

Last time we discussed criteria for self-adjointness and essential self-adjointness of a densely defined symmetric linear operator $(H, \mathcal{D}(H))$.

We found that

(i) H is self-adjoint. \Leftrightarrow (ii) H is closed and $\ker(H^* \pm i) = \{0\}$.

\Leftrightarrow (iii) $\text{im}(H \pm i) = \mathcal{H}$.

(i) H is essentially self-adjoint. \Leftrightarrow (ii) $\ker(H^* \pm i) = \{0\}$.

\Leftrightarrow (iii) $\overline{\text{im}(H \pm i)} = \mathcal{H}$.

Today, we will deal with the possibility of multiple self-adjoint extensions (as we had for $\mathcal{D}_{\min} = -i \frac{d}{dx}$). For that, we need to look a bit closer at $\ker(H^* \pm i)$ and $\text{im}(H \pm i)$.

Note that $\ker(H^* \mp i) = \text{im}(H \pm i)^\perp$ by definition of H^* . The dimensions of these spaces have names:

$$\eta \in \ker(H^* \mp i) \Leftrightarrow (H^* \mp i)\eta = 0 \Leftrightarrow \langle (H^* \mp i)\eta, \psi \rangle = 0 \quad \forall \psi \in \mathcal{D}(H) \Leftrightarrow \langle \eta, (H \pm i)\psi \rangle = 0 \quad \forall \psi \in \mathcal{D}(H)$$

Definition 3.82: Let $(H, \mathcal{D}(H))$ be a densely defined symmetric linear operator. Then

- $\mathcal{L}^\pm := \ker(H^* \mp i) = \text{im}(H \pm i)^\perp$ are called **deficiency spaces** of H ,
- $\mathcal{N}^\pm := \dim \mathcal{L}^\pm$ are called **deficiency indices** of H .

So essential self-adjointness $\Leftrightarrow \mathcal{N}^+ = \mathcal{N}^- = 0$ ($\mathcal{H} = \overline{\text{im}(H \pm i)} \oplus \mathcal{L}^\pm$).

What we want to show next is that existence of self-adjoint extensions $\Leftrightarrow \mathcal{N}^+ = \mathcal{N}^-$
(but not necessarily = 0)

These can be nicely studied with the following map:

Definition 3.84: Let $(H, \mathcal{D}(H))$ be a densely defined symmetric linear operator. Then we define its **Cayley transform** $U: \text{im}(H+i) \rightarrow \text{im}(H-i)$ as $U := (H-i)(H+i)^{-1}$.

Note: • U is clearly surjective

• U is also isometric, since

$$\|U\psi\| = \|U(H+i)\varphi\| = \|(H-i)\varphi\| = \sqrt{\|H\varphi\|^2 + \|\varphi\|^2} = \|(H+i)\varphi\| = \|\psi\|$$

by def. $\psi = (H+i)\varphi$
for some φ

Now, let us skip the details, and just give a summary of main result concerning the Cayley transform. This is:

Lemma 3.86: There is a one-to-one correspondence between the symmetric extensions of H and isometric extensions of its Cayley transform U .

Then, the following also holds:

Lemma 3.90: H self-adjoint \Leftrightarrow Cayley transform U is unitary on \mathcal{H} .

These two lemmas imply:

Theorem 3.89: H has self-adjoint extensions $\Leftrightarrow \mathcal{N}^+ = \mathcal{N}^-$.

In this case the extensions are parametrized by $u \in \mathcal{U}(\mathcal{N}^+)$ (the unitary group, i.e., unitary $n \times n$ matrices).

We skipped the proofs, but let us look at examples:

- $D_{\min} = -i \frac{d}{dx}$ on $\mathcal{H} = L^2([0,1])$ with $\mathcal{D}(D_{\min}) = C_0^\infty((0,1))$. We already found before that $\varphi_\pm = e^{\mp x} \in \mathcal{D}(D_{\min}^*) = H^1([0,1])$, so $L^\pm = \text{span}\{\varphi_\pm\}$, i.e., $N^+ = N^- = 1$. So D_{\min} has self-adjoint extensions parametrized by $U(1)$, i.e., multiplication with $e^{i\alpha}$.

- Translations on the half-line. Let $D_{[0,\infty)} = -i \frac{d}{dx}$ on $\mathcal{H} = L^2([0,\infty))$ with domain $\mathcal{D}(D_{[0,\infty)}) = C_0^\infty((0,\infty))$. Integration by parts shows that $D_{[0,\infty)}$ is indeed symmetric, and $\mathcal{D}(D_{[0,\infty)}^*) = H^1([0,\infty))$. Now consider $L^\pm = \ker(D_{[0,\infty)}^* \mp i)$, i.e., we need to find solutions to $D_{[0,\infty)}^* \varphi_\pm = \pm i \varphi_\pm$.

The only solutions are $\varphi_\pm = e^{\mp x}$. Now $\varphi_+ \in \mathcal{D}(D_{[0,\infty)}^*)$ since it goes to 0 at ∞ . Thus $L^+ = \text{span}\{e^{-x}\}$ and $N^+ = 1$. But φ_- is not even in $L^2([0,\infty))$, so $L^- = \{0\}$ and $N^- = 0$.

Therefore, $D_{[0,\infty)}$ has no self-adjoint extensions. This makes sense because it is clearly impossible to define a unitary group of translations on $L^2([0,\infty))$.

But note that $-\Delta$ on $L^2([0,\infty))$ can be defined as a self-adjoint operator, so the Schrödinger equation on the half-line makes sense, as we will see shortly.

Finally, let us mention a very useful criterion to check whether $N^+ = N^-$. For this, recall the following:

Definition 3.93: An anti-linear map $C: \mathcal{H} \rightarrow \mathcal{H}$ (meaning that $C(\alpha\psi + \varphi) = \bar{\alpha}C(\psi) + C(\varphi)$) is called a conjugation if $\|C\psi\| = \|\psi\| \forall \psi \in \mathcal{H}$ and $C^2 = \text{id}_{\mathcal{H}}$.

Examples: • Of course, complex conjugation $\psi(x) \mapsto \overline{\psi(x)}$ is a conjugation.

- For Dirac spinors $\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)$ that come up in relativistic quantum physics, $\psi(x) \mapsto J \overline{\psi(x)}$ for any 4×4 matrix J with $J \bar{J} = \text{id}$, is a conjugation.

Then it follows relatively straightforwardly that the following holds:

Theorem 3.95: von Neumann-theorem

Let $(H, \mathcal{D}(H))$ be a densely defined symmetric linear operator. If there is a conjugation C with $C\mathcal{D}(H) \subset \mathcal{D}(H)$ and $CHe = HCe \ \forall e \in \mathcal{D}(H)$, then $N^+ = N^-$ (i.e., H has self-adjoint extensions).

- Examples:
- $D_{[0, \infty)} = -i \frac{d}{dx}$ on $C_0^\infty([0, \infty))$ does not commute with complex conjugation, and in fact not with any conjugation.
 - But $-\Delta$ on $C_0^\infty([0, \infty))$ does commute with complex conjugation, so indeed it has self-adjoint extensions.

The last technical tool that we need is the resolvent. This is a very important operator especially in spectral theory, but it will also be useful for us here.

Recall that for $n \times n$ matrices A we defined eigenvalues λ and eigenvectors $\vec{x} \neq 0$ as solutions to $A\vec{x} = \lambda\vec{x}$, i.e., $(A - \lambda \text{id})\vec{x} = 0$. These exist if $(A - \lambda)$ is not invertible.

This we can generalize to unbounded operators.

Definition 3.97: Let $(T, \mathcal{D}(T))$ be a linear operator on \mathcal{H} . Then we define the resolvent set $\rho(T) := \{z \in \mathbb{C} : (T-z) : \mathcal{D}(T) \rightarrow \mathcal{H} \text{ is bijective with continuous inverse}\}$.

For $z \in \rho(T)$ we call $R_z(T) := (T-z)^{-1} \in \mathcal{L}(\mathcal{H})$ the resolvent of T at z .

The spectrum of T is $\sigma(T) = \mathbb{C} \setminus \rho(T)$ (the complement of the resolvent set).

We differentiate further:

a) $\sigma_p(T) := \{z \in \mathbb{C} : T-z \text{ is not injective}\}$ is called the **point spectrum**, and any $z \in \sigma_p(T)$ is called eigenvalue of T .

b) $\sigma_c(T) := \{z \in \mathbb{C} : T-z \text{ is injective, but not surjective, but has dense image}\}$ is called the **continuous spectrum**.

c) $\sigma_r(T) := \{z \in \mathbb{C} : T-z \text{ is injective, but not surjective, and the image is not dense}\}$ is called **residual spectrum**.

Before we discuss examples, let us note the following:

Theorem 3.98:

- T closed $\Rightarrow \rho(T) = \{z \in \mathbb{C} : (T-z) : \mathcal{D}(T) \rightarrow \mathcal{H} \text{ is bijective}\}$ and for $z \in \rho(T)$ we have that $(T-z)^{-1} : \mathcal{H} \rightarrow (\mathcal{D}(T), \|\cdot\|_{\mathcal{D}(T)})$ is bounded.
- T not closed $\Rightarrow \rho(T) = \emptyset$.

Proof: If T is closed, $(\mathcal{D}(T), \|\cdot\|_{\mathcal{D}(T)})$ is complete, i.e., a Hilbert space. And by definition, $T: (\mathcal{D}(T), \|\cdot\|_{\mathcal{D}(T)}) \rightarrow \mathcal{H}$ is bounded, in fact by 1 in norm:

$$\|T\psi\|_{\mathcal{H}}^2 \leq \|T\psi\|_{\mathcal{H}}^2 + \|\psi\|_{\mathcal{H}}^2 = \|\psi\|_{\mathcal{D}(T)}^2.$$

Now one can use the **open mapping theorem**: Let $A: X \rightarrow Y$ be a continuous linear operator, where X, Y are Banach spaces. If A is surjective, then A is an open map (i.e., it maps open sets into open sets).

So here, if $T-z: (\mathcal{D}(T), \|\cdot\|_{\mathcal{D}(T)}) \rightarrow \mathcal{H}$ is surjective, it is also open. So if $T-z$ is bijective, then $(T-z)^{-1}: \mathcal{H} \rightarrow (\mathcal{D}(T), \|\cdot\|_{\mathcal{D}(T)})$ is continuous (preimages of open sets are open).

For the second statement one can show $\rho(T) \neq \emptyset \Rightarrow T$ closed. If $\rho(T) \neq \emptyset$, then there is a $z \in \mathbb{C}$ s.t. the resolvent $R_z(T): \mathcal{H} \rightarrow \mathcal{D}(T)$ exists. Using the definition of closedness one can then infer that T is indeed closed; let us skip the details. \square

So for closed T we do not need the requirement of continuous inverse in the definition of $\rho(T)$, and thus $\sigma(T) = \underbrace{\sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T)}_{\text{they are disjoint}}$.

And for $\dim \mathcal{H} < \infty$, $T-z$ injective $\Leftrightarrow T-z$ surjective, so $\sigma(T) = \sigma_p(T)$, the eigenvalues.