Last time: • For <u>bounded operators</u> $H: \mathcal{H} \to \mathcal{H}$, we have:

$$H \text{ symmetric} \iff H \text{ self-adjoint} \iff H \text{ generator of } U(t) = e^{-iHt}$$

We already saw earlier that there are unbounded operators $A: D(A) \to \mathcal{H}$ with dense domain $D(A)$ that satisfy $\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle \ \forall \varphi, \psi \in D(A)$ (i.e., that are symmetric), but that cannot be generators. (The example was $-i\frac{d}{dx}: D_{min} \to L^2([0,1])$.)

Note: The term "unbounded operator" is usually used for a not necessarily bounded operator defined on some domain. More precisely:

<u>Definition 3.49:</u>

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

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

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

E.g., $(H_1, \mathcal{D}(H_1)) = (-\frac{\Delta}{2}, H^2(\mathbb{R}^d))$ is a symmetric densly defined unbounded operator.

$(H_0, \mathcal{D}(H_0)) = (-\frac{\Delta}{2}, C_c^\infty(\mathbb{R}^d))$ also, and $H_1 \supset H_0$ (H_1 extends H_0).

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 $\psi(0) \in \mathcal{D}(H_0)$ 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.

Therefore we define:

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 $(D_{min}, D(D_{min}))$, $D_{min} = -i\frac{d}{dx}$, with $D(D_{min}) = \{\varphi \in H^1[0,1] : \varphi(0) = 0 = \varphi(1)\}$

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

integration by parts, boundary terms vanish on $D(D_{min})$

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

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

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

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

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

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

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

A big result is that indeed the following holds:

$\boxed{\text{\underline{Theorem 3.58:} A densly defined operator } (H, D(H)) \text{ is generator of a strongly continuous unitary group } U(t) \text{ if and only if it is self-adjoint.}}$

"$\Leftarrow$" follows from the spectral theorem; "$\Rightarrow$" is Stone's theorem

We skip the proofs here.

Finally, let us state Kato-Rellich. The idea is that we often consider operators $H = H_0 + V$, where we know that H_0 is self-adjoint with domain $D(H_0)$ and we want to know whether also H is self-adjoint. Often the V's are such that they do not disturb $D(H_0)$ too much, i.e., they do not introduce new boundary points.

<u>Definition:</u> Let A, B be densly defined linear operators with $D(A) \subset D(B)$ and such that there are $a, b \geq 0$ s.t.

$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \quad \forall \varphi \in D(A)$. Then B is called relatively bounded by A (or A-bounded), and the infimum over all permissible a is called the relative bound.

If the relative bound $= 0$, B is called infinitesimally A-bounded.

Finally:

<u>Theorem (Kato-Rellich):</u> Let A be self-adjoint, B symmetric and A-bounded with relative bound $a < 1$. Then $A+B$ is self-adjoint on $D(A+B) = D(A)$.

Another approach to proving existence of self-adjoint extensions is via the Friedrichs extension. The advantage of this approach is that it is very easy to apply in practice. The disadvantage is that it only gives existence of a self-adjoint extension, and it does not provide information on its domain, nor uniqueness.

It uses the following definition:

Definition 3.114: An operator H is called semibounded if there is a $c \in \mathbb{R}$ s.t. for all $\psi \in \mathcal{D}(H)$, $\langle \psi, H\psi \rangle \geq c\|\psi\|^2$ (from below) or $\langle \psi, H\psi \rangle \leq c\|\psi\|^2$ (from above).

Then we have:

Theorem 3.115 (Friedrichs extension):

Any densly defined semibounded operator H has a self-adjoint extension, which satisfies the same upper/lower bound.

We skip the proof.

E.g., for $-\Delta$ on $C_0^\infty(\Omega)$, $\Omega \subset \mathbb{R}^d$ open, we find $\langle \varphi, (-\Delta)\varphi \rangle = \|\nabla \varphi\|^2 \geq 0 \cdot \|\varphi\|^2$,

so $(-\Delta, C_0^\infty(\Omega))$ has a self-adjoint extension. Same for $-\Delta + V$ with $V \geq 0$.

One can actually define one particular self-adjoint extension uniquely via quadratic forms. This is then called <u>the</u> Friedrichs extension.

(E.g., for $H = -\frac{d^2}{dx^2}$ on $C_0^\infty((0,1))$, the Friedrichs extension is the Dirichlet Laplacian. But there are other extensions with other boundary conditions, e.g., Neumann.)