6 Spectrum of bounded linear operators

6.1 Spectrum of bounded operators on Banach spaces

Definition 9. Let V be a Banach space. The *spectrum* of $T \in \mathcal{B}(V)$ is defined to be

$$\sigma(T) := \{\lambda \in \mathbb{C} \,:\, \lambda - T \text{ not invertible in } \mathcal{B}(V)\}, \tag{6.1}$$

and the complement

$$\rho(T) := \mathbb{C} \setminus \sigma(T)$$

is the *resolvent set* of T.

Remark. Usually, when we say that $T \in \mathcal{B}(V)$ is invertible, we mean that it has an inverse in $\mathcal{B}(V)$. Actually, if $T \in \mathcal{B}(V)$ is invertible set-theoretically, then the set-theoretic inverse (which is linear) is automatically bounded! This remarkable fact is called the *bounded inverse theorem*, which is one of the famous core theorems of functional analysis; see Chapter III.5 of Reed–Simon for a proof.

Recall that λ is an *eigenvalue* of T if $\lambda - T$ is non-injective; in this case, T possesses a non-zero *eigenspace* of *eigenvectors* v such that $Tv = \lambda v$. In finite dimensions, the spectrum is the same thing as the set of eigenvalues, and every matrix has an eigenvalue (over $\mathbb{C}$). In infinite dimensions, the latter statement is replaced by Corollary 6.5 below. The set of eigenvalues is called the *point spectrum*, denoted

$$\sigma_{\mathrm{p}} = \{\lambda \in \mathbb{C} \,:\, \lambda - T \,\text{not injective}\}.$$

Obviously, $\sigma_{\mathrm{p}}(T) \subset \sigma(T)$. But not all elements of $\sigma(T)$ are eigenvalues!

Exercise 6.1. Consider the Banach space $\ell^2(\mathbb{Z})$, with canonical basis vectors

$$e_n = (\ldots, 0, \underbrace{1}_{n\text{-th}}, 0 \ldots), \qquad n \in \mathbb{Z}.$$

Let R be the right shift operator on $\ell^2(\mathbb{Z})$ taking each e_n to e_{n+1}.

- Show that $\sigma_{\mathrm{p}}(R)$ is empty.

- Let λ be a unit complex number, $|\lambda| = 1$. Find a sequence of unit vectors $v_1, v_2, \ldots \in \ell^2(\mathbb{Z})$, such that

$$\lim_{n\to\infty} ||Rv_n - \lambda v_n|| = 0.$$

  (Thus λ is an approximate eigenvalue, see Definition 11.)

- Deduce that $\{\lambda \in \mathbb{C} : |\lambda| = 1\} \subset \sigma(T)$.

Proposition 6.1 (Neumann series)**.** *Let V be a Banach space and $T \in \mathcal{B}(V)$. If $|\lambda| > ||T||_{\text{op}}$, then $\lambda \in \rho(T)$.*

Proof. By scaling, we may assume $\lambda = 1$ and $||T||_{\text{op}} < 1$. Then sub-multiplicativity of $||\cdot||_{\text{op}}$ implies that the Neumann series

$$\sum_{n=0}^{\infty} T^n$$

converges in $\mathcal{B}(V)$, and it is the inverse of $(1 - T)$, since

$$(1 - T)(1 + T + \ldots + T^n) = 1 - T^{n+1}, \qquad n \geq 1.$$

□

Proposition 6.2 (Compactness of spectrum)**.** *Let V be a Banach space and $T \in \mathcal{B}(V)$. Then $\sigma(T)$ is a compact subset of $\mathbb{C}$.*

Proof. Fix any $\mu \in \rho(T)$. Then

$$\begin{aligned} ||1 - (\mu - T)^{-1}(\lambda - T)|| &= ||(\mu - T)^{-1}\big((\mu - T) - (\lambda - T)\big)|| \\ &= ||(\mu - T)^{-1}|| \cdot |\mu - \lambda|, \qquad \lambda \in \mathbb{C}. \end{aligned}$$

In particular, for all λ sufficiently close to μ, the inequality

$$||1 - (\mu - T)^{-1}(\lambda - T)|| < 1$$

holds, and Prop. 6.1 says that

$$1 - (1 - (\mu - T)^{-1}(\lambda - T)) = (\mu - T)^{-1}(\lambda - T)$$

is invertible. Thus $\lambda \in \rho(T)$. Since $\mu \in \rho(T)$ was arbitrary, we have shown that $\rho(T)$ is open, thus $\sigma(T)$ is closed. Due to Prop. 6.1, $\sigma(T)$ is bounded; thus it is compact. □

Exercise 6.2. Let V be a Banach space, and $T \in \mathcal{B}(V)$. Show that

- The spectrum is invariant under a similarity transformation,

$$\sigma(T) = \sigma(ATA^{-1}).$$

- If T is invertible, then

$$\sigma(T^{-1}) = \sigma(T)^{-1} := \{\lambda^{-1} \,:\, \lambda \in \sigma(T)\}.$$

- If p is a polynomial, then

$$\sigma(p(T)) = p(\sigma(T)) = \{p(\lambda) \,:\, \lambda \in \sigma(T)\}.$$

We end this section with a useful characterization of invertibility.

Proposition 6.3. *Let V be a Banach space, and $T \in \mathcal{B}(V)$. Then T is invertible iff T is bounded below and has dense range.*

Proof. Suppose T is invertible. Obviously it has dense range. Furthermore, for any $v \in V$,

$$||v|| = ||T^{-1}Tv|| \leq ||T^{-1}|| \cdot ||Tv||,$$

so T is bounded below by $||T^{-1}||^{-1}$.

Conversely, suppose that (i) the range of T is dense, and (ii) there exists some $\alpha > 0$ such that $||Tv|| \geq \alpha||v||$ for all $v \in V$. It follows from (ii) that T has closed range: if $Tv_n = y_n \to y$, then

$$||v_n - v_m|| \leq \alpha^{-1}||Tv_n - Tv_m|| = \alpha^{-1}||y_n - y_m||,$$

so $\{v_n\}$ is Cauchy, and has a limit $v \in V$; continuity of T means $Tv = y$. Combining this closed range property with (i), we see that T is surjective.

For injectivity, suppose $Tv = Tv'$, then $0 = ||T(v - v')|| \geq \alpha||v - v'||$, which implies $v = v'$. Thus the set-theoretic inverse T^{-1} exists (and is linear). It is straightforward to check that T^{-1} is bounded (in fact, $||T^{-1}||_{\text{op}} \leq \alpha^{-1}$.) $\square$

6.1.1 Existence of spectrum (optional)

Theorem 6.4. *Let V be a Banach space, and $T \in \mathcal{B}(V)$. The assignment of resolvents,*

$$\begin{aligned} \rho(T) &\to \mathcal{B}(V) \\ \lambda &\mapsto R_\lambda(T) := (\lambda - T)^{-1} \end{aligned}$$

is analytic on each component of $\rho(T)$.

Proof. For each $\mu \in \rho(T)$, let us find a power series expansion for $R_\lambda(T)$ near μ. Formally,

$$\begin{aligned} R_\lambda(T) \text{“}=\text{”} \frac{1}{\lambda - T} = \frac{1}{(\mu - T) - (\mu - \lambda)} &= \frac{1}{\mu - T}\left(1 - \frac{\mu - \lambda}{\mu - T}\right)^{-1} \\ &= \frac{1}{\mu - T}\left(\sum_{n=0}^{\infty}\left(\frac{\mu - \lambda}{\mu - T}\right)^n\right) \\ &\text{“}=\text{”} \sum_{n=0}^{\infty}(\mu - \lambda)^n (R_\mu(T))^{n+1}. \end{aligned}$$

Using the sub-multiplicativity of the operator norm, the above power series converges to $R_\lambda(T)$ for λ in the open ball

$$|\lambda - \mu| < ||R_\mu(T)||^{-1}.$$

□

Corollary 6.5. *Let V be a Banach space. For any $T \in \mathcal{B}(V)$, the spectrum $\sigma(T)$ is non-empty (and compact).*

Proof. For large $|\lambda| > ||T||_{\text{op}}$, the Neumann series for $R_\lambda(T)$ shows that $||R_\lambda(T)||_{\text{op}} \to 0$ as $\lambda \to \infty$. Fix $\mu \in \rho(T)$. Since linear functionals separate elements[12] of $\mathcal{B}(V)$, we can choose $\Phi \in (\mathcal{B}(V))^*$ such that $\Phi(R_\mu(T)) \neq 0$.

[12] One form of the *Hahn–Banach theorem* states:

> Let V be a normed vector space, and $v, v' \in V$ be distinct. Then there exists $\Phi \in V^*$ such that $\Phi(v) \neq \Phi(v')$.

This is another non-trivial core theorem in functional analysis.

Suppose $\sigma(T)$ is empty. Then the map

$$\mathbb{C} \to \mathbb{C}, \qquad \lambda \mapsto \Phi \circ R_\lambda(T)$$

will be a bounded analytic function tending to 0 at infinity, thus identically zero by Liouville's theorem in complex analysis. In particular, $\Phi(R_\mu(T)) = 0$, which is a contradiction. □

Remark. The complex analysis proofs of non-emptiness of spectrum is the standard approach appearing in most textbooks. It is not so well-known that "elementary" proofs also exist, see, e.g. [Rickart, C., Michigan Math. J. 5 75–78 (1958)] or Kaniuth, E., A Course in Commutative Banach Algebras, pp. 12-13. For self-adjoint operators on Hilbert space, see Prop. 6.10 for a simpler proof.

6.2 Spectrum of normal operators on Hilbert spaces

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

Definition 10. An operator $T \in \mathcal{B}(\mathcal{H})$ is *normal* if $TT^* = T^*T$. Particular classes of normal operators are:

- *Self-adjoint*, if $T = T^*$;
- *Unitary*, if $TT^* = 1 = T^*T$;
- *(Orthogonal) projection*, if $T = T^* = T^2$.

There is a useful equivalent criterion for normality:

Proposition 6.6. *An operator $T \in \mathcal{B}(\mathcal{H})$ is normal iff $||T\psi|| = ||T^*\psi||$ for all $\psi \in \mathcal{H}$.*

Proof. A preparatory result is that $\langle\psi|T\psi\rangle = 0$ for all $\psi \in \mathcal{H}$ implies $T = 0$. To see this, observe that $0 = \langle\psi' + \psi|T(\psi' + \psi)\rangle = \langle\psi'|T\psi\rangle + \langle\psi|T\psi'\rangle$ as well. Replace ψ by $i\psi$ to get $0 = \langle\psi'|T\psi\rangle - \langle\psi|T\psi'\rangle$. Thus $0 = \langle\psi|T\psi'\rangle$ for all $\psi, \psi' \in \mathcal{H}$, and $T = 0$ follows readily.

Now, we have the equations

$$\begin{aligned} ||T\psi||^2 &= \langle T\psi|T\psi\rangle = \langle\psi|T^*T\psi\rangle, \\ ||T^*\psi||^2 &= \langle T^*\psi|T^*\psi\rangle = \langle\psi|TT^*\psi\rangle, \qquad \forall\psi \in \mathcal{H}. \end{aligned}$$

So $||T\psi|| = ||T^*\psi||$ for all $\psi \in \mathcal{H}$ iff $\langle\psi|(T^*T - TT^*)\psi\rangle = 0$ for all $\psi \in \mathcal{H}$ iff $T^*T - TT^* = 0$ iff T is normal. □

Note that any $T \in \mathcal{B}(\mathcal{H})$, can be decomposed as

$$T = \underbrace{\frac{1}{2}(T + T^*)}_{\text{real part}} + i \underbrace{\frac{1}{2i}(T - T^*)}_{\text{imaginary part}},$$

with the real/imaginary part being self-adjoint. This mimics the decomposition of a complex number. The key difference is that the real/imaginary parts of T are operators, so they are not guaranteed to commute with each other. In fact, they commute iff T is normal (Exercise).

Exercise 6.3. Let $T \in \mathcal{B}(\mathcal{H})$. Check that

$$\sigma(T^*) = \sigma(T)^* := \{\bar{\lambda} \,:\, \lambda \in \sigma(T)\}. \tag{6.2}$$

Exercise 6.4. Show that an invertible $T \in \mathcal{B}(\mathcal{H})$ preserves inner products iff it is unitary. (Thus unitaries are the automorphisms of Hilbert spaces.)

Exercise 6.5. Show that if U is unitary, then $\sigma(U)$ is a subset of the unit circle.

Normal operators are well-behaved from the viewpoint of spectral theory. At the level of eigenvalues, there is the following easy result:

Exercise 6.6. For a bounded normal operator, show that the eigenspaces for distinct eigenvalues are orthogonal to each other.

Next, consider the following generalization of eigenvalue:

Definition 11. Let $T \in \mathcal{B}(\mathcal{H})$. We say that $\lambda \in \mathbb{C}$ is an *approximate eigenvalue* of T if for each $\epsilon > 0$, there exists a unit vector $\psi \in \mathcal{H}$ such that $||(\lambda - T)\psi|| \leq \epsilon$. The set of approximate eigenvalues of T is its *approximate point spectrum*, denoted $\sigma_{\text{ap}}(T)$.

Exercise 6.7. Check that $\sigma_{\text{p}}(T) \subset \sigma_{\text{ap}}(T) \subset \sigma(T)$.

Theorem 6.7. *Let $T \in \mathcal{B}(\mathcal{H})$ be a normal operator. Then $\sigma(T) = \sigma_{\text{ap}}(T)$.*

Proof. The inclusion $\sigma_{\text{ap}}(T) \subset \sigma(T)$ is Exercise 6.7.

For the reverse inclusion, suppose $\lambda \notin \sigma_{\text{ap}}(T)$. So there exists $\alpha > 0$ such that $||(\lambda - T)\psi|| \geq \alpha||\psi||$ for all $\psi \in \mathcal{H}$, i.e., $\lambda - T$ is bounded below. By Prop. 6.3, it suffices to show that $\lambda - T$ has dense range, to deduce that it is invertible, thus $\lambda \in \sigma(T)$.

To that end, suppose $\varphi \in (\mathrm{Ran}(\lambda - T))^\perp$. Thus

$$0 = \langle \varphi | (\lambda - T)\psi \rangle = \langle (\bar{\lambda} - T^*)\varphi | \psi \rangle, \qquad \forall \psi \in \mathcal{H},$$

so $(\bar{\lambda} - T^*)\varphi = 0$. Now $\lambda - T$ is normal, so Prop. 6.6 says that

$$||(\bar{\lambda} - T^*)\varphi|| = ||(\lambda - T)\varphi|| \geq \alpha ||\varphi||$$

also holds. We learn that φ has to be zero. Thus $(\mathrm{Ran}(\lambda - T))^\perp = \{0\}$, which is the dense range condition. □

For non-normal operators, Theorem 6.7 is not true; the spectrum will generally include some rather mysterious elements.

Exercise 6.8. On $\ell^2 = \ell^2(\mathbb{N})$, consider the *unilateral* shift,

$$S : (x_1, x_2, x_3 \ldots) \mapsto (0, x_1, x_2, \ldots).$$

- What is the adjoint operator S^*?
- Show that $S^*S = 1$. What is SS^*? Is S normal?
- Determine the operator norm of S.
- Does S have any eigenvalues?

Let $\lambda \in \mathbb{C}$ with $|\lambda| < 1$.

- Show that λ is an eigenvalue of S^*.
- Show that $\lambda - S$ does not have dense range. Is λ an approximate eigenvalue of S?

6.3 Bounded self-adjoint operators and quantum observables

It follows immediately from (6.2) that the spectrum of a self-adjoint operator is symmetric under reflection in the real axis. We will improve this observation below.

Proposition 6.8. *$T \in \mathcal{B}(\mathcal{H})$ is self-adjoint iff $\langle \psi | T\psi \rangle \in \mathbb{R}$ for all $\psi \in \mathcal{H}$.*

Proof. Let f_T be the sesquilinear form for T (Lemma 5.6). It determines a quadratic form

$$\hat{f}_T : \psi \mapsto f_T(\psi, \psi) = \langle \psi | T\psi \rangle.$$

Similarly, for T^*, we have the sesquilinear form f_{T^*} with associated quadratic form

$$\hat{f}_{T^*} : \psi \mapsto f_{T^*}(\psi, \psi) = \langle \psi | T^*\psi \rangle = \langle T\psi | \psi \rangle.$$

So $\hat{f}_{T^*} = \hat{f}_T$ iff $\langle \psi | T\psi \rangle$ is real-valued for all $\psi \in \mathcal{H}$.

Now, the polarization identity (Eq. (4.7)) is actually a general procedure for recovering a sesquilinear form from its associated quadratic form. Thus $T = T^*$ iff $f_T = f_{T^*}$ iff $\langle \psi | T\psi \rangle$ is real-valued for all $\psi \in \mathcal{H}$. □

Theorem 6.9. *If $T \in \mathcal{B}(\mathcal{H})$ is self-adjoint, then $\sigma(T) \subset \mathbb{R}$.*

Proof. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$. For any unit vector $\psi \in \mathcal{H}$,

$$\begin{aligned} 0 < |\lambda - \bar{\lambda}| = |\lambda - \bar{\lambda}| \cdot ||\psi||^2 &= \big|\langle \psi | (\lambda - \bar{\lambda}\psi) \rangle\big| \\ &= \big|\langle \psi | (\bar{\lambda} - T)\psi \rangle - \langle \psi | (\lambda - T)\psi \rangle\big| \\ &= \big|\langle (\lambda - T)\psi | \psi \rangle - \langle \psi | (\lambda - T)\psi \rangle\big| \\ &\leq 2||(\lambda - T)\psi|| \cdot ||\psi|| \\ &= 2||(\lambda - T)\psi||. \end{aligned}$$

Thus λ is not an approximate eigenvalue of T. But T is normal, so Theorem 6.7 says that λ is not in the spectrum of T. □

The following is called the *spectral radius formula*.

Proposition 6.10. *If $T \in \mathcal{B}(\mathcal{H})$ is self-adjoint, then*

$$||T|| = \sup_{\lambda \in \sigma(T)} |\lambda|.$$

Proof. By definition of operator norm, there is a sequence of unit vectors ψ_n such that $||T\psi_n|| \to ||T||$. For these unit vectors,

$$\begin{aligned} ||(||T||^2 - T^2)\psi_n||^2 &= \big\langle \|T\|^2\psi_n - T^2\psi_n \big| \|T\|^2\psi_n - T^2\psi_n \big\rangle \\ &= ||T||^4 - \big\langle T^2\psi_n \big| \|T\|^2\psi_n \big\rangle - \big\langle \|T\|^2\psi \big| T^2\psi_n \big\rangle + ||T^2\psi_n||^2 \\ &= \|T\|^4 - 2\|T\|^2\langle T\psi_n | T\psi_n \rangle + \|T^2\psi_n\|^2 \\ &\leq ||T||^4 - 2||T||^2||T\psi_n||^2 + ||T||^2||T\psi_n||^2 \\ &= ||T||^2(||T||^2 - ||T\psi_n||^2), \end{aligned}$$

which tends to zero since the factor in round brackets tends to zero by construction. This shows that $||T||^2 \in \sigma_{\rm ap}(T^2) = \sigma(T^2)$. (Note that T^2 is self-adjoint so Theorem 6.7 applies). Now, we also saw from an exercise that polynomial spectral mapping holds,

$$\sigma(T^2) = \sigma(T)^2.$$

So $||T||$ and/or $-||T||$ belong to $\sigma(T)$. Thus $\sup_{\lambda\in\sigma(T)} |\lambda| \geq ||T||$. The reverse inequality is a general result proved in Prop. 6.1. □

6.3.1 Observables in quantum mechanics

In quantum mechanics, "observables" are modelled as bounded (and possibly unbounded) self-adjoint operators, partly because it makes sense to interpret

$$\langle\psi|T\psi\rangle \in \mathbb{R}, \qquad ||\psi|| = 1$$

as the expectation value of the T for the normalized state $\psi \in \mathcal{H}$. Why this actually works well is due to a further *orthogonal spectral decomposition* property of self-adjoint operators. Let us illustrate this in the finite-dimensional case.

In linear algebra, we learn that an $n \times n$ self-adjoint matrix $T = T^*$ can be unitarily diagonalized, with real eigenvalues. The eigenspaces for distinct eigenvalues are mutually orthogonal. For simplicity, assume non-degenerate eigenvalues. Thus T has an orthonormal basis of eigenvectors e_i, with respective eigenvalues λ_i. In ket-bra notation, the orthogonal projection onto the i-th eigenspace is $|e_i\rangle\langle e_i|$, and we may write

$$T = \sum_{i=1}^{n} \lambda_i |e_i\rangle\langle e_i|. \tag{6.3}$$

For a normalized $\psi \in \mathcal{H} \cong \mathbb{C}^n$ ("state"), the expectation value of T is thus

$$\langle\psi|T\psi\rangle = \sum_{i=1}^{n} \lambda_i \langle\psi|e_i\rangle\langle e_i|\psi\rangle = \sum_{i=1}^{n} \lambda_i |\langle e_i|\psi\rangle|^2.$$

The real number $|\langle e_i|\psi\rangle|^2$ is the probability that the i-th outcome λ_i occurs when measuring the observable T for the state ψ. The sum of all the probabilities is 1, because of the normalization condition on ψ.

In practice, an actual measurement produces only "yes/no" answers. The question of whether the i-th outcome occurs is itself an observable, with 1 ("yes") or 0 ("no") as outcomes. For example, one sets up a detector whose position coordinate (say 3.14) was measured/calibrated previously with a ruler. If "yes, detected" occurs, we formally say that "position coordinate 3.14 occurred". The physical system in question does not know about the labels attached to the detector. For "energy measurements", one has a detector already established to be sensitive to a particular frequency ν of electromagnetic radiation, then if "yes, detected" occurs, we formally say that energy (jump of) "$h\nu$ was detected".

In this sense, "observables" with distinct outcomes $\lambda_1, \ldots, \lambda_n$ are often really composites of "irreducible observables" having only $\{0, 1\}$ as outcomes. The state which has outcome λ_i with 100% certainly is called $|e_i\rangle$ (up to a U(1) phase). The minimal Hilbert space $\mathcal{H}$ for modelling the setup is spanned by these $|e_i\rangle$. The rank-1 projection operators $P_i = |e_i\rangle\langle e_i|$ have the property

$$\langle e_j | P_i e_j \rangle = \begin{cases} 1, & j = i, \\ 0, & j \neq i, \end{cases}$$

consistent with the requirement that $|e_j\rangle$ has 0% chance of realizing the i-th outcome for i distinct from j. The sum

$$\sum_{i=1}^{n} P_i = \sum_{i=1}^{d} |e_i\rangle\langle e_i| = \mathbf{1}_{\mathcal{H}}$$

gives a distinguished "resolution of identity". After attaching the numerical outcome labels λ_i, we get the operator T in (6.3). The operators which have the form (6.3) for some orthonormal basis $\{e_i\}_{i=1,\ldots,n}$ are precisely the *normal operators*; If we restrict to real λ_i, we get the self-adjoint operators.

Some other "observable" may also be set up, modelled by $T' = \sum_{i=1}^{d} \mu_i |e'_i\rangle\langle e'_i|$. There is no assumption that T' and T commute. Some thought reveals that the commutativity question pertains to the eigenprojections $|e_i\rangle\langle e_i|$ and $|e'_j\rangle\langle e'_j|$, rather than the labels λ_i, μ_j.

From the above discussion, "observables" should be modelled by operators that admit an orthogonal eigen-decomposition (6.3), with the eigenvalues λ_i being the real numerical outcome labels. This expectation carries over to the setting of infinite-dimensional Hilbert space, which is needed for more complicated systems (e.g. scattering into the environment). Theorem 6.9 verifies

that self-adjoint operators satisfy this reals spectrum condition. (Later on, we address the question of orthogonal eigen-decomposition for self-adjoint operators.)

7 Unbounded operators on Hilbert space

7.1 Basic definitions for unbounded operators

With differential operators in mind, we make the following generalization:

Definition 12. An *operator* on a Banach space V is a linear map $T : \mathrm{Dom}(T) \to V$, whose *domain* $\mathrm{Dom}(T)$ is some subspace of V. Its *graph* is the subset

$$\Gamma_T = \{(\psi, T\psi) \,:\, \psi \in \mathrm{Dom}(T)\} \subset V \oplus V.$$

T is said to be

- *Closed*, if $\Gamma_T = \overline{\Gamma_T}$ is a closed set;
- *Closable*, if $\overline{\Gamma_T}$ remains the graph of some operator. In this case, that operator is called the *closure* $\overline{T}$ of T; thus $\overline{\Gamma_T} = \Gamma_{\overline{T}}$.

Definition 13. Let T, T' be operators on a Banach space. By default,

$$\begin{aligned}\mathrm{Dom}(TT') &= \{v \in \mathrm{Dom}(T') \,:\, T'v \in \mathrm{Dom}(T)\} \\ \mathrm{Dom}(T + T') &= \mathrm{Dom}(T) \cap \mathrm{Dom}(T').\end{aligned}$$

If

$$\mathrm{Dom}(T) \subset \mathrm{Dom}(T'), \qquad T'|_{\mathrm{Dom}(T)} = T,$$

we write $T \subset T'$.

Exercise 7.1. Let $S \in \mathcal{B}(V)$ be bounded, and $T : \mathrm{Dom}(T) \to V$ be a closed operator.

- Show that TS and $T + S$ are closed operators.
- Suppose $\mathrm{Ran}(S) \subset \mathrm{Dom}(T)$. Deduce that $TS \in \mathcal{B}(V)$.

Definition 14. Let T be a closed operator on a Banach space V. Its *resolvent set* is

$$\rho(T) = \{\lambda \in \mathbb{C} \,:\, (\lambda - T)^{-1} : V \to \mathrm{Dom}(T) \text{ exists}\},$$

and the operator

$$R_\lambda(T) := (\lambda - T)^{-1}, \qquad \lambda \in \rho(T),$$

is called the *resolvent of* T *at* λ. The *spectrum* of T is

$$\sigma(T) = \mathbb{C} \setminus \rho(T).$$

The *point spectrum* $\sigma_{\mathrm{p}}(T)$ is the set of eigenvalues, while the *approximate point spectrum* $\sigma_{\mathrm{ap}}(T)$ is the set of approximate eigenvalues,

$$\sigma_{\mathrm{ap}}(T) = \{\lambda \in \mathbb{C} \,:\, \exists \psi_n \in \mathrm{Dom}(T), ||\psi_n|| = 1, \text{ such that } (\lambda - T)\psi_n \to 0\}.$$

Remark. Since T is closed, its resolvents $R_\lambda(T)$ have closed graphs, and are defined on all of V. So they are actually bounded operators on V, due to the *closed graph theorem*[13].

Remark. Following the proof of Theorem 6.4, one deduces that $\rho(T)$ is open, and thus $\sigma(T)$ is a closed subset of $\mathbb{C}$.

Remark. In the concrete setting of differential operators, T has an initial domain of smooth functions, and is only a closable operator. The closure $\overline{T}$ is not always easy to describe explicitly.

Example 7.1. Let us try to define a "momentum operator"

$$T = -i\frac{d}{dx} : \mathrm{Dom}(T) \subset L^2[0,1] \to L^2[0,1].$$

The following are two possible domains, comprising absolutely continuous functions (see Section 7.1.1 for some properties of such functions),

$$\mathrm{Dom}(T_1) = \{\psi \in \mathrm{AC}[0,1] \,:\, \psi' \in L^2[0,1]\},$$
$$\mathrm{Dom}(T_2) = \{\psi \in \mathrm{Dom}(T_1) \,:\, \psi(0) = 0\},$$

with the understanding that ψ' means the almost-everywhere derivative. It may be shown that T_1, T_2 are closed operators. Their spectra are

$$\sigma(T_1) = \mathbb{C}, \qquad \sigma(T_2) = \emptyset.$$

The first claim follows from the simple observation that for each $\lambda \in \mathbb{C}$, the function $x \mapsto e^{i\lambda x}$ lies in $\mathrm{Dom}(T_1)$, and is clearly an eigenfunction of T_1. For the second claim, we leave it as an exercise to check that the resolvent $R_\lambda(T_2)$ at $\lambda \in \mathbb{C}$ is given by the operator

$$(R_\lambda(T_2)\varphi)(x) = -i\int_0^x e^{i\lambda(x-s)}\varphi(s)\,ds, \qquad \varphi \in L^2[0,1].$$

[13]If a Banach space operator $V \to V$ has closed graph, then it is continuous. The closed graph theorem is equivalent to the bounded inverse theorem.

Example 7.1 shows that $\mathrm{Dom}(T_1)$ is too large for T_1 to be a reasonable momentum observable — there are eigenfunctions with imaginary eigenvalues. So we must impose some boundary conditions to cut down the domain. The "Dirichlet" condition at $x = 0$ is unsuitable, as can be seen by the trivial spectrum of T_2. A "balanced" boundary condition is required to achieve a real spectrum, and we shall see that there is no unique choice — different choices describe different physical situations.

7.1.1 Note on absolutely continuous functions

Details can be found, e.g., in Section 7.5 of Ziemer's Modern Real Analysis book.

A function $\psi : [a, b] \to \mathbb{C}$ is *absolutely continuous* if, given any $\epsilon > 0$, there exists $\delta > 0$ such that for any finite collection of disjoint intervals $[x_i, x_i'] \subset [a, b]$ with total length less than δ, one has $\sum_i |\psi(x_i') - \psi(x_i)| < \epsilon$. Absolutely continuous functions are, in particular, uniformly continuous. We write $\mathrm{AC}[a, b]$ for the set of absolutely continuous functions on $[a, b]$.

The Fundamental Theorem of (Lebesgue integral) Calculus is:

Theorem 7.1. *Let $\psi \in \mathrm{AC}[a, b]$. Then ψ is almost everywhere differentiable, and its almost-everywhere defined derivative ψ' satisfies*

$$\psi' \in L^1[a, b], \qquad \psi(x) - \psi(a) = \int_a^x \psi'(\tilde{x})\, d\tilde{x}.$$

Conversely, let $f \in L^1[a, b]$. Then $F(x) := \int_a^x f(\tilde{x})\, d\tilde{x}$ is absolutely continuous, with $F' = f$ almost everywhere.

Suppose $\psi, \varphi \in \mathrm{AC}[a, b]$, then $\psi\varphi \in \mathrm{AC}[a, b]$ as well, and $(\psi\varphi)' = \psi'\varphi + \psi\varphi'$ almost everywhere, and is L^1. Integrating over $[a, b]$ gives the integration-by-parts rule,

$$\int_a^b \psi\varphi' = \psi(b)\varphi(b) - \psi(a)\varphi(a) - \int_a^b \psi'\varphi.$$

7.2 Adjoints of unbounded operators on Hilbert space

The adjoint operation generalizes to densely-defined operators on Hilbert spaces.

Definition 15. Let $T : \mathrm{Dom}(T) \to \mathcal{H}$ be a densely-defined operator. Define $\mathrm{Dom}(T^*)$ to be the set of $\varphi \in \mathcal{H}$ such that there exists (a unique[14]) $\eta_\varphi \in \mathcal{H}$ obeying the condition

$$\langle \eta_\varphi | \psi \rangle = \langle \varphi | T\psi \rangle, \qquad \forall \psi \in \mathrm{Dom}(T).$$

The *adjoint* operator $T^* : \mathrm{Dom}(T^*) \to \mathcal{H}$ is then defined as

$$T^*\varphi := \eta_\varphi, \qquad \varphi \in \mathrm{Dom}(T^*).$$

By design, the adjoint's domain is the maximal one for which the formal adjointness condition is true,

$$\langle T^*\varphi | \psi \rangle = \langle \varphi | T\psi \rangle, \qquad \forall \psi \in \mathrm{Dom}(T),\ \varphi \in \mathrm{Dom}(T^*). \tag{7.1}$$

Notice that the larger $\mathrm{Dom}(T)$ is, the smaller $\mathrm{Dom}(T^*)$ will become,

$$T \subset T' \ \Rightarrow\ T'^* \subset T^*. \tag{7.2}$$

The basic relation (5.5) continues to hold in the unbounded setting:

Lemma 7.2. *Let T be a densely-defined operator on a Hilbert space $\mathcal{H}$. Then* $\mathrm{Ran}(T)^\perp = \ker(T^*)$

Proof. For any $\varphi \in \ker(T^*)$,

$$\langle \varphi | T\psi \rangle = \langle T^*\varphi | \psi \rangle = 0, \qquad \forall\, \psi \in \mathrm{Dom}(T). \tag{7.3}$$

Thus $\ker(T^*) \subset \mathrm{Ran}(T)^\perp$. Conversely, suppose $\varphi \in \mathrm{Ran}(T)^\perp$, i.e.,

$$\langle \varphi | T\psi \rangle = 0 = \langle 0 | \psi \rangle, \qquad \forall\, \psi \in \mathrm{Dom}(T).$$

By definition, $\varphi \in \mathrm{Dom}(T^*)$ with $T^*\varphi = 0$. Thus $\mathrm{Ran}(T)^\perp \subset \ker(T^*)$. □

Passing from T to T^* is somewhat like taking orthogonal complements at the level of their graphs (together with a swap). More precisely:

$$\begin{aligned} (\varphi, \eta) \in \Gamma_{T^*} &\Leftrightarrow \langle \eta | \psi \rangle - \langle \varphi | T\psi \rangle \qquad\qquad \forall \psi \in \mathrm{Dom}(T) \\ &\Leftrightarrow \big\langle (\eta, \varphi) \big| (\psi, -T\psi) \big\rangle_{\mathcal{H}\oplus\mathcal{H}} = 0 \quad \forall \psi \in \mathrm{Dom}(T) \\ &\Leftrightarrow (\eta, \varphi) \in \Gamma_{-T}^\perp \end{aligned} \tag{7.4}$$

Note that the above calculation shows that Γ_{T^*} is an orthogonal complement (taken in the Hilbert space $\mathcal{H} \oplus \mathcal{H}$. Therefore,

[14]The dense domain is used here to ensure uniqueness of such an η_φ.

Lemma 7.3. *The adjoint of a densely-defined operator is a closed operator.*

We can take the double adjoint, T^{**}, provided T^* is densely defined.

Proposition 7.4. *Let $T : \mathrm{Dom}(T) \to \mathcal{H}$ be a densely-defined operator. Then T is closable iff $\mathrm{Dom}(T^*)$ is dense. In this case, $\overline{T} = T^{**}$.*

Proof. From (7.4), $\Gamma_T^\perp$ coincides with Γ_{T^*} up to a swap.
($\Leftarrow$) If $\mathrm{Dom}(T^*)$ is dense, T^{**} makes sense, and we can write

$$\overline{\Gamma_T} = \Gamma_T^{\perp\perp} = ((\mathrm{swap}(\Gamma_{T^*}))^\perp = \Gamma_{T^{**}}.$$

This means that $\overline{T}$ exists and coincides with T^{**}.
($\Rightarrow$) Suppose $\mathrm{Dom}(T^*)$ is not dense, then we can pick a nonzero $\psi \in \mathrm{Dom}(T^*)^\perp$. For this ψ,

$$\begin{aligned}
\langle\psi|\varphi\rangle = 0 \quad \forall\varphi \in \mathrm{Dom}(T^*) &\Rightarrow \big\langle (\psi,0) \big| (\varphi, T^*\varphi) \big\rangle = 0 \quad \forall\varphi \in \mathrm{Dom}(T^*) \\
&\Leftrightarrow (\psi,0) \in \Gamma_{T^*}^\perp \\
&\Leftrightarrow (0,\psi) \in \underbrace{(\Gamma_{-T}^\perp)^\perp}_{=\overline{\Gamma_T}} \qquad \text{(Eq. (7.4)).}
\end{aligned}$$

But $(0,\psi)$ does not lie in the graph of any linear operator, so the above calculation says that $\overline{\Gamma_T}$ does not arise as the graph of any operator. Thus T is not closable. □

Another tricky issue is the adjoint of a product.

Exercise 7.2. Let S, T, as well as ST be densely-defined operators on a Hilbert space. Show that

$$T^*S^* \subset (ST)^*.$$

7.3 Formal self-adjointness

Definition 16. A densely-defined operator H is *symmetric*, or *formally self-adjoint*, if $H \subset H^*$; explicitly,

$$\langle H\varphi|\psi\rangle = \langle\varphi|H\psi\rangle, \qquad \forall\varphi,\psi \in \mathrm{Dom}(H). \tag{7.5}$$

Exercise 7.3. Show that the eigenvalues of a symmetric operator are real, and that the eigenspaces for distinct eigenvalues are orthogonal to each other.

7.3.1 Formal harmonic oscillator

Let us revisit the harmonic oscillator with more precise language at our disposal.

First of all, a standard result in function theory, stated without proof, is that $\mathscr{S}(\mathbb{R})$ is dense in $L^p(\mathbb{R})$, $1 \leq p < \infty$. This is also true over $\mathbb{R}^d$, where the *Schwartz space* $\mathscr{S}(\mathbb{R}^d)$ is defined as the space of smooth functions $f : \mathbb{R}^d \to \mathbb{C}$ such that

$$\sup_{x \in \mathbb{R}^d} |x^\alpha D^\beta(x)| < \infty,$$

for all multi-indices $\alpha = (\alpha_1, \ldots, \alpha_d)$ and $\beta = (\beta_1, \ldots, \beta_d)$, where

$$x^\alpha := x_1^{\alpha_1} \ldots x_d^{\alpha_d}$$
$$D^\beta f := \partial_1^{\beta_1} \ldots \partial_d^{\beta_d}.$$

The *formal position operator* X and *formal momentum operator* P are defined on the domain $\mathscr{S}(\mathbb{R})$, by the formulae

$$(X\psi)(x) = x\psi(x), \qquad x \in \mathbb{R},$$
$$P\psi = -i\frac{d}{dx}\psi.$$

The *formal creation/annihilation operators* are, respectively, the operators

$$A^\dagger := X - iP, \qquad A = X + iP.$$

It is a simple matter to check that X and P are symmetric operators, which map $\mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$. So $A, A^\dagger, A^\dagger A, AA^\dagger$ are all densely-defined operators with domain $\mathscr{S}(\mathbb{R})$. In particular, the harmonic oscillator Hamiltonian $H = \frac{1}{2}(A^\dagger A + 1)$ is symmetric on $\mathscr{S}(\mathbb{R})$. So its eigensystem (which we had deduced quite abstractly) enjoys the nice properties guaranteed by Exercise 7.3.

However, being symmetric does not guarantee completeness, in the sense of the eigenvectors providing an orthonormal *basis*.

Exercise 7.4. Let H be a symmetric operator. Suppose H^* has eigenvalue i. Show that the i-eigenspace of H^* is orthogonal to all the eigenspaces of H.

The completeness of harmonic oscillator eigenspaces cannot be deduced simply by formal algebraic arguments. Completeness turns out to be true in

this case, and one textbook way to show this is to examine the explicit eigenfunctions in detail. From Exercise 3.2, we know that these eigenfunctions are of the form $p_n(x) \times e^{-x^2/2}$ for some polynomials, called *Hermite polynomials* (after a suitable normalization convention). With some Fourier analysis, one verifies that the span of $p_n(x) \times e^{-x^2/s}$ is indeed dense in $L^2(\mathbb{R})$.

For general symmetric operators, there would be no hope of finding all the eigenfunctions explicitly. Indeed, we might not even be dealing with Hilbert spaces arising as concrete function spaces!