DEF: Schrödinger operators
are operators of the form $-\Delta + V : D \subset L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n)$
where $\underbrace{V = T_v}_{\text{abuse of notation...}}$ is a multiplication operator.

THM 3.6: (Some Sobolev inequalities)

(i) Let $n \geq 3$ and $1 < p < n$. There exists a constant $C_{n,p} > 0$ such that for $q = \frac{pn}{n-p}$: $\|\nabla f\|_{L^p} \geq C_{n,p} \|f\|_{L^q}$
for any measurable $f: \mathbb{R}^n \to \mathbb{C}$ (possibly one or both sides $= +\infty$).

(ii) Let $f \in H^s(\mathbb{R}^n)$ and $k \in \mathbb{N}$ with $k + \frac{n}{2} < s$.
Then $\sup_{|\alpha| \leq k} \|\partial^\alpha f\|_{L^\infty} \leq C_{n,s,k} \|f\|_{H^s}$.

(A Sobolev inequality is an inequality that allows to go to a smaller L^p-exponent at the cost of introducing derivatives. There are many variations, see e.g. Lieb & Loss: "Analysis".)

THM 3.7: Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$
(i.e. $\exists V_2 \in L^2(\mathbb{R}^3)$ and $V_\infty \in L^\infty(\mathbb{R}^3)$ such that $V(x) = V_2(x) + V_\infty(x)$)
and realvalued.

Then $-\Delta + V : D \subset L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3)$
is selfadjoint on $D = H^2(\mathbb{R}^3)$ and essentially selfadjoint on $\mathcal{S}(\mathbb{R}^3)$.

PROOF: By Kato-Rellich suffices to show: $\exists a<1, b \in \mathbb{R}$ such that
$\|V\varphi\| \le a\|\Delta\varphi\| + b\|\varphi\| \quad \forall \varphi \in H^2(\mathbb{R}^3)$.

W.l.o.g. the L^2-part of V is arbitrarily small:
Let $\varepsilon > 0$, then $\exists V_2^\varepsilon, V_\infty^\varepsilon$: $V = V_2^\varepsilon + V_\infty^\varepsilon$ with $\|V_2^\varepsilon\|_{L^2} < \varepsilon$.

See ~~Assignment~~.

So $\|V\varphi\| \le \|V_2^\varepsilon\varphi\| + \|V_\infty^\varepsilon\varphi\|$

$\le \|V_2^\varepsilon\|_{L^2}\|\varphi\|_{L^\infty} + \|V_\infty^\varepsilon\|_{L^\infty}\|\varphi\|_{L^2}$ Hölder inequ.

$\le \varepsilon\|\varphi\|_{L^\infty} + \|V_\infty^\varepsilon\|_{L^\infty}\|\varphi\|_{L^2}$

$\left(\|\varphi\|_{L^\infty} \underset{\text{Sobolev inequ. (ii)}}{\le} C\|\varphi\|_{H^2} \underset{\text{easy}}{\le} C\sqrt{2}\,(\|\Delta\varphi\| + \|\varphi\|) \right)$

$\le \underbrace{\varepsilon \cdot C\sqrt{2}}_{<1 \text{ for } \varepsilon \text{ small enough}}\|\Delta\varphi\| + (\varepsilon C\sqrt{2} + \|V_\infty^\varepsilon\|_\infty)\|\varphi\|.$

$\blacksquare$

EXAMPLE: The Coulomb potential

$$V(x) = \begin{cases} \pm \frac{1}{|x|} & x \in \mathbb{R}^3 \setminus \{0\} \\ 0 & x = 0 \end{cases} \quad \text{is in } L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3).$$

$\longrightarrow$ Assignment.

REMARK: Introduce mult. op V_{ik} as:

$$(V_{ik}\varphi)(x_1, \ldots x_N) = V_{ik}(x_i - x_k)\varphi(x_1, \ldots x_N).$$

Introduce $\left((V_{ext})_k \varphi\right)(x_1 \ldots x_N) = V_{ext}(x_k)\, \varphi(x_1, \ldots x_k).$

This is a model for molecules:

$$V_{ext}(x) = -\frac{1}{|x|} \quad \text{(attractive atomic nuclei)}$$

$$V(x) = +\frac{1}{|x|} \quad \text{(pairwise repulsion between electrons)}.$$

The N-electron operator

$$H_N = \sum_{k=1}^{N} -\Delta_k + \sum_{k=1}^{N} (V_{ext})_k + \sum_{i=1}^{N}\sum_{k>i}^{N} V_{ik} : H^2(\mathbb{R}^{3N}) \subset L^2(\mathbb{R}^{3N}) \longrightarrow L^2(\mathbb{R}^{3N})$$

is selfadjoint.

IV EXISTENCE OF SOLUTIONS TO (SE). UNITARY GROUPS

[Teschl 5.1, but missing the construction of the unitary group.]

DEF: Let X, Y be Banach spaces. A sequence of bounded operators, $A_n \in \mathcal{L}(X,Y)$, <u>converges strongly</u> to $A \in \mathcal{L}(X,Y)$ if $A_n x \longrightarrow Ax \quad (n\to\infty) \quad \forall x \in X$.

We write: $\quad A = \underset{n\to\infty}{\text{s-lim}}\, A_n$. ... just a fancy word for pointwise convergence.

WARNING: Norm convergence $\|A_n - A\| \to 0$ is <u>stronger</u> than strong convergence. Norm conv. implies strong conv., but not the other way around!

LEMMA 4.1: Let X, Y, Z be Banach spaces.

(i) If $A = \underset{n\to\infty}{\text{s-lim}}\, A_n$ in $\mathcal{L}(X,Y)$ and $B = \underset{n\to\infty}{\text{s-lim}}\, B_n$ in $\mathcal{L}(Y,Z)$, then $\underset{n\to\infty}{\text{s-lim}}\, B_n A_n = BA$.

(ii) If $(A_n)_{n\in\mathbb{N}}$ is a <u>bounded</u> sequence in $\mathcal{L}(X,Y)$ and $(A_n x)_{n\in\mathbb{N}}$ is convergent for all x in a <u>dense</u> $D \subset X$, then $\underset{n\to\infty}{\text{s-lim}}\, A_n$ exists.

i.e. uniformly: $\|A_n\| \le C < \infty$, C independent of n.

PROOF: (i) simple.
(ii) an $\varepsilon/3$-argument using the uniform-boundedness principle. ■

DEF: Let $\mathcal{H}$ a Hilbert space. A <u>strongly continuous unitary group</u> (SCUG) is a map $U: \mathbb{R} \longrightarrow \mathcal{L}(\mathcal{H})$ such that

(i) $U(t)$ is unitary and $U(t+s) = U(t)U(s) \quad \forall s,t \in \mathbb{R}$.

(ii) $U(t)\psi \to \psi \quad (t\to 0) \quad \forall \psi \in \mathcal{H}$.

RMK: $U(0) = U(0+0) = U(0)U(0) \Rightarrow U(0) = \mathbb{1}$.

RMK: $U: \mathbb{R} \to \mathcal{L}(\mathcal{H})$ is generally not continuous, only $U(t)\varphi$ is continuous.

In fact, we have a counterexample:

Let $\mathcal{H} := L^2(\mathbb{R})$ and $[U(t)\varphi](x) := \varphi(x-t)$ $(\varphi \in \mathcal{H})$.

<u>We verify that U is a SCUG:</u>

(i) is trivial.

(ii) by 4.1 it's enough to verify it on a dense set;
so let $\varphi \in C_0^\infty(\mathbb{R}^n)$:

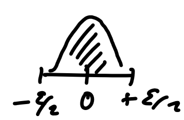
$$\| U(t)\varphi - \varphi \|_{L^2}^2 = \int |\varphi(x-t) - \varphi(x)|^2 \, dx \longrightarrow 0 \quad (t \to \infty)$$

by dominated convergence.

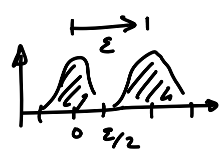
<u>Now we show that U is not continuous.</u>

<u>We show: $\|U(t) - \mathbb{1}\| \not\to 0$.</u>

For $\varepsilon > 0$, pick a $\varphi_\varepsilon \in C_0(\mathbb{R})$ s.th. $\|\varphi_\varepsilon\| = 1$, $\operatorname{supp} \varphi_\varepsilon \subset B_{\varepsilon/2}(0)$.



Then: $U(\varepsilon)\varphi_\varepsilon \perp \varphi_\varepsilon$:



no overlap!

so $\|(U(\varepsilon) - \mathbb{1})\varphi_\varepsilon\|^2 = \langle U(\varepsilon)\varphi, U(\varepsilon)\varphi \rangle + \langle \varphi, \varphi \rangle = 2$.