PROP. 2.8: Let $H : D \subset \mathcal{H} \to \mathcal{H}$ symmetric and closed.
If for every $u \in D$ there is a global solution $\psi : \mathbb{R} \to \mathcal{H}$ of (SE), then $H = H^*$.

PROOF: It's sufficient to show $\mathrm{Ker}(H^* \pm i) = \{0\}$.

Let $(H^* + i)\omega = 0$. (*)

Let $u \in D$, let $\psi(t)$ solve (SE) with $\psi(0) = u$. Then:

$$\underline{\frac{d}{dt}\langle \omega, \psi(t)\rangle} = \langle \omega, -iH\psi(t)\rangle = \langle H^*\omega, -i\psi(t)\rangle$$

$$\overset{\text{by } (*)}{=} \langle \bar{i}\omega, -i\psi(t)\rangle = \underline{\langle \omega, \psi(t)\rangle}$$

This is a simple ODE for $\langle \omega, \psi(t)\rangle$ —— solution: exponential.

$$\Rightarrow \quad \langle \omega, \psi(t)\rangle = \langle \omega, u\rangle e^{t}.$$

by the previous lemma, since $H \subset H^*$

On the other hand: $|\langle \omega, \psi(t)\rangle| \le \|\omega\| \, \|\psi(t)\| = \|\omega\| \, \|u\|$.
How can this agree with the exponential solution?
The only way is:
$$\langle \omega, u\rangle = 0 \quad \forall u \in D$$
Since D is dense, this implies $\omega = 0$.
For $H^* - i$: same argument. ∎

REMARK: If H is bounded, the solution of (SE) is easy:
$$\psi(t) = e^{-iHt}u := \sum_{n=0}^{\infty} \frac{1}{n!}(-iHt)^n u. \qquad (**)$$
For unbounded op., in general not even H^2 is well-defined.
But later we are going to make sense of (**).

SELFADJOINT EXTENSIONS

RMK: A is selfadjoint $\Leftrightarrow$ A is maximal in the following sense: if $A = A^*$ and B is symmetric with $B \supset A$, then $B = A$.

PROOF: $A \subset B \subset B^* \subset A^* = A \Rightarrow A = B$. $\blacksquare$

RMK: If you start with a very small domain, it is easy to make sense of your operator, but it will typically be only symmetric.

Then in a 2nd step, you want to increase the domain until it becomes selfadjoint (hopefully).

TYPICAL WORKFLOW:

1) Given: formal expression for Hamiltonian H (based on physical ideas).
2) Find good domain (nicely behaved functions) s.th. $H \subset H^*$.
3) Find s.a. extension.
4) start solving physical problems:
   - what is the spectrum?
   - what is the scattering theory?
   - what do eigenfunctions look like?
   - ...

There can be <u>no</u> or <u>many</u> s.a. extensions.

Classification of s.a. extensions: <u>Neumann defect indices.</u>

If there are several different s.a. extensions, they often correspond to different boundary conditions.

We need physics knowledge to pick the right one.

For now we look at $L^2(\mathbb{R}^3)$ — on all of $\mathbb{R}^3$ — the only reasonable boundary condition is decay at infinity.

$\Rightarrow$ usually there will be a unique s.a. extension for us.

A particularly comfortable situation is if we have essential selfadjointness.

DEF: $A : D \subset X \to X$ is <u>closable</u> if $\exists$ closed $B \supset A$.
The smallest closed extension is called <u>closure</u>, $\overline{A}$.

DEF: Let $A : D \subset \mathcal{H} \to \mathcal{H}$ symmetric.
Notice: Since $A \subset A^*$ and A^* is always closed, A is closable.
A is <u>essentially selfadjoint</u> if $\overline{A}$ is selfadjoint.

THM 2.10: (Kato-Rellich II) Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ essentially selfadjoint, B symmetric and $D(B) \supset D(A)$.
Assume
$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \quad \forall \varphi \in D(A),$$
with $b \in \mathbb{R}$, $a < 1$.

Then $A + B : D(A) \subset \mathcal{H} \to \mathcal{H}$ is essentially selfadjoint and $D(\overline{A+B}) = D(\overline{A})$, $\overline{A+B} = \overline{A} + \overline{B}$.

RMK: In some situations we don't know $D(\overline{A})$, but we have a $D(A)$ on which our operator is essentially selfadjoint. Often one can do all calculations on a nice $D(A)$ and then extend later.

no closedness is assumed!

PROP 2.11: Let $H : D \subset \mathcal{H} \to \mathcal{H}$ symmetric. If for every $u \in D$
$$\begin{cases} i\frac{d}{dt}\varphi(t) = H\varphi(t) \\ \varphi(0) = u \end{cases}$$
has a solution $\varphi : \mathbb{R} \to \mathcal{H}$, then H is essentially selfadjoint.

III SCHRÖDINGER OPERATORS

GOAL: Define $H = -\Delta + V$.

Idea: define $-\Delta$ by Fourier transform, then use Kato-Rellich to add V as a perturbation.

RECALL: An operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ is <u>unitary</u> if $U^* = U^{-1}$.

If U is unitary: $\langle Uf, Ug \rangle = \langle f, U^* U g \rangle$
$= \langle f, U^{-1} U g \rangle = \langle f, g \rangle$.

In particular: $\|Uf\| = \|f\|$, so $\|U\| = 1$.

THM 3.1: (Fourier transform)
There is a unique unitary $\mathcal{F} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ with

$$(\mathcal{F} f)(p) = \lim_{R \to \infty} \frac{1}{(2\pi)^{n/2}} \int_{|x| \leq R} e^{-ip \cdot x} f(x)\, dx.$$

(this regularization is necessary because a general $f \in L^2$ need not be integrable.)

RMK: • Notation: $\mathcal{F} f =: \hat{f}$. $\quad \mathcal{F}^{-1} f = \mathcal{F}^* f =: \check{f}$.

• Key property: $\left[\mathcal{F} \left(-i \frac{\partial}{\partial x_j} f \right) \right](p) = p_j \hat{f}(p)$. $\quad (*)$

• Generalized derivative:
For $\alpha \geq 0$: $\left(-i \frac{\partial}{\partial x_j} \right)^\alpha f := \mathcal{F}^{-1} p_j^\alpha \mathcal{F} f$

SKETCH OF PROOF OF THM 3.1:

- using (*) one shows that $\mathcal{F}\mathcal{S}(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$.

- use the Fourier inversion formula and the fact
$\hat{g} = g$ for $g(x) = e^{-x^2/2}$
to show that $\mathcal{F}$ is 1-to-1:
$$(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ip\cdot x} \hat{f}(p)\, dp = \lim_{\varepsilon \downarrow 0} (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ip\cdot x} e^{-\varepsilon p^2/2} \hat{f}(p)\, dp$$
$$= f(x).$$

- Plancherel: $\langle \mathcal{F} f, \mathcal{F} g \rangle = \langle f, g \rangle \quad \forall f, g \in \mathcal{S}(\mathbb{R}^n)$,
in particular: $\|\mathcal{F}\| \leq 1$.

- extend from $\mathcal{S}(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ by continuity. ∎

DEF: Sobolev spaces: Let $s \geq 0$.

$$H^s(\mathbb{R}^n) := \{ u \in L^2(\mathbb{R}^n) : \int |\hat{u}(p)|^2 (1+p^2)^s \, dp < \infty \}$$
$$\langle u, v \rangle_{H^s} := \int \overline{\hat{u}(p)}\, \hat{v}(p)\, (1+p^2)^s \, ds.$$

RMK:
- $H^0(\mathbb{R}^n) = L^2(\mathbb{R}^n)$,
- for $s > s'$: $H^s(\mathbb{R}^n) \subset H^{s'}(\mathbb{R}^n)$.

DEF: Let $f: \mathbb{R}^n \longrightarrow \mathbb{C}$ measurable. The <u>multiplication op.</u> T_f is

$$T_f : D_f \subset L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n) \quad \text{with}$$

$$D_f := \{ \varphi \in L^2(\mathbb{R}^n) : f\varphi \in L^2(\mathbb{R}^n) \}$$ ← the biggest reasonable domain

and

$$(T_f \varphi)(x) = f(x)\, \varphi(x) \quad \text{(almost everywhere).}$$

RMK: A multiplication op. is the analogue of a diagonal matrix.

RMK: If $f \in L^\infty(\mathbb{R}^n)$, then $D_f = L^2(\mathbb{R}^n)$ and $\|T_f\| \leq \|f\|_\infty$.

DEF: Let X a Banachspace, $A : D \subset X \longrightarrow X$ an operator. Let $\lambda \in \mathbb{C}$.

A sequence $(x_n)_{n\in\mathbb{N}}$ in D with $\|x_n\| = 1 \ \forall n \in \mathbb{N}$ and $\|(A-\lambda)x_n\| \longrightarrow 0 \ (n \to \infty)$ is called a <u>Weyl sequence</u> for λ.

LEMMA 3.2: (Weyl criterion)

If there exists a Weyl sequence for λ, then $\lambda \in \sigma(A)$.

If $\lambda \in \sigma(A)$ and $\lambda \in \partial S(A)$, then there exists a Weyl sequence for λ.

PROOF: Part 1: see assignment.

Part 2: Let $\lambda \in \sigma(A)$ and $\lambda \in \partial \rho(A)$.

Recall that $\|R_z(A)\| \geq \frac{1}{\operatorname{dist}(z, \sigma(A))}$ $\forall z \in \rho(A)$.

$\Rightarrow \exists z_n \in \rho(A): z_n \longrightarrow \lambda$ and $\exists \varphi_n \in X$ s.th.

$$\|R_{z_n}(A)\varphi_n\| \geq \underbrace{\frac{1}{\operatorname{dist}(z_n, \sigma(A))}}_{\longrightarrow \infty \ (n \to \infty)} \|\varphi_n\| \qquad (*)$$

Let $\psi_n := R_{z_n}(A)\varphi_n$. We rescale ψ_n:

Set $\tilde{\varphi}_n := \frac{1}{\|R_{z_n}(A)\varphi_n\|}\varphi_n$ and $\tilde{\psi}_n := R_{z_n}(A)\tilde{\varphi}_n$.

By $(*)$ we have $\|\tilde{\varphi}_n\| \longrightarrow 0$, $\|\tilde{\psi}_n\| = 1$

and

$$\begin{aligned} \|(A-\lambda)\tilde{\psi}_n\| &= \|(A-z_n)\tilde{\psi}_n + (z_n-\lambda)\tilde{\psi}_n\| \\ &= \|\tilde{\varphi}_n + (z_n-\lambda)\tilde{\psi}_n\| \\ &\leq \|\tilde{\varphi}_n\| + |z_n-\lambda| \longrightarrow 0. \end{aligned}$$

So ψ_n is a Weyl sequence for λ. ∎

PRP. 3.3: Let $f: \mathbb{R}^n \longrightarrow \mathbb{C}$ measurable,
and $T_f: D_f \subset L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n)$. Then:

$$\sigma(T_f) = \underbrace{\{ z \in \mathbb{C} : \underset{\substack{\uparrow \\ \text{Lebesgue measure}}}{m} \left(f^{-1}(B_\varepsilon(z)) \right) > 0 \quad \forall \varepsilon > 0 \}}_{=: W_f}.$$

(If f is continuous, W_f is just the image of f.)

PROOF: • Let $z \in \omega_f$.

$\forall k \in \mathbb{N}\setminus\{0\}$: $\quad E_k := f^{-1}(B_{1/k}(z))$.

Make a drawing!

$$\varphi_k := \frac{1}{\sqrt{m(E_k)}} \chi_{E_k}.$$

χ_{E_k}: characteristic fct. of E_k, $=0$ outside E_k, $=1$ inside E_k.

(If $m(f^{-1}(B_{1/k}(z))) = \infty$, let E_k be a subset with $0 < m(E_k) < \infty$.)

Check that: $\varphi_k \in D(T_f)$ and $\|\varphi_k\| = 1$.

Now $$\|(T_f - z)\varphi_k\| = \Big(\int_{E_k} \underbrace{|f(x)-z|^2}_{\substack{\le 1/k^2 \\ \text{by def. of } E_k}} \frac{1}{m(E_k)}\,dx\Big)^{1/2} \le \frac{1}{k}\|\varphi_k\| \longrightarrow 0 \quad (k\to\infty).$$

$\Rightarrow \varphi_k$ is a Weyl sequence $\Rightarrow z \in \sigma(T_f)$.

• Let $z \notin \omega_f$. We show $z \notin \sigma(T_f)$ by constructing the resolvent explicitly.

$z \notin \omega_f \Rightarrow \exists \varepsilon > 0$: $m(f^{-1}(B_\varepsilon(z))) = 0$.

Our candidate for the resolvent is T_g, with

$$g(x) := \begin{cases} (f(x)-z)^{-1} & f(x) \notin B_\varepsilon(z) \\ 0 & f(x) \in B_\varepsilon(z) \leftarrow \text{zero measure,} \rightsquigarrow \text{irrelevant.} \end{cases}$$

We have $g \in L^\infty(\mathbb{R}^n)$, so T_g is bounded.
Now for $\varphi \in D_f$:

$$T_g(T_f - z)\varphi(x) = g(x)(f(x)-z)\varphi(x) = \varphi(x) \quad \text{a.e.}$$

Further: $fg \in L^\infty(\mathbb{R}^n)$, so $T_g L^2(\mathbb{R}^n) \subset D_f$, so for $\varphi \in D_f$:

$$(T_f - z)T_g\varphi(x) = (f(x)-z)g(x)\varphi(x) = \varphi(x) \quad \text{a.e.}$$

$\Rightarrow T_g = R_z(T_f)$ and $z \in \rho(T_f)$. ∎

LEMMA 3.4: If f is real-valued, T_f is self-adjoint.

PROOF: T_f is obviously symmetric.
By 3.3: $\sigma(T_f) \subset \mathbb{R}$. So by the basic criterion: s.a. $\blacksquare$

PROP. 3.5: (Unitary equivalence)

If $A: D(A) \subset \mathcal{H} \to \mathcal{H}$ selfadjoint and $U \in \mathcal{L}(\mathcal{H})$ is unitary, then $B := UAU^{-1}: UD(A) \subset \mathcal{H} \to \mathcal{H}$ is selfadjoint and $\sigma(A) = \sigma(B)$.

PROOF: B is symmetric.

We show $\sigma(A) = \sigma(B)$, then s.a. follows by the basic criterion:

Let $z \in \rho(A)$. Then $U(A-z)^{-1}U^{-1}$ is the resolvent of B at z.
$\Rightarrow z \in \rho(B)$.
For $z \in \rho(B)$, $U^{-1}(B-z)^{-1}U$ is the resolvent of A at z.
$\Rightarrow \rho(B) = \rho(A)$. $\blacksquare$

EXAMPLES:

- The momentum operator $-i\frac{d}{dx}: H^1(\mathbb{R}) \subset L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R})$ is defined as:
$$-i\frac{d}{dx} := \mathcal{F}^{-1} T_f \mathcal{F}, \quad f(p) = p.$$
It is selfadjoint and $\sigma(-i\frac{d}{dx}) = \mathbb{R}$.

- The Laplace operator (kinetic energy) $-\Delta: H^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n)$ is defined as $-\Delta := \mathcal{F}^{-1} T_f \mathcal{F}$, $f(p) = p^2 = \sum_{j=1}^{n} p_j^2$.

  It is selfadjoint on $D(\mathcal{F}^{-1} T_f \mathcal{F}) = H^2(\mathbb{R}^n)$.

  Spectrum: $\sigma(-\Delta) = [0, \infty)$.

  It is essentially selfadjoint on $\mathcal{S}(\mathbb{R}^n)$.

INTERPRETATION:

$H = -\frac{\Delta}{2m}$, $m > 0$, describes the energy of a free particle of mass m.

The momentum in 3 dimensions: $-i\nabla = \begin{pmatrix} -i\,\partial/\partial x_1 \\ -i\,\partial/\partial x_2 \\ -i\,\partial/\partial x_3 \end{pmatrix}$.

$$-\frac{\Delta}{2m} = \frac{1}{2m}(-i\nabla)^2$$

c.f. Hamilton fct. in classical mechanics:

$$H(\underbrace{p}_{\text{momentum of particle}}, \underbrace{q}_{\text{position of particle}}) = \frac{p^2}{2m}.$$

- Classical charged particle attracted by a fixed charge:

$$H(p,q) = \frac{p^2}{2m} - \frac{1}{|q|}$$

Coulomb potential.

Next goal: write the s.a. Hamilton operator for this system: this becomes an example of Schrödinger operators.

DEF: <u>Schrödinger operators</u> are operators of the form $-\Delta + V : D \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ where $V = T_V$ is a multiplication operator.