Session 19
April 15, 2020

Last time we covered bounded operators. For these the domain is all of $\mathcal{H}$, and $\underbrace{\text{symmetry}}_{\langle\psi, A\varphi\rangle = \langle A\psi, \varphi\rangle\ \forall \psi,\varphi\in\mathcal{H}}$ is the same as $\underbrace{\text{self-adjointness}}_{A^* = A}$.

Bounded self-adjoint operators H always generate the strongly continuous unitary one-parameter group $U(t) = e^{-iHt}$ (which is even uniformly continuous, a trait that is surely not true for unbounded operators as we have seen for $-\Delta$ and the free propagator).

Next: We would also hope that unbounded operators such as $H = -\Delta + V$ for some multiplication operator V, are generators. For a densly defined operator it is indeed true that H being a generator is equivalent to H being self-adjoint ("$\Leftarrow$" follows from the spectral theorem, "$\Rightarrow$" (i.e., every unitary group has a generator) is Stone's theorem, which we might prove later depending on time). But for unbounded H we still need to define what self-adjointness means: it is definitely not just $\langle\psi, H\varphi\rangle = \langle H\psi, \varphi\rangle$ $\forall \varphi, \psi \in \mathcal{D}(H)$, because we saw that this is a necessary but not sufficient condition when we discussed the example of the translation operator.

So next, we define self-adjointness for unbounded operators, and develop criteria to determine whether a given operator is self-adjoint (the most important one is called Kato-Rellich). This will be more technical, and will occupy us for several class sessions.

Let us first characterize unbounded operators ($\sup_{\substack{\psi\in\mathcal{H}\\ \|\psi\|=1}} \|H\psi\|_{\mathcal{H}} < C$ does <u>not</u> hold) a bit better:

Definition 3.49:

a) An unbounded operator is a pair $(T, \mathcal{D}(T))$ of a subspace $\mathcal{D}(T) \subset \mathcal{H}$ (the domain of T) and a linear operator $T: \mathcal{D}(T) \to \mathcal{H}$. If $\mathcal{D}(T)$ is dense in $\mathcal{H}$ (i.e., $\underbrace{\overline{\mathcal{D}(T)}}_{\text{the closure of } \mathcal{D}(T)} = \mathcal{H}$), then T is called densly defined.

the closure of $\mathcal{D}(T)$, i.e., $\mathcal{D}(T)$ and all limit points

b) $(S, \mathcal{D}(S))$ is called an extension of $(T, \mathcal{D}(T))$ if $\mathcal{D}(S) \supset \mathcal{D}(T)$ and $S|_{\mathcal{D}(T)} = T$. This is denoted $S \supset T$.

c) $(T, \mathcal{D}(T))$ is called symmetric if $\langle \varphi, T\psi \rangle = \langle T\varphi, \psi \rangle \; \forall \varphi, \psi \in \mathcal{D}(T)$.

We already discussed that $H_0 = -\frac{1}{2}\Delta$ with domain $\mathcal{D}(H_0) = H^2(\mathbb{R}^d)$ is a symmetric, unbounded densly defined operator. $H_1 = -\frac{1}{2}\Delta$ with domain $\mathcal{D}(H_1) = H^4(\mathbb{R}^d)$ is also a symmetric, unbounded densly defined operator, and $H_0 \supset H_1$.

Now, recall the example of $-i\frac{d}{dx}$ on $[0,1]$. We need to choose $-i\frac{d}{dx}$ symmetric, but the domain must not be too small: e.g., the Schrödinger evolution leads initial conditions in D_{min} out of D_{min} (D_{min} was not invariant under any T_θ). So where exactly do they go?

Consider more generally some symmetric $(H_0, \mathcal{D}(H_0))$ and a symmetric extension $(H_1, \mathcal{D}(H_1))$. Suppose the solution to $i\frac{d}{dt}\psi(t) = H_1\psi(t)$ for initial data $\psi(0) \in H_0$ stays in $\mathcal{D}(H_1)$, at least for some small time, but not necessarily in $\mathcal{D}(H_0)$. For $\varphi \in \mathcal{D}(H_0)$ we have

$\langle H_1\psi(t), \varphi \rangle = \langle \psi(t), H_1\varphi \rangle = \langle \psi(t), H_0\varphi \rangle$. So this expression still makes sense even if $\psi(t) \notin \mathcal{D}(H_0)$. Naturally we would use this expression to define the adjoint.

So our idea is that "e^{-iHt}" makes $\Psi(0) \in \mathcal{D}(H_0)$ evolve into the domain of the (to be properly defined) adjoint. If the domain of the adjoint is the same as the domain of the operator the Schrödinger evolution leaves the domain invariant and all is good.

Let us define these things more precisely:

Definition 3.53:

Let $(T, \mathcal{D}(T))$ be a densly defined linear operator on $\overbrace{\mathcal{H}}^{\text{always some Hilbert space}}$. Then we define

$$\mathcal{D}(T^*) := \{\psi \in \mathcal{H} : \exists \eta \in \mathcal{H} \text{ s.t. } \langle \psi, T\varphi \rangle = \langle \eta, \varphi \rangle \ \forall \varphi \in \mathcal{D}(T)\}.$$

Since $\mathcal{D}(T)$ is dense, η is determined uniquely and we define the **adjoint operator** as

$$T^* : \mathcal{D}(T^*) \to \mathcal{H}, \ \psi \mapsto T^*\psi = \eta \quad (\eta \text{ as in the def. of } \mathcal{D}(T^*)).$$

Note: • For bounded operator, this definition coincides with the adjoint as previously defined.

- Due to Riesz, the def. of $\mathcal{D}(T^*)$ is equivalent to

$$\mathcal{D}(T^*) = \{\psi \in \mathcal{H} : \varphi \mapsto \langle \psi, T\varphi \rangle \text{ is continuous on } \mathcal{D}(T)\}.$$

- By this def., $(T^*, \mathcal{D}(T^*))$ is linear (but not necessarily densly defined) and of course $\langle \psi, T\varphi \rangle = \langle T^*\psi, \varphi \rangle \ \forall \psi \in \mathcal{D}(T^*), \varphi \in \mathcal{D}(T)$.

Definition 3.56:

Let $(T, \mathcal{D}(T))$ be a densly defined linear operator on $\mathcal{H}$. $(T, \mathcal{D}(T))$ is called **self-adjoint** if $\mathcal{D}(T^*) = \mathcal{D}(T)$ and $T^* = T$ on $\mathcal{D}(T)$.

Let us exemplify the definitions with $-i\frac{d}{dx}$ on $[0,1]$ again.

↳ First, consider $(D_{min}, \mathcal{D}(D_{min}))$ (recall $\mathcal{D}(D_{min}) = \{\varphi \in H^1[0,1] : \varphi(0) = 0 = \varphi(1)\}$).

Then $\forall \varphi \in \mathcal{D}(D_{min})$:

$$\langle \psi, D_{min}\varphi\rangle = \int_0^1 \overline{\psi(x)} \left(-i\frac{d}{dx}\varphi(x)\right) dx = \int_0^1 \overline{\left(-i\frac{d}{dx}\psi(x)\right)} \varphi(x) dx = \langle \underbrace{-i\frac{d}{dx}\psi}_{=\eta}, \varphi\rangle,$$

which works for all $\frac{d\psi(x)}{dx} \in L^2$, i.e., $\psi \in H^1([0,1])$.

So $\mathcal{D}(D^*_{min}) = H^1([0,1]) \neq \mathcal{D}(D_{min})$, and $(D_{min}, \mathcal{D}(D_{min}))$ is not self-adjoint).

↳ For $D_\theta = -i\frac{d}{dx}$ with $\mathcal{D}(D_\theta) = \{\varphi \in H^1([0,1]) : e^{i\theta}\varphi(1) = \varphi(0)\}$ we find $\forall \varphi \in \mathcal{D}(D_\theta)$:

$$\langle \psi, D_\theta \varphi\rangle = i\left(\overline{\psi(0)}\varphi(0) - \overline{\psi(1)}\varphi(1)\right) + \langle \underbrace{-i\frac{d}{dx}\psi}_{\eta}, \varphi\rangle,$$ so in order to get

$\langle \psi, D_\theta\varphi\rangle = \langle \eta, \varphi\rangle$ we need $\psi \in H^1([0,1])$ <u>and</u> $\overline{\psi(0)}\varphi(0) = \overline{\psi(1)}\varphi(1) \iff$

$\frac{\overline{\psi(0)}}{\overline{\psi(1)}} = \frac{\varphi(1)}{\varphi(0)} = e^{-i\theta}$ (by def.).

So $\mathcal{D}(D^*_\theta) = \mathcal{D}(D_\theta)$ and $D^*_\theta = D_\theta$, so D_θ is self-adjoint.

Next time, we will develop nicer criteria for self-adjointness, or at least the existence of unique self-adjoint extensions.