Lecture 9: Schrödinger operators

Sources: ·) Weidmann: Linear operators in Hilbert spaces, Chap. 9, 10

·) Reed/Simon: Methods of Modern Mathematical physics, Vol. II: Chap. X.2, Vol. IV: Chap. XIII.4

Reminder: $-\Delta : L^2(\mathbb{R}^d) \supset H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ self-adjoint

Spectrum: $\sigma(-\Delta) = [0,\infty) = \sigma_c(-\Delta)$, i.p. no eigenvalues.

Goal for today: Study Schrödinger operators $-\Delta + V$ in $L^2(\mathbb{R}^d)$

$$(-\Delta + V)u := -\Delta u + Vu \qquad V \text{ real-valued}$$

Relatively bounded perturbations

If $A = A^*$ in Hilbert space $\mathcal{H}$ and $V = V^*$, when is $A+V$ self-adjoint? ($\operatorname{dom}(A+V) = \operatorname{dom} A \cap \operatorname{dom} V$ may be small)

<u>Definition</u> Let A, V linear operators in $\mathcal{H}$. We call V *A-bdd.* (or relatively bdd. w.r.t. A) if $\operatorname{dom} A \subset \operatorname{dom} V$ and $\exists\, a, b \geq 0$:

$$\|Vf\| \leq a\|f\| + b\|Af\| \quad \forall f \in \operatorname{dom} A. \qquad (*)$$

The infimum over all b s.t. $\exists\, a$ s.t. $(*)$ holds is called <u>A-bound</u> *of V.*

<u>Notes</u>: .) If V bdd with $\operatorname{dom} V = \mathcal{H}$, then V is A-bdd. with A-bound 0.

.) If V is A-bdd. with A-bound b then $\forall \varepsilon > 0\ \exists\, a_\varepsilon > 0$:

$$\|Vf\| \leq a_\varepsilon \|f\| + (b+\varepsilon)\|Af\| \quad \forall f \in \operatorname{dom} A,$$

but not necessarily for $\varepsilon = 0$.

.) V A-bdd. $\Leftrightarrow \exists\, \alpha, \beta > 0$: $\|Vf\|^2 \leq \alpha\|f\|^2 + \beta\|Af\|^2\ \forall f \in \operatorname{dom} A$, and the inf over all $\sqrt{\beta}$ s.t. $\exists\, \alpha$ s.t. .... is the A-bound of V.

Lemma Let $A = A^*$ in $\mathcal{H}$ and let V a linear op. in $\mathcal{H}$ with $\operatorname{dom} A \subset \operatorname{dom} V$. Let

$$c_\pm := \limsup_{\eta \to \pm\infty} \| V(A - i\eta)^{-1} \| .$$

$(\eta \in \mathbb{R})$

(With the norm being ∞ if $V(A-i\eta)^{-1}$ unbdd.). Then

$$V \ A\text{-bdd.} \iff c_+ < \infty \iff c_- < \infty .$$

In this case, $c_+ = c_- =$ A-bound of V.

Proof: (of a part) Assume that V A-bdd, i.e. $\exists\, a, b > 0$ s.t. $\|Vf\|^2 \le a^2 \|f\|^2 + b^2 \|Af\|^2 \quad \forall f \in \operatorname{dom} A$.

Then for $\eta > 0$ and $f \in \mathcal{H}$:

$$\|V(A \pm i\eta)^{-1} f\|^2 \le a^2 \|(A \pm i\eta)^{-1} f\|^2 + b^2 \|A(A \pm i\eta)^{-1} f\|^2$$

$$= b^2 \left(\frac{a^2}{b^2} \|(A \pm i\eta)^{-1} f\|^2 + \|A(A \pm i\eta)^{-1} f\|^2 \right)$$

$$= b^2 \left\| \left(A \pm i \frac{a}{b}\right)(A \pm i\eta)^{-1} f \right\|^2$$

write $\|\cdot\|^2$ as scalar prod and use $A = A^*$.

Choose $\eta = \frac{a}{b}$. We get that $V(A \pm i\frac{a}{b})^{-1}$ is bdd. with

$$\|V(A \pm i\tfrac{a}{b})^{-1}\| \le b.$$

Since this is true for each suff. large a, $c_\pm \le b$.

This is true for any $b >$ A-bound of V. $\Rightarrow$ $c_\pm \le$ A-bound of V. □

<u>Kato-Rellich theorem</u> Let $A = A^*$ in $\mathcal{H}$ and let $V \subseteq V^*$ be A-bounded with A-bound < 1. Then $(A+V)^* = A+V$.

<u>Proof</u> By the lemma there ex. $\eta > 0$ s.t. $\|V(A \pm i\eta)^{-1}\| < 1$.
Then by Neumann series, $I + V(A \pm i\eta)^{-1}$ is invertible with a bounded, everywhere defined inverse. Hence,

$$A + V \pm i\eta = (I + V(A \pm i\eta)^{-1})(A \pm i\eta)$$

is boundedly invertible with

$$(A + V \pm i\eta)^{-1} = (A \pm i\eta)^{-1}(I + V(A \pm i\eta)^{-1})^{-1}.$$

$\Rightarrow$ $\pm i\eta \in \rho(A+V)$ $\Rightarrow$ $A+V$ self-adjoint. □

Compact perturbations

Definition Let $A = A^*$ in $\mathcal{H}$. The set

$$\sigma_d(A) := \{ \lambda \in \sigma_p(A) : \dim \ker(A-\lambda) < \infty,\ \exists \varepsilon > 0 \text{ s.t. } (\lambda - \varepsilon, \lambda + \varepsilon) \cap \sigma(A) = \{\lambda\} \}$$

is called *discrete spectrum* of A, and $\sigma_{ess}(A) := \sigma(A) \setminus \sigma_d(A)$ *essential spectrum*.

Theorem (Weyl) Let $A = A^*$, $B = B^*$ in $\mathcal{H}$. Assume

$$(A-\mu)^{-1} - (B-\mu)^{-1}$$

is compact operator for some $\mu \in \rho(A) \cap \rho(B)$. Then

$$\sigma_{ess}(A) = \sigma_{ess}(B).$$

Remark: B will play the role of $A+V$.

Schrödinger operators

Lemma $H^2(\mathbb{R}^3) \subseteq L^\infty(\mathbb{R}^3)$ and $\forall \varepsilon > 0 \ \exists\, b > 0$:

$$\|\varphi\|_\infty \le \varepsilon \|\Delta\varphi\|_{L^2} + b\|\varphi\|_{L^2} \qquad \forall\, \varphi \in H^2(\mathbb{R}^3).$$

Proof Note: if $u \in L^2(\mathbb{R}^3)$ s.t. $(1+|\cdot|^2)u \in L^2(\mathbb{R}^3)$ then

$$u(x) = \underbrace{\frac{1}{1+|x|^2}}_{\in L^2} \underbrace{(1+|x|^2)\,u(x)}_{\in L^2} \in L^1(\mathbb{R}^3)$$

and

$$\|u\|_{L^1} = \int_{\mathbb{R}^3} \frac{1}{1+|x|^2}(1+|x|^2)\,|u(x)|\,dx$$

$$\overset{\text{Hölder}}{\le} \underbrace{C}_{=: \left\|\frac{1}{1+|\cdot|^2}\right\|_{L^2}} \|(1+|\cdot|^2)\,u\|_{L^2} \le C\left(\|u\|_{L^2} + \||\cdot|^2 u\|_{L^2}\right).$$

Now let $r > 0$ and $\varphi \in H^2(\mathbb{R}^3)$, and set $\hat{\varphi}_r(x) := r^3(\mathcal{F}\varphi)(rx)$.

Then $(1+|\cdot|^2)\,\hat{\varphi}_r \in L^2(\mathbb{R}^3)$ and

$$\|\hat{\varphi}_r\|_{L^1} = \|\mathcal{F}\varphi\|_{L^1}, \qquad \|\hat{\varphi}_r\|_{L^2} = r^{3/2}\|\mathcal{F}\varphi\|_{L^2},$$

$$\| |\cdot|^2 \hat{\varphi}_r\|_{L^2} = r^{-1/2} \| |\cdot|^2 \mathcal{F}\varphi\|_{L^2}.$$

$$\Rightarrow \quad \|\mathcal{F}\varphi\|_{L^1} \lesssim C \left(r^{3/2} \underbrace{\|\mathcal{F}\varphi\|_{L^2}}_{=\|\varphi\|_{L^2}} + r^{-1/2} \underbrace{\| |\cdot|^2 \mathcal{F}\varphi\|_{L^2}}_{=\|\Delta\varphi\|_{L^2}} \right).$$

Choose r large and

noting $\|\varphi\|_\infty = \|\mathcal{F}^{-1}\mathcal{F}\varphi\|_\infty \leq \frac{1}{(2\pi)^{3/2}} \|\mathcal{F}\varphi\|_{L^1}$

(Riemann-Lebesgue lemma). $\square$

<u>Theorem</u> Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$, real-valued. Then $-\Delta + V$ is self-adjoint in $L^2(\mathbb{R}^3)$.

Note: $(-\Delta + V)u := -\Delta u + Vu$, i.e., $-\Delta + V = -\Delta + M_V$,

where $M_V u = Vu$, $\operatorname{dom} M_V = \{u \in L^2(\mathbb{R}^3) : Vu \in L^2(\mathbb{R}^3)\}$.

Proof Let $\varphi \in H^2(\mathbb{R}^3)$. Then $\forall a > 0 \; \exists b > 0$:

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

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

$\Rightarrow$ $\varphi \in \operatorname{dom} M_V$ and M_V is $-\Delta$-bounded with $-\Delta$-bound zero.

$\Rightarrow$ (Kato Rellich) $-\Delta + V$ self-adjoint. $\square$

Ex. $V(x) = -\dfrac{1}{|x|}$ leads to $-\Delta + V$ self-adjoint.

Theorem Let $V \in L^2(\mathbb{R}^3)$ real-valued. Then

$$\sigma_{ess}(-\Delta + V) = \sigma_{ess}(-\Delta) = [0, \infty).$$

Proof $$\left((-\Delta + 1)^{-1} g \right)(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-|x-y|}}{|x-y|} g(y)\, dy.$$

Hence $$V(x) \left((-\Delta + 1)^{-1} g \right)(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} V(x) \frac{e^{-|x-y|}}{|x-y|} g(y)\, dy,$$

hence $M_V(-\Delta+1)^{-1}$ is an integral operator with integral kernel $V(x)\frac{e^{-|x-y|}}{4\pi|x-y|}$, which belongs to $L^2(\mathbb{R}^3\times\mathbb{R}^3)$ since $V\in L^2(\mathbb{R}^3)$.

$\Rightarrow$ $M_V(-\Delta+1)^{-1}$ compact. $\Rightarrow$ $M_V(-\Delta-\lambda)^{-1}$ compact for each $\lambda<0$.

Now for $\lambda<0$ suff. negative, $\lambda\in\rho(-\Delta+V)$ and

$$\underbrace{(-\Delta+V-\lambda)^{-1}\underbrace{M_V(-\Delta-\lambda)^{-1}}_{\text{compact}}}_{\text{compact}} = (-\Delta+V-\lambda)^{-1}\big(-\Delta+V-\lambda-(-\Delta-\lambda)\big)(-\Delta-\lambda)^{-1}$$
$$= (-\Delta-\lambda)^{-1}-(-\Delta+V-\lambda)^{-1}.$$

$\square$

<u>Remarks</u>

.) $-\Delta+V$ with $V\in L^2(\mathbb{R}^3)$ can have discrete EV below zero, they can only converge to zero.

.) $\sigma(-\Delta+V)$ has a finite lower bound for $V\in L^2(\mathbb{R}^3)$ ("$-\Delta+V$ is bounded from below")