligned}$$

as $t \to 0$ shows $\psi_\tau \in \mathfrak{D}(A)$. As in the proof of the previous theorem, we can show that A is symmetric and that $U(t)\mathfrak{D}(A) = \mathfrak{D}(A)$.

Next, let us prove that A is essentially self-adjoint. By Lemma 2.7 it suffices to prove $\mathrm{Ker}(A^* - z^*) = \{0\}$ for $z \in \mathbb{C}\backslash\mathbb{R}$. Suppose $A^*\varphi = z^*\varphi$. Then for each $\psi \in \mathfrak{D}(A)$ we have

$$\frac{d}{dt}\langle\varphi, U(t)\psi\rangle = \langle\varphi, -\mathrm{i}AU(t)\psi\rangle = -\mathrm{i}\langle A^*\varphi, U(t)\psi\rangle = -\mathrm{i}z\langle\varphi, U(t)\psi\rangle$$

and hence $\langle\varphi, U(t)\psi\rangle = \exp(-\mathrm{i}zt)\langle\varphi,\psi\rangle$. Since the left-hand side is bounded for all $t \in \mathbb{R}$ and the exponential on the right-hand side is not, we must have $\langle\varphi,\psi\rangle = 0$ implying $\varphi = 0$ since $\mathfrak{D}(A)$ is dense.

So A is essentially self-adjoint and we can introduce $V(t) = \exp(-\mathrm{i}t\overline{A})$. We are done if we can show $U(t) = V(t)$.

Let $\psi \in \mathfrak{D}(A)$ and abbreviate $\psi(t) = (U(t) - V(t))\psi$. Then

$$\lim_{s\to 0}\frac{\psi(t+s) - \psi(t)}{s} = \mathrm{i}\overline{A}\psi(t)$$

and hence $\frac{d}{dt}\|\psi(t)\|^2 = 2\,\mathrm{Re}\langle\psi(t), \mathrm{i}A\psi(t)\rangle = 0$. Since $\psi(0) = 0$, we have $\psi(t) = 0$ and hence $U(t)$ and $V(t)$ coincide on $\mathfrak{D}(A)$. Furthermore, since $\mathfrak{D}(A)$ is dense, we have $U(t) = V(t)$ by continuity. □

As an immediate consequence of the proof we also note the following useful criterion.

Corollary 5.3. *Suppose $\mathfrak{D} \subseteq \mathfrak{D}(A)$ is dense and invariant under $U(t)$. Then A is essentially self-adjoint on $\mathfrak{D}$.*

Proof. As in the above proof it follows that $\langle\varphi,\psi\rangle = 0$ for any $\psi \in \mathfrak{D}$ and $\varphi \in \mathrm{Ker}(A^* - z^*)$. □

Note that by Lemma 4.9 two strongly continuous one-parameter groups commute,

$$[\mathrm{e}^{-\mathrm{i}tA}, \mathrm{e}^{-\mathrm{i}sB}] = 0, \tag{5.5}$$

if and only if the generators commute.

Clearly, for a physicist, one of the goals must be to understand the time evolution of a quantum mechanical system. We have seen that the time evolution is generated by a self-adjoint operator, the Hamiltonian, and is given by a linear first order differential equation, the Schrödinger equation. To understand the dynamics of such a first order differential equation, one must understand the spectrum of the generator. Some general tools for this endeavor will be provided in the following sections.

Problem 5.1. *Let* $\mathfrak{H} = L^2(0, 2\pi)$ *and consider the one-parameter unitary group given by* $U(t)f(x) = f(x - t \mod 2\pi)$. *What is the generator of* U*?*