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. $\diamond$

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). $\diamond$

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,

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

in the sense that $\langle \psi, P(\Omega_1)\psi\rangle \leq \langle \psi, P(\Omega_2)\psi\rangle$ 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) $P(\lambda_1) \leq P(\lambda_2)$ for $\lambda_1 \leq \lambda_2$.

(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, $|\mu_{\varphi,\psi}(\Omega)| \leq \|\varphi\| \, \|\psi\|$.

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 $P(f_n) \xrightarrow{s} P(f)$ 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

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

which implies

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

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

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

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

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

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

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

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

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

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

Now observe that to every projection-valued measure P we can assign a self-adjoint operator $A = \int_{\mathbb{R}} \lambda dP(\lambda)$. The question is whether we can invert this map. To do this, we consider the resolvent $R_A(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} dP(\lambda)$. From (3.17) the corresponding quadratic form is given by

$$F_\psi(z) = \langle \psi, R_A(z)\psi \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda), \tag{3.40}$$

which is know as the **Borel transform** of the measure μ_ψ. By

$$\mathrm{Im}(F_\psi(z)) = \mathrm{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} d\mu_\psi(\lambda), \tag{3.41}$$

we infer that $F_\psi(z)$ is a holomorphic map from the upper half plane into itself. Such functions are called **Herglotz** or **Nevanlinna functions** (see Section 3.4). Moreover, the measure μ_ψ can be reconstructed from $F_\psi(z)$ by the **Stieltjes inversion formula**

$$\mu_\psi(\lambda) = \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{-\infty}^{\lambda+\delta} \mathrm{Im}(F_\psi(t + \mathrm{i}\varepsilon))dt. \tag{3.42}$$

(The limit with respect to δ is only here to ensure right continuity of $\mu_\psi(\lambda)$.) Conversely, if $F_\psi(z)$ is a Herglotz function satisfying $|F_\psi(z)| \le \frac{M}{\mathrm{Im}(z)}$, then it is the Borel transform of a unique measure μ_ψ (given by the Stieltjes inversion formula) satisfying $\mu_\psi(\mathbb{R}) \le M$.

So let A be a given self-adjoint operator and consider the expectation of the resolvent of A,

$$F_\psi(z) = \langle \psi, R_A(z)\psi\rangle. \tag{3.43}$$

This function is holomorphic for $z \in \rho(A)$ and satisfies

$$F_\psi(z^*) = F_\psi(z)^* \quad \text{and} \quad |F_\psi(z)| \le \frac{\|\psi\|^2}{\mathrm{Im}(z)} \tag{3.44}$$

(see (2.69) and Theorem 2.18). Moreover, the first resolvent formula (2.81) shows that it maps the upper half plane to itself:

$$\mathrm{Im}(F_\psi(z)) = \mathrm{Im}(z)\|R_A(z)\psi\|^2; \tag{3.45}$$

that is, it is a Herglotz function. So by our above remarks, there is a corresponding measure $\mu_\psi(\lambda)$ given by the Stieltjes inversion formula. It is called the **spectral measure** corresponding to ψ.

More generally, by polarization, for each $\varphi, \psi \in \mathfrak{H}$ we can find a corresponding complex measure $\mu_{\varphi,\psi}$ such that

$$\langle \varphi, R_A(z)\psi\rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{\varphi,\psi}(\lambda). \tag{3.46}$$

The measure $\mu_{\varphi,\psi}$ is conjugate linear in φ and linear in ψ. Moreover, a comparison with our previous considerations begs us to define a family of operators via the sesquilinear forms

$$s_\Omega(\varphi, \psi) = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{3.47}$$

Since the associated quadratic form is nonnegative, $q_\Omega(\psi) = s_\Omega(\psi, \psi) = \mu_\psi(\Omega) \ge 0$, the Cauchy–Schwarz inequality for sesquilinear forms (Problem 0.16) implies $|s_\Omega(\varphi, \psi)| \le q_\Omega(\varphi)^{1/2} q_\Omega(\psi)^{1/2} = \mu_\varphi(\Omega)^{1/2}\mu_\psi(\Omega)^{1/2} \le$

$\mu_\varphi(\mathbb{R})^{1/2}\mu_\psi(\mathbb{R})^{1/2} \le \|\varphi\|\,\|\psi\|$. Hence Corollary 1.9 implies that there is indeed a family of nonnegative ($0 \le \langle\psi, P_A(\Omega)\psi\rangle \le 1$) and hence self-adjoint operators $P_A(\Omega)$ such that

$$\langle\varphi, P_A(\Omega)\psi\rangle = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{3.48}$$

Lemma 3.6. *The family of operators $P_A(\Omega)$ forms a projection-valued measure.*

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

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

Proof. Existence has already been established. Moreover, Lemma 3.5 shows that $P_A((\lambda - z)^{-1}) = R_A(z)$, $z \in \mathbb{C}\backslash\mathbb{R}$. Since the measures $\mu_{\varphi,\psi}$ are uniquely determined by the resolvent and the projection-valued measure is uniquely determined by the measures $\mu_{\varphi,\psi}$, we are done. □

The quadratic form of A is given by

$$q_A(\psi) = \int_{\mathbb{R}} \lambda d\mu_\psi(\lambda) \tag{3.50}$$

and can be defined for every ψ in the **form domain**

$$\mathfrak{Q}(A) = \mathfrak{D}(|A|^{1/2}) = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} |\lambda| d\mu_\psi(\lambda) < \infty\} \tag{3.51}$$

(which is larger than the domain $\mathfrak{D}(A) = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} \lambda^2 d\mu_\psi(\lambda) < \infty\}$). This extends our previous definition for nonnegative operators.

Note that if A and $\tilde{A}$ are unitarily equivalent as in (3.30), then $UR_A(z) = R_{\tilde{A}}(z)U$ and hence

$$d\mu_\psi = d\tilde{\mu}_{U\psi}. \tag{3.52}$$

In particular, we have $UP_A(f) = P_{\tilde{A}}(f)U$, $U\mathfrak{D}(P_A(f)) = \mathfrak{D}(P_{\tilde{A}}(f))$.

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 $\lambda_0 \in \rho(A)$. □

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*

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

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.*

Problem 3.11 (Polar decomposition)**.** *Let A be a closed operator and set $|A| = \sqrt{A^*A}$ (recall that, by Problem 2.12, A^*A is self-adjoint and $\mathfrak{Q}(A^*A) = \mathfrak{D}(A)$). Show that*

$$\||A|\psi\| = \|A\psi\|.$$

Conclude that $\mathrm{Ker}(A) = \mathrm{Ker}(|A|) = \mathrm{Ran}(|A|)^\perp$ and that

$$U = \begin{cases} \varphi = |A|\psi \mapsto A\psi & \text{if } \varphi \in \mathrm{Ran}(|A|), \\ \varphi \mapsto 0 & \text{if } \varphi \in \mathrm{Ker}(|A|) \end{cases}$$

extends to a well-defined **partial isometry***; that is, $U : \mathrm{Ker}(U)^\perp \to \mathrm{Ran}(U)$ is unitary, where $\mathrm{Ker}(U) = \mathrm{Ker}(A)$ and $\mathrm{Ran}(U) = \mathrm{Ker}(A^*)^\perp$.*

In particular, we have the **polar decomposition**

$$A = U|A|.$$

Problem 3.12. *Compute $|A| = \sqrt{A^*A}$ for the rank one operator $A = \langle\varphi, .\rangle\psi$. Compute $\sqrt{AA^*}$ also.*

Next we recall the unique decomposition of μ with respect to Lebesgue measure,

$$d\mu = d\mu_{ac} + d\mu_s, \tag{3.72}$$

where μ_{ac} is **absolutely continuous** with respect to Lebesgue measure (i.e., we have $\mu_{ac}(B) = 0$ for all B with Lebesgue measure zero) and μ_s is **singular** with respect to Lebesgue measure (i.e., μ_s is supported, $\mu_s(\mathbb{R}\backslash B) = 0$, on a set B with Lebesgue measure zero). The singular part μ_s can be further decomposed into a **(singularly) continuous** and a **pure point** part,

$$d\mu_s = d\mu_{sc} + d\mu_{pp}, \tag{3.73}$$

where μ_{sc} is continuous on $\mathbb{R}$ and μ_{pp} is a step function. Since the measures $d\mu_{ac}$, $d\mu_{sc}$, and $d\mu_{pp}$ are mutually singular, they have mutually disjoint supports M_{ac}, M_{sc}, and M_{pp}. Note that these sets are *not* unique. We will choose them such that M_{pp} is the set of all jumps of $\mu(\lambda)$ and such that M_{sc} has Lebesgue measure zero.

To the sets M_{ac}, M_{sc}, and M_{pp} correspond projectors $P^{ac} = \chi_{M_{ac}}(A)$, $P^{sc} = \chi_{M_{sc}}(A)$, and $P^{pp} = \chi_{M_{pp}}(A)$ satisfying $P^{ac} + P^{sc} + P^{pp} = \mathbb{I}$. In other words, we have a corresponding direct sum decomposition of both our Hilbert space

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sc}) \oplus L^2(\mathbb{R}, d\mu_{pp}) \tag{3.74}$$

and our operator

$$A = (AP^{ac}) \oplus (AP^{sc}) \oplus (AP^{pp}). \tag{3.75}$$

The corresponding spectra, $\sigma_{ac}(A) = \sigma(\mu_{ac})$, $\sigma_{sc}(A) = \sigma(\mu_{sc})$, and $\sigma_{pp}(A) = \sigma(\mu_{pp})$ are called the absolutely continuous, singularly continuous, and pure point spectrum of A, respectively.

It is important to observe that $\sigma_{pp}(A)$ is in general not equal to the set of eigenvalues

$$\sigma_p(A) = \{\lambda \in \mathbb{R} | \lambda \text{ is an eigenvalue of } A\} \tag{3.76}$$

since we only have $\sigma_{pp}(A) = \overline{\sigma_p(A)}$.

Example. Let $\mathfrak{H} = \ell^2(\mathbb{N})$ and let A be given by $A\delta_n = \frac{1}{n}\delta_n$, where δ_n is the sequence which is 1 at the n'th place and zero otherwise (that is, A is a diagonal matrix with diagonal elements $\frac{1}{n}$). Then $\sigma_p(A) = \{\frac{1}{n} | n \in \mathbb{N}\}$ but $\sigma(A) = \sigma_{pp}(A) = \sigma_p(A) \cup \{0\}$. To see this, just observe that δ_n is the eigenvector corresponding to the eigenvalue $\frac{1}{n}$ and for $z \notin \sigma(A)$ we have $R_A(z)\delta_n = \frac{n}{1-nz}\delta_n$. At $z = 0$ this formula still gives the inverse of A, but it is unbounded and hence $0 \in \sigma(A)$ but $0 \notin \sigma_p(A)$. Since a continuous measure cannot live on a single point and hence also not on a countable set, we have $\sigma_{ac}(A) = \sigma_{sc}(A) = \emptyset$. ◇

Next, we want to introduce the splitting (3.74) for arbitrary self-adjoint operators A. It is tempting to pick a spectral basis and treat each summand in the direct sum separately. However, since it is not clear that this approach is independent of the spectral basis chosen, we use the more sophisticated definition

$$\begin{aligned}
\mathfrak{H}_{ac} &= \{\psi \in \mathfrak{H} | \mu_\psi \text{ is absolutely continuous}\},\\
\mathfrak{H}_{sc} &= \{\psi \in \mathfrak{H} | \mu_\psi \text{ is singularly continuous}\},\\
\mathfrak{H}_{pp} &= \{\psi \in \mathfrak{H} | \mu_\psi \text{ is pure point}\}.
\end{aligned} \tag{3.83}$$

Lemma 3.19. *We have*

$$\mathfrak{H} = \mathfrak{H}_{ac} \oplus \mathfrak{H}_{sc} \oplus \mathfrak{H}_{pp}. \tag{3.84}$$

There are Borel sets M_{xx} such that the projector onto $\mathfrak{H}_{xx}$ is given by $P^{xx} = \chi_{M_{xx}}(A)$, $xx \in \{ac, sc, pp\}$. In particular, the subspaces $\mathfrak{H}_{xx}$ reduce A. For the sets M_{xx} one can choose the corresponding supports of some maximal spectral measure μ.

The **absolutely continuous**, **singularly continuous**, and **pure point spectrum** of A are defined as

$$\sigma_{ac}(A) = \sigma(A|_{\mathfrak{H}_{ac}}), \quad \sigma_{sc}(A) = \sigma(A|_{\mathfrak{H}_{sc}}), \quad \text{and} \quad \sigma_{pp}(A) = \sigma(A|_{\mathfrak{H}_{pp}}), \tag{3.85}$$

respectively. If μ is a maximal spectral measure, we have $\sigma_{ac}(A) = \sigma(\mu_{ac})$, $\sigma_{sc}(A) = \sigma(\mu_{sc})$, and $\sigma_{pp}(A) = \sigma(\mu_{pp})$.

If A and $\tilde{A}$ are unitarily equivalent via U, then so are $A|_{\mathfrak{H}_{xx}}$ and $\tilde{A}|_{\tilde{\mathfrak{H}}_{xx}}$ by (3.52). In particular, $\sigma_{xx}(A) = \sigma_{xx}(\tilde{A})$.

Problem 3.19. *Compute* $\sigma(A)$, $\sigma_{ac}(A)$, $\sigma_{sc}(A)$, *and* $\sigma_{pp}(A)$ *for the multiplication operator* $A = \frac{1}{1+x^2}$ *in* $L^2(\mathbb{R})$. *What is its spectral multiplicity?*

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

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

by the dominated convergence theorem.

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

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

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?*

13.3 Quantum Return Probability

Let T be self-adjoint, $\eta, \xi \in \mathcal{H}$ and $\mu_\xi = \mu_\xi^T$, $\mu_{\xi,\eta} = \mu_{\xi,\eta}^T$ the corresponding spectral measures. Without loss of generality the initial condition of the Schrödinger equation

$$i\frac{d\xi}{dt}(t) = T\xi(t), \qquad \xi(0) = \xi \in \operatorname{dom} T,$$

will be supposed to be given at initial time $t_0 = 0$. The main quantities considered to probe the large time behavior of the dynamics $e^{-itT}\xi$ will be:

1. The (quantum) *return probability* to the initial condition ξ, at time t,

$$p_\xi(t) := \left|\left\langle \xi, e^{-itT}\xi \right\rangle\right|^2,$$

   and more generally $p_{\eta,\xi}(t) := \left|\left\langle \eta, e^{-itT}\xi \right\rangle\right|^2$.

2. The *average return probability* up to time $t \neq 0$,

$$\langle p_\xi \rangle (t) := \frac{1}{t}\int_0^t p_\xi(s)\, ds,$$

   and similarly one defines $\langle p_{\eta,\xi} \rangle (t)$.

A crucial relation for what follows comes from the spectral theorem

$$p_\xi(t) = |\hat{\mu}_\xi(t)|^2 := \left| \int_{\sigma(T)} e^{-itx} \, d\mu_\xi(x) \right|^2 .$$

$\hat{\mu}_\xi(t) = \int_{\sigma(T)} e^{-it\lambda} \, d\mu_\xi(\lambda)$ is called the *Fourier transform of the measure* μ_ξ, so that the behavior of the return probability and expectation values of test operators are naturally related to spectral measures of T through $\langle \xi, e^{-itT}\xi \rangle = \hat{\mu}_\xi(t)$. Two general results on Borel measures over $\mathbb{R}$ are important here: the Riemann-Lebesgue lemma (around 1900) and the Wiener lemma (around 1935).

Lemma 13.3.2 (Riemann-Lebesgue). *If $f \in \mathrm{L}^1(\mathbb{R})$ and $\hat{f}$ denotes its Fourier transform, then $\hat{f}$ is continuous and $\lim_{|p|\to\infty} \hat{f}(p) = 0$; in other symbols $\hat{f} \in C_\infty(\hat{\mathbb{R}})$.*

Theorem 5.4 (Wiener). *Let μ be a finite complex Borel measure on $\mathbb{R}$ and let*

$$\hat{\mu}(t) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda} d\mu(\lambda) \tag{5.8}$$

be its Fourier transform. Then the Cesàro time average of $\hat{\mu}(t)$ has the limit

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\hat{\mu}(t)|^2 dt = \sum_{\lambda\in\mathbb{R}} |\mu(\{\lambda\})|^2, \tag{5.9}$$

where the sum on the right-hand side is finite.

Proof. By Fubini we have

$$\begin{aligned}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 dt &= \frac{1}{T}\int_0^T \int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}(x-y)t} d\mu(x) d\mu^*(y) dt \\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} \left(\frac{1}{T}\int_0^T \mathrm{e}^{-\mathrm{i}(x-y)t} dt\right) d\mu(x) d\mu^*(y).\end{aligned}$$

The function in parentheses is bounded by one and converges pointwise to $\chi_{\{0\}}(x-y)$ as $T \to \infty$. Thus, by the dominated convergence theorem, the limit of the above expression is given by

$$\int_{\mathbb{R}}\int_{\mathbb{R}} \chi_{\{0\}}(x-y) d\mu(x) d\mu^*(y) = \int_{\mathbb{R}} \mu(\{y\}) d\mu^*(y) = \sum_{y\in\mathbb{R}} |\mu(\{y\})|^2,$$

which finishes the proof. $\square$

Now a prominent result with respect to the large-time behavior of the return probability will be presented. Some dynamical differences between point and continuous subspaces are noteworthy.

Theorem 13.3.7. *Let T be self-adjoint.*

i) *For any $\xi \in \mathcal{H}$ the limit*

$$\mathfrak{X}_\xi := \lim_{t\to\infty} \langle p_\xi \rangle (t)$$

exists. Furthermore, $\mathfrak{X}_\xi = 0$ iff $\xi \in \mathcal{H}_{\mathrm{c}}(T)$.

ii) *If $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$, then $\lim_{t\to\infty} p_\xi(t) = 0$.*

Proof. i) It follows immediately by the Wiener Lemma 13.3.5 and the crucial relation on page 359. In particular, $\mathfrak{X}_\xi = 0$ iff μ_ξ is a continuous measure and, by Theorem 12.1.2, iff $\xi \in \mathcal{H}_{\mathrm{c}}(T)$.

ii) One has $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$ iff $\mu_\xi \ll \ell$ iff there exists $f \in \mathrm{L}^1(\mathbb{R})$, $f \geq 0$, with $\frac{d\mu_\xi}{d\ell} = f$. Thus

$$p_\xi(t) = \langle \xi, e^{-itT}\xi \rangle = \int_{\mathbb{R}} e^{-itx}\, d\mu_\xi(x) = \int_{\mathbb{R}} e^{-itx} f(x)\, dx,$$

which vanishes as $t \to \infty$ by Riemann-Lebesgue 13.3.2. $\square$

Such results are interpreted as follows. Under time evolution $e^{-itT}\xi$, any state η (in particular the initial state ξ) is completely abandoned in time average if $\xi \in \mathcal{H}_c(T)$, since $\langle p_{\eta,\xi}\rangle(t) \to 0$ as $t \to \infty$; for elements of $\mathcal{H}_{ac}(T)$ the time average is not necessary. Sometimes such properties are associated with instabilities, e.g., atomic ionization. On the other hand, for elements $\xi \in \mathcal{H}_p(T)$ one has $\mathfrak{X}_\xi > 0$ and so the initial state is not "forgotten," in accordance with their almost periodic trajectories, as discussed in Section 13.2.

Remark 13.3.10. All occurrences of $t \to \infty$ above can be replaced by $t \to -\infty$.

Remark 13.2.7. The following reasoning gives some insight into precompact orbits and almost periodic trajectories for vectors in the point subspace of T, i.e., $\xi = \sum_{j=1}^{\infty} a_j \xi_j$, $T\xi_j = \lambda_j \xi_j$, $\forall j$, and (ξ_j) orthonormal. By Example 5.4.10 its time evolution is $\xi(t) = \sum_{j=1}^{\infty} a_j e^{-it\lambda_j} \xi_j$.

1. For all $t \in \mathbb{R}$ one has

$$\|\xi(t)\|^2 = \sum_{j=1}^{\infty} |e^{-it\lambda_j} a_j|^2 = \sum_{j=1}^{\infty} |a_j|^2.$$

   Given $\varepsilon > 0$ there is N so that $\sum_{j=1}^{N} |e^{-it\lambda_j} a_j|^2 > (1-\varepsilon)$, $\forall t$, and a large part of the orbit lives in a finite-dimensional subspace (of dimension $\leq N$). Compare with Lemma 13.1.5.

2. Note that in Hilbert space, $\xi(t) = \lim_{M\to\infty} \xi^M(t)$ with uniform convergence in t, where $\xi^M(t) = \sum_{j=1}^{M} a_j e^{-it\lambda_j} \xi_j$ is quasiperiodic, i.e., a linear combination of (finitely many) periodic trajectories. The almost periodicity "is obtained in the limit of infinitely many periods $M \to \infty$."

Now we want to draw some additional consequences from Wiener's theorem. This will eventually yield a dynamical characterization of the continuous and pure point spectrum due to Ruelle, Amrein, Gorgescu, and Enß. But first we need a few definitions.

An operator $K \in \mathfrak{L}(\mathfrak{H})$ is called a **finite rank operator** if its range is finite dimensional. The dimension

$$\operatorname{rank}(K) = \dim \operatorname{Ran}(K)$$

is called the **rank** of K. If $\{\psi_j\}_{j=1}^n$ is an orthonormal basis for $\operatorname{Ran}(K)$, we have

$$K\psi = \sum_{j=1}^{n} \langle \psi_j, K\psi \rangle \psi_j = \sum_{j=1}^{n} \langle \varphi_j, \psi \rangle \psi_j, \tag{5.10}$$

where $\varphi_j = K^*\psi_j$. The elements φ_j are linearly independent since $\mathrm{Ran}(K) = \mathrm{Ker}(K^*)^\perp$. Hence every finite rank operator is of the form (5.10). In addition, the adjoint of K is also finite rank and is given by

$$K^*\psi = \sum_{j=1}^{n} \langle \psi_j, \psi\rangle \varphi_j. \tag{5.11}$$

The closure of the set of all finite rank operators in $\mathfrak{L}(\mathfrak{H})$ is called the set of **compact operators** $\mathfrak{C}(\mathfrak{H})$. It is straightforward to verify (Problem 5.2)

Lemma 5.5. *The set of all compact operators $\mathfrak{C}(\mathfrak{H})$ is a closed $*$-ideal in $\mathfrak{L}(\mathfrak{H})$.*

13.4 RAGE Theorem and Test Operators

The RAGE theorem is an important tool in the study of the time asymptotics of expectation values of test operators, which were introduced in Section 13.3.

Theorem 13.4.1 (RAGE). *Let T be a self-adjoint operator in $\mathcal{H}$.*

i) $\xi \in \mathcal{H}_{\mathrm{c}}(T)$ *iff for every compact operator* $K : \mathcal{H} \hookleftarrow$,

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \left\| K e^{-iTs} \xi \right\|^2 ds = 0.$$

ii) *If* $\xi \in \mathcal{H}_{\mathrm{ac}}(T)$, *then for every compact operator* $K : \mathcal{H} \hookleftarrow$,

$$\lim_{t\to\infty} K e^{-itT} \xi = 0.$$

Proof. K can be approximated in the norm of $\mathrm{B}(\mathcal{H})$ by finite-rank operators, and by induction and the triangle inequality, it is sufficient to consider rank-one operators

$$K\xi = \langle \eta, \xi \rangle \zeta,$$

for some $\eta, \zeta \in \mathcal{H}$. In this case

$$\|K e^{-itT} \xi\| = \|\langle \eta, e^{-itT} \xi \rangle \zeta\| = \|\zeta\| \, |\langle \eta, e^{-itT} \xi \rangle|,$$

and the result follows by Corollary 13.3.8. □

Exercise 13.4.2. Discuss the missing details in the proof of Theorem 13.4.1.

Remark 13.4.3. The term RAGE comes from the initials of D. Ruelle, W.O. Amrein, V. Georgescu and V. Enss. The RAGE theorem has applications to localization in scattering theory in $\mathbb{R}^n$; see Section 13.6.

Important compact operators are the projections onto finite-dimensional subspaces of $\mathcal{H}$; so the elements of $\mathcal{H}_{\mathrm{c}}(T)$ can be interpreted as those whose trajectories escape, in time average, from every finite-dimensional subspace (again, the average is not necessary for the absolutely continuous subspace). Compare with the corresponding remark about the point subspace on page 356.