

(last time: For  $A \in \mathcal{S}(\mathcal{H})$ , the adjoint  $A^*$  is the unique operator determined by

$$\langle \psi, A\varphi \rangle = \langle A^*\psi, \varphi \rangle \quad \forall \psi, \varphi \in \mathcal{H}.$$

$A \in \mathcal{S}(\mathcal{H})$  selfadjoint  $\Leftrightarrow A^* = A \Leftrightarrow A$  symmetric

Unitary operators can be nicely characterized via the adjoint:

Proposition 3.45:  $U \in \mathcal{S}(\mathcal{H})$  is unitary if and only if  $U^* = U^{-1}$ .

surjective + isometric

Proof: " $\Rightarrow$ " We compute  $\langle U^*U\psi - \psi, \varphi \rangle = \langle U^*U\psi, \varphi \rangle - \langle \psi, \varphi \rangle$

$$\begin{aligned} &= \langle U\psi, U\varphi \rangle - \langle \psi, \varphi \rangle \\ &= \langle \psi, \varphi \rangle - \langle \psi, \varphi \rangle \\ &= 0 \quad \forall \psi, \varphi \in \mathcal{H}, \text{ so } U^*U = \text{id} \end{aligned}$$

since  $U$  surjective  $UU^*U = U$  implies  $UU^* = \text{id}$ , so  $U^{-1} = U^*$ .

" $\Leftarrow$ " If  $U^* = U^{-1}$  then  $U$  is surjective.

Isometry?  $\langle U\psi, U\varphi \rangle = \langle U^*U\psi, \varphi \rangle = \langle U^*U\psi, \varphi \rangle = \langle \psi, \varphi \rangle \quad \checkmark$

□

Now we can make the connection to generators:

Theorem 3.48: Let  $H \in \mathcal{S}(\mathcal{H})$  be self-adjoint. Then  $e^{-iHt} = \sum_{n=0}^{\infty} \frac{(-iHt)^n}{n!}$  defines

a unitary group with generator  $H$  with domain  $D(H) = \mathcal{H}$ . Moreover

$U: \mathbb{R} \rightarrow \mathcal{S}(\mathcal{H}), t \mapsto e^{-iHt}$  is (uniformly) differentiable.

Proof: HW Sketch:

- Well-definedness: Show that  $\sum_{n=0}^k \frac{(-iHt)^n}{n!}$  is a Cauchy sequence (in  $\mathcal{S}_0(\mathcal{H})$  norm).
- Group property: direct computation.
- Unitarity: Carefully compute  $\langle \varphi, e^{-iHt}\psi \rangle$  to find  $(e^{-iHt})^*$ ; show it equals  $(e^{-iHt})^{-1}$ .
- Uniform differentiability: Need to check only at  $t=0$  (why?). Estimate  $\lim_{t \rightarrow 0} \left\| \frac{U(t) - id_{\mathcal{H}}}{t} - (-iH) \right\|_{\mathcal{S}_0(\mathcal{H})}$ .
- Schrödinger eq. clear from uniform differentiability.

So for bounded linear  $H: \mathcal{H} \rightarrow \mathcal{H}$ , we can make sense of  $e^{-iHt}\psi(0)$  being the solution to  $i \frac{d}{dt} \psi(t) = H\psi(t)$ , and we have

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

For unbounded  $H$  (e.g.,  $H$  containing differential operators) we will have a similar connection, but the definition of self-adjointness is more subtle.

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

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

### 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  $T: \mathcal{D}(T) \rightarrow \mathcal{H}$ . If  $\mathcal{D}(T)$  is dense in  $\mathcal{H}$  (i.e.,  $\overline{\mathcal{D}(T)} = \mathcal{H}$ ), then  $T$  is called **densely 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  $S > T$ .
- c)  $(T, \mathcal{D}(T))$  is called **symmetric** if  $\langle \varphi, T\psi \rangle = \langle T\varphi, \psi \rangle \quad \forall \varphi, \psi \in \mathcal{D}(T)$ .

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

$(H_0, \mathcal{D}(H_0)) = \left(-\frac{\Delta}{2}, C_c^\infty(\mathbb{R}^d)\right)$  also, and  $H_1 > H_0$  ( $H_1$  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  $\mathcal{D}_{\min}$  out of  $\mathcal{D}_{\min}$  ( $\mathcal{D}_{\min}$  was not invariant under any  $T_0$ ). 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 densely defined linear operator on  $\mathbb{H}$ . Then we define

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

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

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

- Note:
- For bounded operators, this definition coincides with the adjoint as previously defined.
  - Due to Riesz, the def. of  $\mathcal{D}(T^*)$  is equivalent to

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

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

Definition 3.56:

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