Session 25
May 6, 2020

Let us add one more nice criterion for essential self-adjointness:

Proposition 3.104: Let H be densly defined and symmetric. If H has an orthonormal basis (φ_n) of eigenvectors, i.e., $\varphi_n \in \mathcal{D}(H)$ and $H\varphi_n = \lambda_n \varphi_n$ for some $\lambda_n \in \mathbb{R}$, then H is essentially self-adjoint and $\sigma(\overline{H}) = \overline{\{\lambda_n : n \in \mathbb{N}\}}$.

Proof: Let us compute the deficiency indices. If $\varphi \in \mathcal{L}^{\pm} = \ker(H^* \mp i)$, then

$$\lambda_n \langle \varphi, \varphi_n \rangle = = \langle \varphi, \lambda_n \varphi_n \rangle = \langle \varphi, H\varphi_n \rangle = \langle H^* \varphi, \varphi_n \rangle = \langle \pm i\varphi, \varphi_n \rangle = \mp i \langle \varphi, \varphi_n \rangle.$$

But $\lambda_n \in \mathbb{R}$ since H is symmetric, so $\langle \varphi, \varphi_n \rangle = 0$ $\forall n \in \mathbb{R}$, which implies $\varphi = 0$ since $(\varphi_n)_n$ is an ONB (Proposition 3.10). So $\mathcal{N}^+ = \mathcal{N}^- = 0$ and with Theorem 3.89 H is essentially self-adjoint.

Now, $\overline{H}\varphi_n = \lambda_n \varphi_n$ still holds, and $\sigma(\overline{H})$ is closed (Theorem 3.100), so $\overline{\{\lambda_n : n \in \mathbb{N}\}} \subset \sigma(\overline{H})$.
What about $\lambda \notin \overline{\{\lambda_n : n \in \mathbb{N}\}}$? Let us define the bounded operator R_λ by
$R_\lambda \varphi_n = \frac{1}{\lambda_n - \lambda} \varphi_n$ $\forall n \in \mathbb{N}$. (The action on the ONB vectors φ_n defines R_λ on all of $\mathcal{H}$.)

If we can show that $R_\lambda = (\overline{H} - \lambda)^{-1}$, then $\lambda \in \rho(\overline{H})$ and thus $\lambda \notin \sigma(\overline{H})$, which proves the statement.
Writing $\mathcal{H} \ni \varphi = \sum_{n=1}^{\infty} \alpha_n \varphi_n$, we find

$\overline{H}$ closed, so we can pull it inside the limit

$$(\overline{H} - \lambda) R_\lambda \varphi = (\overline{H} - \lambda) \sum_{n=1}^{\infty} \left(\frac{\alpha_n}{\lambda_n - \lambda} \right) \varphi_n = \sum_{n=1}^{\infty} \left(\frac{\alpha_n}{\lambda_n - \lambda} \right) (\lambda_n - \lambda) \varphi_n = \sum_{n=1}^{\infty} \alpha_n \varphi_n = \varphi \quad \checkmark \qquad \square$$

Examples: • Dirichlet Laplacian on $[0, \pi]$:

$$H = -\frac{d^2}{dx^2} \text{ on } [0, \pi] \text{ with } \mathcal{D}(H) = \{ \psi \in H^2([0,\pi]) : \overbrace{\psi(0) = 0 = \psi(1)}^{\text{Dirichlet boundary conditions}} \}$$

Note: • specifying the value of a function at the boundary is called Dirichlet boundary condition.
• specifying the derivative of a function at the boundary is called Neumann boundary condition.
• specifying some combination $\alpha\psi + \beta\psi'$ at the boundary is called Robin boundary condition.

We have $-\frac{d^2}{dx^2}\left(\sqrt{\frac{2}{\pi}}\sin(nx)\right) = \underbrace{n^2}_{\lambda_n} \underbrace{\sqrt{\frac{2}{\pi}}\sin(nx)}_{\varphi_n}$, and these $(\varphi_n)_n$ are an ONB of $L^2([0,\pi])$ (Fourier series). So H is essentially self-adjoint and $\sigma(\bar{H}) = \{n^2 : n \in \mathbb{N}\}$.

- Harmonic oscillator: $H = -\frac{d^2}{dx^2} + x^2$ on $L^2(\mathbb{R})$. The eigenfunctions are the Hermite functions of the form $\varphi_n(x) = \text{const} \cdot e^{-x^2} H_n(x)$, where $H_n(x)$ are the Hermite polynomials; the eigenvalues are $\lambda_n = n + \frac{1}{2}$. $(\varphi_n)_n$ is an ONB, so H is essentially self-adjoint.

Let us come back to one of the main results of this chapter, the Kato-Rellich theorem.

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

Proof: We use Theorem 3.78 and show that $\mathrm{im}(A+B \pm i\mu_0) = \mathcal{H}$ for a suitable $\mu_0 > 0$. This implies that $\frac{A+B}{\mu_0}$ is self-adjoint on $D(A)$ and then so is $A+B$.

The goal is to show that $B(A+i\mu_0)^{-1}$ is bounded with $\|B(A+i\mu_0)^{-1}\| < 1$ for some μ_0. Then Proposition 3.101 (Neumann series) tells us that $1 + B(A+i\mu_0)^{-1} = 1 - (-B(A+i\mu_0)^{-1})$ is continuously invertible and in particular $\mathrm{im}(1+B(A+i\mu_0)^{-1}) = \mathcal{H}$. But then, for all $\varphi \in D(A)$, $(A+B+i\mu_0)\varphi = (1+B(A+i\mu_0)^{-1})(A+i\mu_0)\varphi$, and A is self-adjoint, so $\mathrm{im}(A+i\mu_0) = \mathcal{H}$. So together, $\mathrm{im}(A+B+i\mu_0) = \mathcal{H}$. The same argument holds for $A+B-i\mu_0$ and we would be done.

It remains to show that $\|B(A+i\mu_0)^{-1}\| < 1$ for some μ_0. For that, we use boundedness of the resolvent $(A+i\mu)^{-1}$ for any $0 \neq \mu \in \mathbb{R}$ (Theorem 3.102) and then the relative A-boundedness of B.

Let $\varphi \in \mathcal{D}(A)$ and $\mu > 0$. Later we will choose μ such that we can use the Neumann series argument. Note that

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

Let $\psi \in \mathcal{H}$ and set $\varphi = (A+i\mu)^{-1}\psi$. Then

$$\|\psi\|^2 \geq \|A(A+i\mu)^{-1}\psi\|^2 \quad \text{and} \quad \|\psi\|^2 \geq \mu^2 \|(A+i\mu)^{-1}\psi\|^2.$$

$$\Rightarrow \|A(A+i\mu)^{-1}\| \leq 1 \quad \text{and} \quad \underbrace{\|(A+i\mu)^{-1}\| \leq \frac{1}{\mu}}_{\text{this is also Theorem 3.102}}.$$

Now the A boundedness of B yields

$$\|B(A+i\mu)^{-1}\psi\| \leq a\|A(A+i\mu)^{-1}\psi\| + b\|(A+i\mu)^{-1}\psi\| \leq \left(a + \frac{b}{\mu}\right)\|\psi\|.$$

So for $\mu > \frac{b}{1-a} > 0$ (↑ $a<1$), we indeed have $\|B(A+i\mu)^{-1}\| < 1$, which proves the theorem with the argument above. Note that such μ only exist if $1-a>0$, i.e., $a<1$. $\square$

Example: $-\frac{1}{2}\Delta + V$ with $V \in L^\infty(\mathbb{R}^d)$ is self-adjoint.

Now, let us apply Kato-Rellich to Schrödinger operators of the form $H = H_0 + V$ with $H_0 = -\frac{1}{2}\Delta$ in three dimensions. One large class of multiplication operators V is covered in the following theorem.

We can often split $V = V_1 + V_2$ with $V_1 \in L^p$ and $V_2 \in L^q$. In this case we write $V \in L^p + L^q$.

Theorem 3.111:

a) For any $a>0$ there is a $b>0$, such that $\forall \varphi \in H^2(\mathbb{R}^3)$, $\|\varphi\|_{L^\infty} \leq a\|\Delta\varphi\|_{L^2} + b\|\varphi\|_{L^2}$.

b) Let $V:\mathbb{R}^3 \to \mathbb{R}$ with $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. For $H_0 = -\frac{1}{2}\Delta$ with $D(H_0) = H^2(\mathbb{R}^3)$, we have that V is infinitesimally H_0 bounded.

Thus, $H_0 + V$ is self-adjoint on $H^2(\mathbb{R}^3)$.

Proof:

in particular, $\varphi \in H^2(\mathbb{R}^3) \Rightarrow \varphi$ continuous and bounded, so $\|\varphi\|_{L^\infty} < \infty$

a) Similarly as in the proof of the Sobolev lemma, we estimate with Cauchy-Schwarz:

$$\|\varphi\|_{L^\infty} \leq \|\hat\varphi\|_{L^1} = \|(1+k^2)^{-1}(1+k^2)\hat\varphi\|_{L^1} \overset{C.-S.}{\leq} \underbrace{\|(1+k^2)^{-1}\|_{L^2}}_{\substack{=\left(4\pi\int_0^\infty (1+r^2)^{-1} r^2\,dr\right)^{\frac{1}{2}} \\ \leq C < \infty}} \|(1+k^2)\hat\varphi\|_{L^2} \leq C\Big(\underbrace{\|\hat\varphi\|_{L^2}}_{=\|\varphi\|_{L^2}} + \underbrace{\|k^2\hat\varphi\|_{L^2}}_{=\|\Delta\varphi\|_{L^2}}\Big)$$

Can we make the estimate such that the constant in front of $\|k^2\hat\varphi\|_{L^2}$ becomes as small as we want? Yes, by scaling $\hat\varphi$ s.t. it keeps its L^1 norm, but decreases $\|k^2\hat\varphi\|_{L^2}$ at the expense of $\|\hat\varphi\|_{L^2}$.

We set $\hat\varphi_\lambda(k) = \lambda^3\hat\varphi(\lambda k)$, $\lambda \neq 0$. Then $\|\hat\varphi_\lambda\|_{L^1} = \int |\hat\varphi_\lambda(k)|\,d^3k = \int |\hat\varphi(k)|\,d^3k = \|\hat\varphi\|_{L^1}$.

Also:
- $\|\hat\varphi_\lambda\|_{L^2}^2 = \int |\hat\varphi_\lambda(k)|^2 d^3k = \lambda^3 \int |\hat\varphi(k)|^2 d^3k = \lambda^3\|\hat\varphi\|_{L^2}^2$
- $\|k^2\hat\varphi_\lambda\|_{L^2}^2 = \int |k^2\hat\varphi_\lambda(k)|^2 d^3k = \lambda^{-4}\lambda^3 \int |k^2\hat\varphi(k)|^2 d^3k = \lambda^{-1}\|k^2\hat\varphi\|_{L^2}^2$

So
$$\|\varphi\|_{L^\infty} \leq \|\hat\varphi\|_{L^1} = \|\hat\varphi_\lambda\|_{L^1} \leq C\left(\|\hat\varphi_\lambda\|_{L^2} + \|k^2\hat\varphi_\lambda\|_{L^2}\right) = C\left(\lambda^{-\frac{1}{2}}\|k^2\hat\varphi\|_{L^2} + \lambda^{\frac{3}{2}}\|\hat\varphi\|_{L^2}\right)$$
$$= C\lambda^{-\frac{1}{2}}\|\Delta\varphi\|_{L^2} + C\lambda^{\frac{3}{2}}\|\varphi\|_{L^2}.$$

Since λ can be chosen arbitrarily large, this proves a).

b) First, is $\mathcal{D}(V)=\{\psi\in L^2(\mathbb{R}^3): V\psi\in L^2\}$ dense in $L^2(\mathbb{R}^3)$? Yes, since $V\in L^2+L^\infty$, $\mathcal{D}(V)$ contains, e.g., bounded L^2 functions, and those are clearly dense in L^2.

Now let $V=V_1+V_2$ with $V_1\in L^2(\mathbb{R}^3)$, $V_2\in L^\infty(\mathbb{R}^3)$. For $\varphi\in H^2(\mathbb{R}^3)$, we find

$$\|V\varphi\|_{L^2}\le \|V_1\varphi\|_{L^2}+\|V_2\varphi\|_{L^2}\le \underbrace{\|\varphi\|_{L^\infty}}_{\le a\|\Delta\varphi\|_{L^2}+b\|\varphi\|_{L^2}}\|V_1\|_{L^2}+\|V_2\|_{L^\infty}\|\varphi\|_{L^2}$$

$$\overset{\text{part a)}}{\le}\left(2\|V_1\|_{L^2}a\right)\|H_0\varphi\|_{L^2}+\left(b+\|V_2\|_{L^\infty}\right)\|\varphi\|_{L^2}$$

for a as small as we want, which is infinitesimal H_0-boundedness. □

Since $\pm\frac{e}{|x|}=\pm\underbrace{\mathbb{1}_{|x|\le R}\frac{e}{|x|}}_{\in L^2(\mathbb{R}^3)}\pm\underbrace{\mathbb{1}_{|x|>R}\frac{e}{|x|}}_{\in L^\infty(\mathbb{R}^3)}$ we have:

$\left(\int_0^R r^{-2}r^2\,dr<\infty\right)$

Theorem 3.113: $H=-\frac{1}{2}\Delta-\frac{e}{|x|}$ for any $e\in\mathbb{R}$ with $\mathcal{D}(H)=H^2(\mathbb{R}^3)$ is self-adjoint.

Analogously, by translation invariance, we immediately get self-adjointness of the Hamiltonian of non-relativistic matter introduced in the beginning of class, at least when the nuclei are static:

Theorem: $H=\sum_{j=1}^{N}\left(-\frac{a}{2}\Delta_j-\sum_{k=1}^{M}\frac{b_k}{|x_j-Y_k|}\right)+\text{const}+\sum_{j<k}\frac{c}{|x_j-x_k|}$ for any $a,b_k,c\in\mathbb{R}$, $Y_k\in\mathbb{R}^3$, with $\mathcal{D}(H)=H^2(\mathbb{R}^{3N})$ is self-adjoint.

at least if you believe me that e^{-iHt} is a strongly cont. unitary one parameter group (see references on website)

The dynamics of non-relativistic matter exists! So we have one thing less to worry about in life ☺

Note that $-\frac{1}{2}\Delta + \frac{e}{|x|}$ is self-adjoint for any coupling constant $e \in \mathbb{R}$. But that is not always the case. E.g., for the Dirac operator $D = \underbrace{D_0}_{\text{first order differential operator}} - \frac{e}{|x|}$, we only find

$\|\frac{e}{|x|}\varphi\| \leq 2e\|D_0\varphi\| + b\|\varphi\|$, so Kato-Rellich only works for $e < \frac{1}{2}$. For $e > \frac{1}{2}$, it turns out that D is no longer self-adjoint on $\mathcal{D}(D_0)$.

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.

It uses the following definition:

<u>Definition 3.114:</u> 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).

Note: In particular, $\langle\psi, H\psi\rangle \in \mathbb{R}$, so H is symmetric with Lemma 3.87.

Then we have:

<u>Theorem 3.115 (Friedrichs extension):</u>

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.)