THM: (Hellinger – Töplitz)

Let $\mathcal{H}$ a Hilbert space and $A: \mathcal{H} \to \mathcal{H}$ linear and symmetric, i.e. $\langle y, Ax \rangle = \langle Ay, x \rangle \ \forall x, y \in \mathcal{H}$.

Then A is bounded.

PROOF: We show that Γ_A is closed, then boundedness follows from the closed-graph theorem.

So take a sequence in Γ_A and show that the limit is also in Γ_A.

So let $x_n \to x$ and $Ax_n \to y$.

Then for all $z \in \mathcal{H}$:

$$\langle z, y \rangle = \lim_{n \to \infty} \langle z, Ax_n \rangle = \lim_{n \to \infty} \langle Az, x_n \rangle$$

$$= \langle Az, x \rangle = \langle z, Ax \rangle.$$

Thus $y = Ax$, thus $(x, y) \in \Gamma_A$. ∎

In QM we typically deal with symmetric and unbounded operators (e.g. position operator).

The message of Hellinger – Töplitz:
We inevitably have to study operators that are only densely defined!

DEF: $C^\infty(\mathbb{R}^n)$:= complex functions with abitrarily many derivatives (smooth functions).

For $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$ („a multiindex") set:

$$\partial_\alpha f := \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}, \quad x^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}, \quad |\alpha| := \alpha_1 + \dots + \alpha_n.$$

<u>Schwartz space:</u>

$$\mathcal{S}(\mathbb{R}^n) := \left\{ f \in C^\infty(\mathbb{R}^n) : \sup_x |x^\alpha \partial_\beta f(x)| < \infty \quad \forall \alpha, \beta \in \mathbb{N}^n \right\}$$

FACTS:

1) $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$, because

$C_0^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$, and $C_0^\infty(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$

[functions with compact support, i.e. vanishing outside a bounded region in $\mathbb{R}^n$ (also denoted $C_c^\infty(\mathbb{R}^n)$).]

2) The Fourier transform is 1-to-1 as a map
$\mathcal{F} : \mathcal{S}(\mathbb{R}^n) \longrightarrow \mathcal{S}(\mathbb{R}^n)$.

EXAMPLE: Let $\mathcal{H} = L^2(\mathbb{R})$, $D(A) = \mathcal{S}(\mathbb{R})$
and $Af = -i\frac{d}{dx}f'$. (Momentum operator)
A is symmetric (but not selfadjoint).

PROOF: Integration by parts:
$$\langle f, Ag\rangle = -i\int \overline{f(x)}\, g'(x)\, dx = \int \overline{(-if')(x)}\, g(x)\, dx = \langle Af, g\rangle$$
$\forall f, g \in \mathcal{S}$.
(no boundary terms because Schwartz fct. and their derivatives $\longrightarrow 0$ as $x \to \pm\infty$)
$\Rightarrow A \subset A^*$. ■

PROP: (Generalized thm. of the bounded inverse)
Let X, Y Banach spaces.
Let $A : D \subset X \longrightarrow Y$ linear, 1-to-1 and closed.
Then A^{-1} is bounded.

RMK:
This theorem is useful because our op. are usually all closed.
If you recall the def. of resolvent set, it says "where the inverse exists <u>and is bounded</u>".
By this theorem here, at least the boundedness part comes for free for closed A (in particular for self-adjoint A).

PROOF: We show that $\Gamma_{A^{-1}}$ is closed.

Since $A : D \subset X \longrightarrow Y$ is 1-to-1: $Y = AD$.

So $\Gamma_{A^{-1}} = \{ (y, A^{-1}y) : y \in Y \}$

$= \{ (Ax, A^{-1}Ax) : x \in D \}$

$= \{ (Ax, x) : x \in D \} = I\,\Gamma_A$,

where $I : X \oplus Y \longrightarrow Y \oplus X$
$(x,y) \longmapsto (y,x)$.

I is 1-to-1 and isometric (i.e. leaves the norm invariant, $\|I(x,y)\| = \|(x,y)\|$).

So $\Gamma_{A^{-1}}$ is closed if and only if Γ_A is closed.

But Γ_A is closed by assumption. $\blacksquare$

LEMMA 2.3: Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ symmetric, $\lambda, \mu \in \mathbb{R}$.
Then for all $\varphi \in D(A)$

$$\| (A - \lambda - i\mu)\varphi \|^2 = \| (A-\lambda)\varphi \|^2 + \mu^2 \|\varphi\|^2.$$

PROOF:

$$\| (A-\lambda - i\mu)\varphi\|^2 = \langle (A-\lambda-i\mu)\varphi, (A-\lambda-i\mu)\varphi \rangle$$
$$= \langle (A-\lambda)\varphi, (A-\lambda)\varphi \rangle$$

2nd line cancels $\longrightarrow$
$$- i\mu \langle \varphi, (A-\lambda)\varphi \rangle + i\mu \langle (A-\lambda)\varphi, \varphi \rangle$$
$$+ \mu^2 \|\varphi\|^2.$$

$\blacksquare$

DEF: $\mathbb{C}_+ := \{ z \in \mathbb{C} \mid \operatorname{Im} z > 0 \}$, $\mathbb{C}_- := \{ z \in \mathbb{C} \mid \operatorname{Im} z < 0 \}$.

PROP 2.4: Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ symmetric.
If there exists a $z \in \mathbb{C}_+$ with $\operatorname{ran}(A - z) = \mathcal{H}$,
then $\mathbb{C}_+ \subset \rho(A)$.

Same for $\mathbb{C}_-$.

PROOF: Let $z \in \mathbb{C}_+$ with $\operatorname{ran}(A-z) = \mathcal{H}$. $(**)$
By previous lemma: $\|(A - z)\varphi\| \geq |\operatorname{Im} z| \, \|\varphi\|$. $(*)$

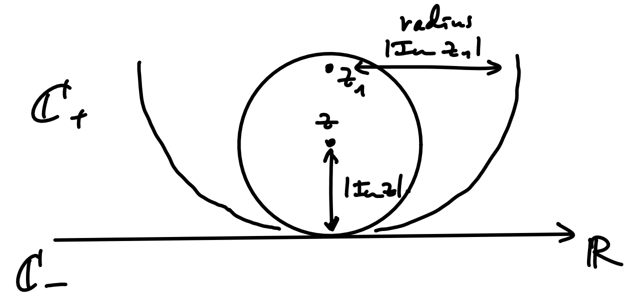
Since $|\operatorname{Im} z| > 0$, $A - z$ is injective,
by $(**)$ it is surjective, and thus bijective.
$\Rightarrow$ Inverse exists. Is it bounded?

Let $\varphi := (A-z)^{-1}\psi$ ($\psi \in \mathcal{H}$ arbitrary) in $(*)$:
$$\Rightarrow \| (A - z)^{-1} \| \leq \frac{1}{|\operatorname{Im} z|}.$$
So $(A-z)^{-1}$ is bounded, and thus $z \in \rho(A)$.

Remains to show that the whole half-plane is in the resolvent set.

Thm. 1.3 $\Rightarrow$ $B_{|\mathrm{Im}\, z|}(z) \subset \rho(A)$.

Iterate:



- ball around z
- bigger ball around z_1
- repeat...

$\Rightarrow \mathbb{C}_+ \subset \rho(A)$.

Same argument for $\mathbb{C}_-$. ∎

THEOREM 2.5: (Basic criterion for self-adjointness)

Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ symmetric. Then the following are equivalent:

(i) $A = A^*$

(ii) $\sigma(A) \subset \mathbb{R}$

(iii) $\operatorname{ran}(A - z_\pm) = \mathcal{H}$ for a $z_+ \in \mathbb{C}_+$ <u>and</u> a $z_- \in \mathbb{C}_-$.

(iv) A is closed and $\ker(A^* - z_\pm) = \{0\}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.

REMARK: $\sigma(A) \subset \mathbb{R} \not\Rightarrow A = A^*$; (already for matrices!)

A has to be symmetric.

REMARK: In QM, $\sigma(A)$ is the set of possible values the observable A can produce in a measurement.

So we have good reason to demand that $\sigma(A)$ be real!

PROOF: (i) $\Rightarrow$ (iv): Since A^* is closed, so is $A = A^{**}$.

By Lm. 2.3: $\|(A-z_+)\psi\| \geq |\mathrm{Im}\, z_+|\,\|\psi\|$.

Since $|\mathrm{Im}\, z_+| > 0$: $(A-z_+)\psi = 0 \Rightarrow \psi = 0 \Rightarrow \ker(A-z_+) = \{0\}$.

By (i): $\ker(A^* - z_+) = \ker(A - z_+) = 0$, q.e.d.

(iv) $\Rightarrow$ (iii): Recall Prp. 2.2: $\mathrm{ran}\,(A - \overline{z}_+)^\perp = \ker(A^* - z_+) = \{0\}$

$$\Rightarrow \underbrace{(\mathrm{ran}\,(A-\overline{z}_+)^\perp)^\perp}_{=\ \overline{\mathrm{ran}\,(A-\overline{z}_+)}} = \{0\}^\perp = \mathcal{H}$$

Let $\varphi \in \mathcal{H}$ arbitrary.

Have to show: $\varphi \in \mathrm{ran}\,(A - \overline{z}_+)$.

We use that A is closed!

By density of $\mathrm{ran}\,(A-\overline{z}_+)$: $\exists\, \psi_n$ in D: $(A-\overline{z}_+)\psi_n \to \varphi$.

Then $((A-\overline{z}_+)\psi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence.

We want to show that $(\psi_n)_{n\in\mathbb{N}}$ is also Cauchy, in order to prove that $(\psi_n)_n$ has a limit.

Consider $\| (A - \bar{z}_+) \varphi_n - (A - \bar{z}_+) \varphi_m \|$

$$= \| (A - \bar{z}_+)(\varphi_n - \varphi_m) \| \geq \underbrace{| \operatorname{Im} \bar{z}_+ |}_{> 0} \| \varphi_n - \varphi_m \| .$$

$\Rightarrow \varphi_n$ is Cauchy,

Because $\mathcal{H}$ is complete: $\varphi = \lim_{n \to \infty} \varphi_n$ exists.

Because $A - \bar{z}_+$ is closed: $\varphi \in D(A)$ and $(A - \bar{z}_+) \varphi = \psi$.

So we have found a φ that maps on ψ, $\Rightarrow \psi \in \operatorname{ran}(A - \bar{z}_+)$.

(iii) $\Rightarrow$ (ii): see Prp. 2.4.

(ii) $\Rightarrow$ (i): $A \subset A^*$ by assumption. to be shown: $D(A^*) \subset D(A)$.

Let $\varphi \in D(A^*)$.

Since $\sigma(A) \subset \mathbb{R}$: $(A + i) : D(A) \longrightarrow \mathcal{H}$ is surjective.

$\Rightarrow \exists \eta \in D(A)$: $(A + i) \eta = (A^* + i) \varphi$.

surjectivity of $A + i$.

$A \subset A^*$ $\rightsquigarrow$ $\|$

$(A^* + i) \eta$

$\Rightarrow (A^* + i)(\eta - \varphi) = 0.$

Recall: $\ker (A^* + i) = \operatorname{ran}(A - i)^\perp = \mathcal{H}^\perp = \{0\}$

because $A - i$ is surjective

$\Rightarrow \varphi = \eta \in D(A)$.

that shows $D(A^*) \subset D(A)$. ∎

The next theorem is a a perturbation theorem for self-adjointness.
It shows that if we add to a selfadjoint operator a „smaller" perturbation, it stays selfadjoint. Later useful for Hamiltonians (Schrödinger operator $H = -\Delta + V$).

THEOREM 2.6: (KATO-RELLICH)
Let $A = A^*$, $B \subset B^*$ and $D(B) \supset D(A)$.
If there exist $a < 1$, $b \in \mathbb{R}$ s.t.

$$\|B\varphi\| \leq a \|A\varphi\| + b \|\varphi\|$$

then $A + B : D(A) \subset \mathcal{H} \to \mathcal{H}$ is selfadjoint.

RMK: $A + B$ makes sense on $D(A)$:
since $D(B) \supset D(A)$, the expression

$$(A+B)\varphi := A\varphi + B\varphi$$

is well-defined for all $\varphi \in D(A)$.

The question answered by Kato-Rellich is whether $A + B$ with the domain $D(A)$ is selfadjoint.

Of course, if for example $D(A) \cap D(B) = \emptyset$ we are in for more serious trouble.

PROOF: $A+B$ is symmetric (trivial to see).

We use the criterion of $A+B-z_\pm$ being surjective, see (iii) above.
(We actually show more, we show that it is invertible.)

As before: $\|(A-i\mu)\psi\|^2 = \|A\psi\|^2 + \mu^2\|\psi\|^2$ for $\forall \psi \in D(A)$, $\mu \in \mathbb{R}, \mu \neq 0$.

Take $\psi = (A-i\mu)^{-1}\varphi$:

$$\Rightarrow \quad \|\varphi\|^2 = \|A(A-i\mu)^{-1}\varphi\|^2 + \mu^2\|(A-i\mu)^{-1}\varphi\|^2.$$

This implies the following two inequalities:

$$(*)\ \begin{cases} \|\varphi\| \geq \|A(A-i\mu)^{-1}\varphi\| \\ \|\varphi\| \geq |\mu|\,\|(A-i\mu)^{-1}\varphi\| \end{cases} \quad \forall \varphi \in \mathcal{H}.$$

(**) We write: $$A+B-i\mu = \underbrace{(\mathbb{1} + B(A-i\mu)^{-1})}_{}\underbrace{(A-i\mu)}_{}.$$

<u>standard trick:</u>
want to use Neumann series to invert $\Rightarrow$ have to show that $\|B(A-i\mu)^{-1}\| < 1$.

resolvent exists because $A = A^*$ and (ii) above

By assumption:

$$\|B(A-i\mu)^{-1}\varphi\| \leq a\|A(A-i\mu)^{-1}\varphi\| + b\|(A-i\mu)^{-1}\varphi\|$$

$$\overset{\text{by } (*)}{\leq} a\|\varphi\| + \frac{b}{|\mu|}\|\varphi\|.$$

$\Rightarrow$ for $|\mu|$ large enough: $\|B(A-i\mu)^{-1}\| \leq 1$ (recall $a<1$).

Then $\mathbb{1} + B(A-i\mu)^{-1}$ is invertible (Neumann series).

$\Longrightarrow$ $A + B - i\mu$ is invertible by $(**)$.

In particular surjective: $(A + B - i\mu)\, D(A) = \mathcal{H}$.

■

THE SCHRÖDINGER EQUATION

RECALL: state of a qu. system $\longleftrightarrow$ $\psi \in \mathcal{H}$ with $\|\psi\| = 1$

time evolution:

(SE) initial value problem
$$\begin{cases} i \dfrac{d}{dt} \psi(t) = H \psi(t) \\ \psi(0) = u \end{cases}$$

H is typically an unbounded operator

A solution is a function $\psi : I \longrightarrow \mathcal{H}$

some interval containing time $t=0$.

s.th.

- $\psi(t) \in D(H) \quad \forall t \in I$
- $\psi(0) = u$
- $\displaystyle\lim_{h \to 0} \frac{\psi(t+h) - \psi(t)}{h} = -iH\psi \quad \forall t \in I.$

Limit taken in the norm of $\mathcal{H}$.

PROP. 2.7: If (SE) has a solution with $\|\psi(t)\| = \|u\|$ $\forall t$, $\forall u \in D(H)$, then $H \subset H^*$.
If $H \subset H^*$, then $\|\psi(t)\|$ is constant, and the solution is unique.

PROOF: Let $\|\psi(t)\| = \|u\|$.
Then: $$0 = \frac{d}{dt} \langle \psi(t), \psi(t) \rangle \Big|_{t=0} = i \left(\langle Hu, u \rangle - \langle u, Hu \rangle \right).$$

$$\Longleftrightarrow \langle Hu, u \rangle = \langle u, Hu \rangle \ \forall u \in D(H) \Longleftrightarrow H \subset H^*.$$

(Check!)

Uniqueness:
Let $\psi(t)$, $\phi(t)$ be two solutions.
Then: $\|\psi(t) - \phi(t)\| = \|\psi(0) - \phi(0)\| = \|u - u\| = 0.$ ■