Our first topic in this chapter is a mathematical analysis of (D). To prepare for this, let T be a self-adjoint operator and let $U(t) = e^{-itT}$. Recall that this is defined via the functional calculus as $U(t) = \int_{\mathbb{R}} e^{-its}\, dE(s)$, where E is the spectral resolution of T. By the properties of the functional calculus, $U(t)$ is unitary for every $t \in \mathbb{R}$ and $U(s+t) = U(s)U(t)$.

Exercise 13.1. Prove these properties of $U(t)$.

In other words, $U(t)$ is a unitary group as in (D). Moreover, $U(t)$ is also *strongly continuous:* this means that for every fixed $x \in H$, the map $\mathbb{R} \to H$, $t \mapsto U(t)x$ is continuous, and this was an additional requirement imposed by (D). To prove this, notice that

$$\|U(t)x - U(s)x\|^2 = \int_{\mathbb{R}} |e^{-itv} - e^{-isv}|^2 \, d\mu_{x,x}(v)$$

by the properties of the functional calculus. Dominated convergence shows that the right-hand side goes to zero as $s \to t$, as claimed.

Exercise 13.2. Let T be a self-adjoint operator on a Hilbert space H, and let $U(t) = e^{-itT}$. Show that the map $\mathbb{R} \to B(H)$, $t \mapsto U(t)$ is continuous if and only if $T \in B(H)$.

Exercise 13.3. Let T be self-adjoint and $U(t) = e^{-itT}$. Suppose that $x \in D(T)$. Show that $U(t)x \in D(T)$ for all $t \in \mathbb{R}$. Then show that the map $t \mapsto U(t)x$ is differentiable in the sense that

$$\frac{d}{dt}U(t)x := \lim_{h\to 0} \frac{1}{h}\left(U(t+h)x - U(t)x\right)$$

exists as a norm limit in H. Finally, show that $(d/dt)U(t)x = -iTU(t)x$. *Hint:* Use an argument similar to the one that was used above to establish the strong continuity of $U(t) = e^{-itT}$.

Stone's Theorem asserts that, conversely, every strongly continuous unitary group is of this type. Recall from (D) that a *unitary group* is a map $U : \mathbb{R} \to B(H)$ such that each $U(t)$ is unitary and $U(s+t) = U(s)U(t)$.

Theorem 13.1 (Stone)**.** *Let $U(t)$ be a strongly continuous unitary group. Then there exists a unique self-adjoint operator T such that $U(t) = e^{-itT}$.*

We call T the *(infinitesimal) generator* of $U(t)$.

Exercise 13.4. Let $U(t)$ be a unitary group. Prove that $U(0) = 1$. Also, prove that $U(t)^* = U(-t)$.

Proof. From Exercise 13.3, we already have at least a vague idea of how to find such a T: we have to "differentiate" $U(t)$. It thus seems natural to define

$$D(S) = \left\{ x \in H : \lim_{h\to 0} \frac{U(h)-1}{h}\, x \text{ exists} \right\},$$

$$Sx = i \lim_{h\to 0} \frac{U(h)-1}{h}\, x. \tag{13.1}$$

It is easy to see that $D(S)$ is a subspace and S is linear. I next claim that $D(S)$ is dense. To show this, we will make use of Hilbert space valued integrals without however carefully developing this subject.

For $x \in H$ and $f \in C_0^\infty(\mathbb{R})$, we want to define

$$x_f = \int_{-\infty}^{\infty} f(t)U(t)x\, dt. \tag{13.2}$$

What exactly do we mean by this? Since the integrand takes values in H, this is certainly not clear right away. Fortunately, several good answers are available. For us, (generalized) Riemann sums provide a convenient interpretation of (13.2): We take $R \in \mathbb{N}$ so large that $\text{supp}\, f \subseteq (-R, R)$, then form $(1/N)\sum_{n=-RN}^{RN} f(n/N)U(n/N)x$ and finally take the limit $N \to \infty$ to define the right-hand side of (13.2). Existence of this limit is an easy consequence of the continuity of the integrand, just as in the elementary theory of the Riemann integral. In the sequel, we will make use of some (very plausible) basic properties of this new integral without worrying too much about their formal verification; see also Exercise 13.7 below.

First of all, I claim that $x_f \in D(S)$ whenever $f \in C_0^\infty(\mathbb{R})$. This follows from the following calculation:

$$\begin{aligned} \frac{U(h)-1}{h}\, x_f &= \frac{1}{h}\int_{\mathbb{R}} f(t)(U(t+h)-U(t))x\, dt \\ &= \int_{\mathbb{R}} \frac{f(t-h)-f(t)}{h} U(t)x\, dt \end{aligned}$$

Now as $h \to 0$, we have $(f(t-h)-f(t))/h \to -f'(t)$, uniformly in $t \in \mathbb{R}$.

Exercise 13.5. Prove this. The point here of course is the *uniform* convergence; convergence at a fixed t just follows from the definition of the derivative.

From this, it follows that $(1/h)(U(h)-1)x_f \to x_{-f'}$; again, that should seem very plausible even without a detailed argument because

Riemann integration can be interchanged with uniform limits. We have shown that $x_f \in D(S)$, as claimed.

Now if $x \in H$ is arbitrary, fix an $f \in C_0^\infty(\mathbb{R})$ with $\int f = 1$, and let $f_n(t) = nf(nt)$, $x_n = x_{f_n}$. Then

$$\|x_n - x\| = \left\| \int_{\mathbb{R}} f_n(t)(U(t)x - x)\, dt \right\| \le \int_{\mathbb{R}} |f_n(t)|\, \|U(t)x - x\|\, dt.$$

Notice that the f_n are supported by $(-R/n, R/n)$, for suitable fixed $R > 0$, and $\sup_{|t|<R/n} \|U(t)x - x\| \to 0$ as $n \to \infty$, by the strong continuity of $U(t)$ and Exercise 13.4. Since $\int |f_n|$ is independent of n, it follows that $x_n \to x$, and, as observed earlier, $x_n \in D(S)$, so $D(S)$ is indeed dense.

Given this, it is now easy to verify that S is symmetric. Let $x, y \in D(S)$. Then, by the continuity of the scalar product and the second part of Exercise 13.4,

$$\begin{aligned} \langle x, Sy \rangle &= i \lim_{h\to 0} \left\langle x, \frac{U(h)-1}{h}\, y \right\rangle = i \lim_{h\to 0} \left\langle \frac{U(-h)-1}{h}\, x, y \right\rangle \\ &= i\langle iSx, y\rangle = \langle Sx, y\rangle. \end{aligned}$$

Next, I claim that $T = \overline{S}$ is self-adjoint. T is symmetric by Exercise 11.14, and we will use Theorem 11.11(b) with $z = i$ to establish self-adjointness. As a preliminary, observe that if $x \in D(S)$, then $U(t)x \in D(S)$ also for all $t \in \mathbb{R}$ because

$$\frac{U(h)-1}{h} U(t)x = U(t)\frac{U(h)-1}{h} x \to -iU(t)Sx.$$

Now suppose that $x \in N(T^* - i) = N(S^* - i)$, fix an arbitrary vector $y \in D(S)$, and let

$$f(t) = \langle x, U(t)y \rangle.$$

By the observation just made, f is differentiable, and in fact

$$f'(t) = \langle x, -iSU(t)y\rangle = -i\langle S^*x, U(t)y\rangle = -i\langle ix, U(t)y\rangle = -f(t).$$

This ODE has the unique solution $f(t) = f(0)e^{-t}$. This is unbounded unless $f(0) = 0$. Since $|f(t)| \le \|x\|\,\|y\|$ is clearly bounded, we conclude that $f(0) = \langle x, y\rangle = 0$, and since $y \in D(S)$ was arbitrary here, we have proved that $x \in D(S)^\perp = 0$. The proof that $N(T^* + i) = 0$ is of course analogous.

Let $V(t) = e^{-itT}$. We want to show that $U(t) = V(t)$. Let $x \in D(S)$, and put $w(t) = U(t)x - V(t)x$. Then w is differentiable, by our discussion from the preceding paragraph (for $U(t)x$) and Exercise 13.3 (for $V(t)x$; also notice that $D(S) \subseteq D(T)$). We have

$$w'(t) = -iSU(t)x + iTV(t)x = -iTw(t).$$

Hence,

$$\frac{d}{dt}\langle w(t), w(t)\rangle = \langle w', w\rangle + \langle w, w'\rangle = i\langle Tw, w\rangle - i\langle w, Tw\rangle = 0,$$

by the symmetry of T.

Exercise 13.6. Formulate and prove the product rule for derivatives of the scalar product that was used here.

Since $w(0) = 0$, this shows that $U(t)x = V(t)x$ for all $t \in \mathbb{R}$. Since this holds for all x from the dense set $D(S)$ and since both $U(t)$ and $V(t)$ are bounded operators, we obtain the desired conclusion $U(t) = V(t)$.

This construction of the infinitesimal generator T also yields uniqueness: If T is the generator constructed in this proof and we also have $U(t) = e^{-itA}$, with $A = A^*$, then Exercise 13.3 with $t = 0$ (and A taking the role of T) shows that $A \subseteq T$. As both A and T are self-adjoint, this implies that $A = T$. □

Exercise 13.7. Provide the omitted details in the first part of the proof. More precisely, clearly state and then prove the properties of integrals of the type $\int \varphi(t)\, dt$ (where $\varphi : \mathbb{R} \to H$ is a compactly supported continuous function) that were used in the proof.

In fact, this proof has shown slightly more than originally stated. By Exercise 13.3 again, the limit from the definition of $D(S)$ exists for *all* $x \in D(T)$, so $S = T$ and the closure operation from the proof turns out to be unnecessary. In other words, (13.1) gives a description of the generator of $U(t)$.

Once we know that every strongly continuous group has an infinitesimal generator, the statement of Exercise 13.3 becomes completely general. It is of particular interest in quantum mechanics, so we formulate it one more time.

Corollary 13.2. *Let $U(t)$ be a strongly continuous unitary group with generator T. Suppose that $\psi \in D(T)$. Then $U(t)\psi \in D(T)$ for all $t \in \mathbb{R}$ and $\psi(t) \equiv U(t)\psi$ satisfies the (Hilbert space valued) differential equation*

$$i\frac{d\psi(t)}{dt} = T\psi(t).$$

In the context of quantum mechanics, this is the famous (time-dependent) *Schrödinger equation.* The self-adjoint operator T is called the *Schrödinger operator* (mathematicians) or the *Hamilton operator* (physicists) of the system. T is at the same time the observable *energy* of the system, which is a satisfying analogy to the time evolution of classical mechanics. We can reformulate (D):

(D') The time-evolved state $\psi(t)$, while no measurement is performed, obeys *Schrödinger's equation*

$$i\,\frac{d}{dt}\psi(t) = T\psi(t),$$

for a self-adjoint operator T, which we call the *Schrödinger operator* of the system.

This description of the dynamics of a quantum system is found in most physics books. Note, however, that we have sacrificed some precision here: The Schrödinger equation can be taken at face value only if $\psi(0) \in D(T)$; otherwise, one has to fall back on the unitary group $U(t) = e^{-itT}$. We can also say that with the help of the unitary group, we can solve the Schrödinger equation, $\psi(t) = e^{-itT}\psi(0)$, and this solution has the added benefit that it works for all $\psi(0) \in H$. Of course, this solution is not very explicit because e^{-itT} is defined via the functional calculus as $e^{-itT} = \int e^{-its}\, dE(s)$, and typically it will not be easy to obtain information on E for a given T.

Note also that only self-adjoint operators are admissible as Schrödinger operators of quantum mechanical systems because only these can be generators of unitary groups. In particular, it is not enough to just come up with some symmetric operator and leave the matter at that. Domain issues need to be discussed very carefully.

Our second set of mathematical results in this chapter will show how to use spectral theory to obtain asymptotic information on the dynamics in cases where a complete analysis of $U(t) = e^{-itT}$ is not possible, which is all cases of interest minus perhaps one or two.

To keep matters digestible, we focus on one-particle systems right away. Then the Hilbert space is usually taken to be $H = L^2(\mathbb{R}^3)$ or even $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ if we want to include electron spin. The variable $x \in \mathbb{R}^3$ is interpreted as space. We will try to avoid some technical problems by instead analyzing discrete analogs of these models. So we will work with $H = \ell^2(\mathbb{Z}^d)$. Again, we want to interpret $n \in \mathbb{Z}^d$ as position, so you should think of a quantum mechanical particle whose position, if it were measured, is restricted to the lattice points $n = (n_1, n_2, \ldots, n_d) \in \mathbb{Z}^d$. We can be more explicit: the observable *jth component of position* is the (unbounded) operator of multiplication by n_j, on its natural domain $D_j = \{\psi \in \ell^2(\mathbb{Z}^d) : n_j\psi(n) \in \ell^2(\mathbb{Z}^d)\}$. Note that all these operators commute for different values of j, so they are simultaneously measurable.

Exercise 13.8. This is a bit imprecise since our operators are unbounded and thus commutators are plagued by domain issues. Show that nevertheless there is a self-adjoint $X \in B(H)$ such that $Q_j = f_j(X)$ for suitable Borel function f_j, with Q_j denoting the operator of multiplication by n_j. *Suggestion:* Take suitable functions of the Q_j to make them bounded.

Easier to deal with and more relevant for our purposes are the corresponding projection operators that describe the measurement of the yes/no questions *is the particle in M?,* for $M \subseteq \mathbb{Z}^d$. These are given by $(P_M\psi)(n) = \chi_M(n)\psi(n)$, with measurement result 1 corresponding to the answer *yes.*

Exercise 13.9. Derive this from the description of the position observables that was given above. *Suggestion:* It suffices to do this for $M = M_1 \times \ldots M_d$ (or in fact for $M = \{m\}$). Show that then $P_M = E_1(M_1) \ldots E_d(M_d)$, where E_j is the spectral resolution of the jth component of the position operator, which is multiplication by n_j.

Notice that P_M indeed projects onto $\{\varphi \in \ell^2 : \varphi(n) = 0 \text{ if } n \notin M\}$; in particular, P_M is self-adjoint, as it must be according to (O). If the system is in the state $\psi \in \ell^2$, $\|\psi\| = 1$, and we measure P_M, then the probabilities are

$$p(1) = \|P_M\psi\|^2 = \sum_{n\in M} |\psi(n)|^2,$$

$$p(0) = \|(1 - P_M)\psi\|^2 = \sum_{n\notin M} |\psi(n)|^2.$$

As discussed, 1 means *the particle is found in M,* and 0 means *the particle is not found in M.* So it turns out that $|\psi(n)|^2$ has a direct physical interpretation as the probability of finding the particle at site n, if we choose to measure this observable (if we don't measure it, then of course any talk about the position of the particle is philosophically risky, as we saw in the last chapter). This, in the continuous version, is often called the *Born rule,* and this is the probabilistic component of quantum mechanics that was historically discovered first; our axioms (O), (C) are essentially due to von Neumann, and they were formulated several years later.

Now suppose we prepare the system in a certain state ψ and we wait a long time before we carry out such a measurement. Where will we, most likely, find the particle? We now classify states according to their long term dynamic behavior in this sense.

Let T be a self-adjoint operator on $\ell^2(\mathbb{Z}^d)$, thought of as the Schrödinger operator of some quantum system. Evolve $\psi \in \ell^2$, according to

(D'), $\psi(t) = e^{-itT}\psi$, and denote the probability of finding the particle in M at time t by $p_M(t) = \sum_{n\in M} |\psi(n,t)|^2$. We will also use the quantity p_M for not necessarily normalized $\psi \in \ell^2$; then $0 \le p_M \le \|\psi\|^2$.

Definition 13.3. Let $\psi \in \ell^2(\mathbb{Z}^d)$. We call ψ a *strong scattering state* if $\lim_{|t|\to\infty} p_M(t) = 0$ for every finite set $M \subseteq \mathbb{Z}^d$. If

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} p_M(t)\, dt = 0$$

for every finite set $M \subseteq \mathbb{Z}^d$, then we call ψ a *weak scattering state.* If for every $\epsilon > 0$, we can find a finite set $M \subseteq \mathbb{Z}^d$ such that $p_{M^c}(t) < \epsilon$ for all $t \in \mathbb{R}$, then we call ψ a *bound state.*

We write H_{ss}, H_{ws}, H_b for the corresponding subsets of ℓ^2.

So, roughly speaking, if the system is in a scattering state, then the particle will leave every bounded set if you just wait long enough. In a weak scattering state, we can only make such a statement about the time averaged probabilities. If the system is in a bound state, on the other hand, it is essentially confined to a bounded set for all times.

Obviously, $H_{ss} \subseteq H_{ws}$. More can be said:

Proposition 13.4. *H_{ss}, H_{ws}, and H_b are closed subspaces and $\ell^2 = H_{ws} \oplus H_b$.*

We postpone the proof because other results that we will develop later will come in handy here.

We want to relate the dynamically defined subspaces H_{ss}, H_{ws}, H_b to spectral subspaces, so we need to discuss this topic first. We do this in an abstract setting.

So let T be a self-adjoint operator on a Hilbert space H. Recall that a Borel measure ρ on $\mathbb{R}$ is called *absolutely continuous* if $\rho(B) = 0$ for all Borel sets $B \subseteq \mathbb{R}$ of Lebesgue measure zero. By the Radon-Nikodym Theorem, ρ is absolutely continuous if and only if $d\rho(t) = f(t)\, dt$ for some density $f \in L^1_{\text{loc}}(\mathbb{R})$, $f \ge 0$. If ρ is supported by a Lebesgue null set (that is, there exists a Borel set $B \subseteq \mathbb{R}$ with $m(B) = \rho(B^c) = 0$), then we say that ρ is *singular.* If ρ is even supported by a countable set, then we call ρ a *(pure) point measure.* We call ρ *continuous* if $\rho(\{x\}) = 0$ for all $x \in \mathbb{R}$, and a *singular continuous* measure is a measure that is both singular and continuous (the standard example being the Cantor measure).

Any Borel measure ρ on $\mathbb{R}$ can be uniquely decomposed into absolutely continuous, singular continuous, and point parts:

$$\rho = \rho_{ac} + \rho_{sc} + \rho_{pp} \tag{13.3}$$

Exercise 13.10. Derive this refined decomposition from Lebesgue's decomposition theorem (see, for example, Folland, Real Analysis, Theorem 3.8), which says that we can, in a unique fashion, write $\rho = \rho_{ac} + \rho_s$, where ρ_{ac} is absolutely continuous and ρ_s is singular. In other words, you need to further break up ρ_s.

We now apply these notions to spectral measures to define the spectral subspaces. We write $d\mu_x(t) = d\|E(t)x\|^2$ for the spectral measure of T and x (we used to denote this by $\mu_{x,x}$).

Definition 13.5. The *absolutely continuous, singular continuous,* and *pure point subspaces* are defined as follows:

$$H_{ac} = \{x \in H : \mu_x \text{ is absolutely continuous}\}$$
$$H_{sc} = \{x \in H : \mu_x \text{ is singular continuous}\}$$
$$H_{pp} = \{x \in H : \mu_x \text{ is a pure point measure}\}$$

Theorem 13.6. *H_{ac}, H_{sc}, H_{pp} are closed subspaces; in fact, they are reducing subspaces for T. Moreover,*

$$H = H_{ac} \oplus H_{sc} \oplus H_{pp}. \tag{13.4}$$

Proof. We first show that the $H_{\dots}$ are closed subspaces and that (13.4) holds. We will make use of the following fact, or rather the version for three subsets.

Exercise 13.11. Let A, B be subsets of a Hilbert space H and suppose that $A \perp B$ and $H = A + B$ (that is, every $x \in H$ can be written in the form $x = a + b$ with $a \in A$, $b \in B$). Show that then $A = B^\perp$, $B = A^\perp$, so A, B are closed subspaces and $H = A \oplus B$.

Let $x \in H$, and decompose μ_x as in (13.3): $\mu_x = \mu_{ac} + \mu_{sc} + \mu_{pp}$. By the defining properties of the individual parts, we can find disjoint Borel sets S_{ac}, S_{sc}, S_{pp} that support the corresponding μ's. Then their union supports μ (or we can just assume that this union is all of $\mathbb{R}$), so

$$x = E(S_{ac} \cup S_{sc} \cup S_{pp})x = E(S_{ac})x + E(S_{sc})x + E(S_{pp})x.$$

Notice that, for example,

$$\begin{aligned} \mu_{E(S_{ac})x}(M) &= \|E(M)E(S_{ac})x\|^2 = \|E(M \cap S_{ac})x\|^2 \\ &= \mu_x(M \cap S_{ac}) = \mu_{ac}(M), \end{aligned}$$

and similarly for the other parts, so $E(S_j)x \in H_j$ for $j = ac, sc, pp$. This proves that $H = H_{ac} + H_{sc} + H_{pp}$. To prove that these sets are orthogonal to each other, let $x \in H_{ac}$, $y \in H_{sc}$, say. As above, the corresponding spectral measures μ_x, μ_y admit disjoint supports S_x, S_y

(because one measure is absolutely continuous, the other is singular). It follows that

$$\langle x, y\rangle = \langle E(S_x)x, E(S_y)y\rangle = \langle x, E(S_x)E(S_y)y\rangle = 0.$$

An argument of this type works in all cases. We have proved (13.4).

To prove that these subspaces are reducing, we will use the criterion from Exercise 11.28(a). So let P be the projection onto H_{ac}, say; we want to show that $PT \subseteq TP$. Notice that Theorem 11.18(c) implies that

$$E(A)T \subseteq TE(A) \tag{13.5}$$

for all Borel sets $A \subseteq \mathbb{R}$.

Let $x \in D(T)$. Fix again a Borel set $S \subseteq \mathbb{R}$ that supports $(\mu_x)_{ac}$ and is given zero weight by the singular part of μ_x. Then, as above, $Px = E(S)x$. Moreover, $E(S)x \in D(T)$, too, so $x \in D(TP)$ and $TPx = TE(S)x$. By (13.5), this equals $E(S)Tx$, so it just remains to show that $E(S)Tx = PTx$. Now (13.5) also implies that

$$d\mu_{Tx}(t) = t^2\, d\mu_x(t). \tag{13.6}$$

From the first part of the proof, we know that we can obtain $P(Tx)$ as $E(M)(Tx)$, where the set $M \subseteq \mathbb{R}$ needs to be chosen such that it supports the ac part of μ_{Tx} and is given zero weight by the singular part of the same measure. By (13.6), a set that works for x will also work for Tx, so we can take $M = S$. □

It is useful to note that H_{pp} has an alternative description. As usual, we call $x \in H$, $x \neq 0$ an *eigenvector* with eigenvalue $t \in \mathbb{R}$ if $x \in D(T)$ and $Tx = tx$.

Proposition 13.7. *H_{pp} is the closed linear span of the eigenvectors of T.*

Exercise 13.12. Prove that $x \neq 0$ is an eigenvector with eigenvalue t if and only if $E(\{t\})x = x$.

Proof. If x is an eigenvector with eigenvalue t, then, by the Exercise, $x = E(\{t\})x$, so

$$\mu_x(M) = \|E(M)x\|^2 = \|E(M \cap \{t\})x\|^2$$

is supported by $\{t\}$ and thus definitely a pure point measure. In other words, $x \in H_{pp}$ for all eigenvectors x. Since H_{pp} is a closed subspace, this implies that the closed linear span of the eigenvectors is contained in H_{pp}.

Conversely, if $x \in H_{pp}$ and $\{t_j : j \in \mathbb{N}\}$ supports μ_x, then

$$x = E(\{t_j : j \in \mathbb{N}\})x = \lim_{N\to\infty} \sum_{j=1}^{N} E(\{t_j\})x, \tag{13.7}$$

and by Exercise 13.12 again, this shows that x is in the closed linear span of the eigenvectors. □

Exercise 13.13. Give a careful argument for the second equality in (13.7).

We now return to the situation where $H = \ell^2(\mathbb{Z}^d)$ and consider the dynamical subspaces from Definition 13.3.

Theorem 13.8. *$H_{ws} = H_c$, $H_b = H_{pp}$. Moreover, $H_{ac} \subseteq H_{ss}$.*

Here, H_c denotes the *continuous subspace* $H_c = H_{ac} \oplus H_{sc}$.

Exercise 13.14. Prove that $x \in H_c$ if and only if μ_x is a continuous measure.

Theorem 13.8 depends on two easy classical results on the Fourier transform of measures; in fact, it could be argued that Theorem 13.8 is essentially a rephrasing of these results. To see why Fourier transforms are relevant here, denote the standard ONB of $\ell^2(\mathbb{Z}^d)$ by $\{\delta_n : n \in \mathbb{Z}^d\}$. So $\delta_n(m) = 1$ if $m = n$ and $\delta_n(m) = 0$ otherwise. Write

$$\widehat{\mu}(t) = \int_{\mathbb{R}} e^{-its}\, d\mu(s)$$

for the Fourier transform of a finite (possibly complex) Borel measure μ. Then

$$p_M(t) = \sum_{n\in M} \left|\langle \delta_n, e^{-itT}\psi\rangle\right|^2 = \sum_{n\in M} |\widehat{\rho_n}(t)|^2,$$

where we use the notation $\rho_n(B) = \langle \delta_n, E(B)\psi\rangle$ for the (complex) spectral measure associated with the vectors δ_n, ψ.

Here are the two results about Fourier transforms that will form the basis of our discussion. Our measures are still assumed to be complex Borel measures on $\mathbb{R}$; in particular, they must be finite if they are positive.

Theorem 13.9 (Riemann-Lebesgue Lemma)**.** *Let μ be an absolutely continuous measure. Then $\lim_{|t|\to\infty} \widehat{\mu}(t) = 0$.*

Theorem 13.10 (Wiener)**.**

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} |\widehat{\mu}(t)|^2\, dt = \sum_{x\in\mathbb{R}} |\mu(\{x\})|^2$$

Existence of the limit is part of the statement in Wiener's Theorem. Note that $\mu(\{x\}) \neq 0$ for at most countably many $x \in \mathbb{R}$, so there are no difficulties involved in defining the sum. We will not use the formula from Wiener's Theorem, but the following immediate Corollary:

Corollary 13.11.

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} |\widehat{\mu}(t)|^2 \, dt = 0$$

if and only if $\mu_{pp} = 0$.

Exercise 13.15. Provide proofs of the Riemann-Lebesgue Lemma and Wiener's Theorem.

Proof of Theorem 13.8 and Proposition 13.4. Notice that

$$|\rho_n(B)| = |\langle \delta_n, E(B)\psi\rangle| \leq \|E(B)\psi\|,$$

so $\rho_n \ll \mu_\psi$. Thus, if $\psi \in H_{ac}$, then the ρ_n ($n \in \mathbb{Z}^d$) are absolutely continuous measures, too. The Riemann-Lebesgue Lemma now shows that

$$p_M(t) = \sum_{n\in M} |\widehat{\rho_n}(t)|^2 \to 0 \quad (t \to \pm\infty)$$

for all finite $M \subseteq \mathbb{Z}^d$, so $H_{ac} \subseteq H_{ss}$.

A similar argument, with Corollary 13.11 replacing the Riemann-Lebesgue Lemma, shows that $H_c \subseteq H_{ws}$. Conversely, if $\psi \in H_{ws}$, then in particular

$$\frac{1}{2T} \int_{-T}^{T} |\widehat{\rho_n}(t)|^2 \, dt \to 0$$

for all $n \in \mathbb{Z}^d$, so, by Corollary 13.11 again, every ρ_n is a continuous measure. But then μ_ψ is a continuous measure, too, because if $x \in \mathbb{R}$ is an arbitrary point, then

$$\begin{aligned}\mu_\psi(\{x\}) = \langle \psi, E(\{x\})\psi\rangle &= \sum \overline{\psi(n)} \langle \delta_n, E(\{x\})\psi\rangle \\ &= \sum \overline{\psi(n)} \rho_n(\{x\}) = 0.\end{aligned}$$

In other words, $\psi \in H_c$. This identification $H_{ws} = H_c$ also proves that H_{ws} is a closed (in fact: reducing, for T) subspace, as claimed in Proposition 13.4.

Next, we show directly that H_b is a closed subspace also. Obviously, $c\psi \in H_b$ if $\psi \in H_b$, and the estimate

$$\left|\langle \delta_n, e^{-itT}(\psi_1 + \psi_2)\rangle\right|^2 \leq 2\left|\langle \delta_n, e^{-itT}\psi_1\rangle\right|^2 + 2\left|\langle \delta_n, e^{-itT}\psi_2\rangle\right|^2$$

makes it clear that also $\psi_1 + \psi_2 \in H_b$ if $\psi_{1,2} \in H_b$. If $\psi_j \in H_b$, $\psi_j \to \psi$, and $\epsilon > 0$ is given, pick first a $j \in \mathbb{N}$ such that $\|\psi_j - \psi\|^2 < \epsilon$ and then $M \subseteq \mathbb{Z}^d$, M finite, so large that

$$\sum_{n \notin M} \left|\langle \delta_n, e^{-itT}\psi_j\rangle\right|^2 < \epsilon$$

for all $t \in \mathbb{R}$ (and this j). Since

$$\sum_{n \in \mathbb{Z}^d} \left|\langle \delta_n, e^{-itT}\psi_j\rangle - \langle \delta_n, e^{-itT}\psi\rangle\right|^2 = \|e^{-itT}(\psi_j - \psi)\|^2 = \|\psi_j - \psi\|^2,$$

by Parseval's identity, it then follows that

$$\sum_{n \notin M} \left|\langle \delta_n, e^{-itT}\psi\rangle\right|^2 < 4\epsilon$$

for all $t \in \mathbb{R}$. Thus $\psi \in H_b$, and H_b is closed.

Exercise 13.16. Prove in a similar way that H_{ss} is a closed subspace.

Next, let ψ be an eigenvector, with eigenvalue s, say. Then $\langle \delta_n, e^{-itT}\psi\rangle = e^{-ist}\langle \delta_n, \psi\rangle$, so

$$p_{M^c}(t) = \sum_{n \notin M} |\langle \delta_n, \psi\rangle|^2,$$

and Parseval's identity ensures that this can be made arbitrarily small by taking M sufficiently large. So all eigenvectors belong to H_b, and H_b is a closed subspace, so Proposition 13.7 shows that $H_{pp} \subseteq H_b$.

Finally, we claim that $H_b \perp H_{ws}$. To prove this, let $\varphi \in H_b$, $\psi \in H_{ws}$. Then

$$\begin{aligned}\langle \varphi, \psi\rangle = \langle e^{-itT}\varphi, e^{-itT}\psi\rangle &= \frac{1}{2T}\int_{-T}^{T} \langle e^{-itT}\varphi, e^{-itT}\psi\rangle\, dt \\ &= \frac{1}{2T}\int_{-T}^{T} \sum_{n \in \mathbb{Z}^d} \langle e^{-itT}\varphi, \delta_n\rangle\langle \delta_n, e^{-itT}\psi\rangle\, dt.\end{aligned}$$

We split this sum into two parts, as follows. Given $\epsilon > 0$, we can find a finite set $M \subseteq \mathbb{Z}^d$ such that $\|\psi\|^2 \sum_{n \notin M} |\langle e^{-itT}\varphi, \delta_n\rangle|^2 < \epsilon^2$ for all $t \in \mathbb{R}$. With the help of the Cauchy-Schwarz inequality and Parseval's identity, we thus see that

$$\left|\sum_{n \notin M} \langle e^{-itT}\varphi, \delta_n\rangle\langle \delta_n, e^{-itT}\psi\rangle\right| < \epsilon,$$

and thus the corresponding time averaged quantity is also $< \epsilon$. Since $\psi \in H_{ws}$, we have $1/(2T)\int_{-T}^{T} |\langle \delta_n, e^{-itT}\psi\rangle|^2\, dt \to 0$ for all $n \in \mathbb{Z}^d$. Now

M is finite, so we can take $T > 0$ so large that also

$$\left| \sum_{n \in M} \frac{1}{2T} \int_{-T}^{T} \langle e^{-itT}\varphi, \delta_n \rangle \langle \delta_n, e^{-itT}\psi \rangle \, dt \right| < \epsilon.$$

We again use the Cauchy-Schwarz inequality here, and in fact we use it twice, to estimate the integral as well as the sum. Our estimates have shown that $|\langle \varphi, \psi \rangle| < 2\epsilon$, and $\epsilon > 0$ was arbitrary here, so $\langle \varphi, \psi \rangle = 0$, as claimed.

Put differently, we have seen that $H_b \subseteq H_{ws}^{\perp}$. We know already that $H_{ws} = H_c$ (see the first part of this proof) and $H_c^{\perp} = H_{pp}$ (see (13.4)), so it follows that $H_b \subseteq H_{pp}$. □

The decomposition from Theorem 13.6 also induces decompositions of the other quantities that are involved here. This makes use of the fact that we have *reducing* subspaces. More specifically, we can write

$$T = T_{ac} \oplus T_{sc} \oplus T_{pp},$$

where, for example, $T_{ac} : H_{ac} \to H_{ac}$, $D(T_{ac}) = D(T) \cap H_{ac}$, and if $x \in D(T_{ac})$, then $T_{ac}x = Tx$. We also define $\sigma_j(T) := \sigma(T_j)$, where $j = ac, sc, pp$. As in Chapter 10 (see especially Proposition 10.9), we then have

$$\sigma(T) = \sigma_{ac}(T) \cup \sigma_{sc}(T) \cup \sigma_{pp}(T).$$

The union is *not* necessarily disjoint, as the following Example shows. We will make use of the following fact, which is of considerable independent interest.

Proposition 13.12. *The (pure) point spectrum, σ_{pp}, is the closure of the set of eigenvalues.*

Recall that (much) earlier, we introduced the notation σ_p for the set of eigenvalues; so we can now say that $\sigma_{pp} = \overline{\sigma_p}$. In particular, σ_{pp} can be much larger than σ_p.

Proof. H_{pp} contains all eigenvectors, so every eigenvalue of T is an eigenvalue of T_{pp} also, so $\sigma_p \subseteq \sigma_{pp}$. Since σ_{pp}, being a spectrum, is closed, we in fact obtain $\overline{\sigma_p} \subseteq \sigma_{pp}$.

Conversely, if $t \in \sigma_{pp} = \sigma(T_{pp})$, then for any $r > 0$, we can find an $x = x_r \in H_{pp}$ such that $E((t-r, t+r))x = x$. Then μ_x is a pure point measure, since $x \in H_{pp}$, and an $s \in \mathbb{R}$ with $E(\{s\}) \neq 0$ is an eigenvalue by Exercise 13.12, so this means that there are eigenvalues arbitrarily close to t, so $t \in \overline{\sigma_p}$. □

Example 13.1. This is in fact very easy from an abstract point of view. We can start out with, let's say, an absolutely continuous operator on one Hilbert space and a pure point operator on a second space and then assemble these by taking the orthogonal sum.

For example, let $H_0 = L^2(0,1)$, $(T_0 f)(x) = xf(x)$. Note that $T_0 \in B(H_0)$, $T_0 = T_0^*$. In fact, T_0 is already given as multiplication by the variable, as in a Spectral Representation, so the spectral theory of T_0 is easy to work out. I claim that $H_{ac} = H_0$ for this operator. Indeed, if $f \in H_0$ is arbitrary, then

$$\mu_f(M) = \|E(M)f\|^2 = \int |\chi_M f|^2 \, dx.$$

In this context, recall the discussion following Proposition 10.10, where the spectral resolution was identified as $E(M)f = \chi_M f$. So $d\mu_f = |f|^2 dx$, and, as claimed, all spectral measures are absolutely continuous. Finally, notice that $\sigma(T_0) = [0,1]$.

Next, let H_1 be an arbitrary separable Hilbert space. Let $\{x_n\}$ be an ONB of H_1, and fix an enumeration $\{q_n\}$ of $\mathbb{Q} \cap [0,1]$. Define $T_1 x_n = q_n x_n$ and extend linearly.

Exercise 13.17. Prove that T_1 is bounded on $L(x_n)$ and thus extends continuously to $\overline{L(x_n)} = H_1$. Show that (the extended) $T_1 \in B(H_1)$, $H_1 = H_{pp}$, $\sigma(T_1) = [0,1]$.

We can now let $H = H_0 \oplus H_1$, $T = T_0 \oplus T_1$. Then, basically by construction, T_0 and T_1 are the absolutely continuous and pure point parts, respectively, of T. In particular, $\sigma_{ac}(T) = \sigma_{pp}(T) = [0,1]$.

Exercise 13.18. Let T be self-adjoint. Prove that every isolated point of $\sigma(T)$ is an eigenvalue of T.

Exercise 13.19. Let $H = \mathbb{C}^n$ be a finite-dimensional Hilbert space. Show that then $H_{pp} = H$, $H_{ac} = H_{sc} = 0$ for every self-adjoint T on H.

Exercise 13.20. Let P be the projection onto the closed subspace $M \subseteq H$, and let $T \in B(H)$ be self-adjoint, $T = \int t \, dE(t)$. Prove that M is a reducing subspace for T if and only if $PE(B) = E(B)P$ for all Borel sets $B \subseteq \mathbb{R}$.
Hint: By Exercise 11.21(a), M is reducing if and only if $PT = TP$.
Remark: The statement also holds for unbounded self-adjoint T, but the proof becomes more technical in this case.

Exercise 13.21. Let $T \in B(H)$ be self-adjoint. Show that a closed invariant subspace M (so $Tx \in M$ for $x \in M$) is reducing.

Exercise 13.22. Let μ be a finite (positive) Borel measure on $\mathbb{R}$, with Lebesgue decomposition $\mu = \mu_{ac} + \mu_{sc} + \mu_{pp}$. Consider the (self-adjoint) operator of multiplication by the variable on $L^2(\mathbb{R},\mu)$:

$$D(M_t)=\{f\in L^2(\mu): tf(t)\in L^2(\mu)\},\quad (M_tf)(t)=tf(t)$$

Prove that H_j may be naturally identified with $L^2(\mathbb{R},\mu_j)$, for $j=ac,sc,pp$. More precisely, proceed as follows: Pick disjoint supports S_j of μ_j, and show that $P_jf=\chi_{S_j}f$, where P_j denotes the projection onto H_j ($j=ac,sc,pp$). Given this, we then indeed have

$$H_j=\{f\in L^2(\mu): f=0\ \mu\text{-a.e. on } S_j^c\},$$

which may be identified with $L^2(S_j,\mu)$ and also with $L^2(\mathbb{R},\mu_j)$.