Lecture 5 Mathematical Physics SS 2013

Note Title 4/18/2013

I.2.6 Self-adjointness of realistic Schrödinger operators

Assume you have N electrons in the field of K (static) nuclei. The positions of the nuclei are at $R_j \in \mathbb{R}^3$, $j = 1, \dots, K$.

and the configuration space of the N electrons is

$$\mathbb{R}^{3N} = \underset{1^{st}}{\mathbb{R}^3} \times \dots \times \underset{N^{th}}{\mathbb{R}^3}$$

$$\mathbb{R}^{3N} \ni x = (x_1, x_2, \dots, x_N), \quad x_j \in \mathbb{R}^3$$

momentum p_j

kinetic energy $p_j^2 = -\Delta_j$ (w.r.t. x_j !)

total kinetic energy

$$\sum_{j=1}^{N} p_j^2 = \sum_{j=1}^{N} -\Delta_j = -\Delta \quad \text{on } \mathbb{R}^{3N}$$

and the Hamiltonian is

$$H = \sum_{j=1}^{N} -\Delta_j \quad + \quad V_n(x) \quad + \quad V_{ee}(x)$$

$$V_n(x) = \sum_{\ell=1}^{N} \sum_{m=1}^{K} \frac{-Z_m}{|x_\ell - R_m|}$$

is the Coulomb attraction of all the nuclei

and

$$V_{ee}(x) = \sum_{1 \le \ell < q \le N} \frac{1}{|x_\ell - x_q|}$$

Coulomb - repulsion of the electrons

Need a theorem which includes these singular potentials. We will do a perturbative approach.

Def 16 Let $H : \mathcal{D}(H) \to \mathcal{H}$ be self-adj. and $V : \mathcal{D}(V) \to \mathcal{H}$ symmetric. The operator A has relative bound $\alpha \geq 0$ w.r.t. H if $\mathcal{D}(A) \supset \mathcal{D}(H)$ and there exists $b < \infty$ s.t.

$$(1) \quad \|V\varphi\| \le \alpha \|H\varphi\| + b \|\varphi\| \quad \forall \varphi \in \mathcal{D}(H).$$

we set

$$\alpha_0 := \inf \{\alpha \mid (1) \text{ holds for some } b < \infty\}$$

and call α_0 the relative bound of V (with respect to H) or the relative H-bound of V.

<u>Lemma 17</u> The definition of relative bound is unchanged if we replace (1) by the seemingly slightly stronger condition

$$(2) \quad \|V\varphi\|^2 \le \alpha^2 \|H\varphi\|^2 + b^2\|\varphi\|^2 \quad \forall \varphi \in \mathcal{D}(H)$$

More precisely, with

$$\alpha_1 := \inf (\alpha \mid (2) \text{ holds})$$

we have $\boxed{\alpha_0 = \alpha_1}$

<u>proof:</u> as done in the homework, but I include it in the note:

(2) $\Rightarrow$ (1): Since for $s, t > 0$

$$(s+t)^{1/2} = \frac{s}{(s+t)^{1/2}} + \frac{t}{(s+t)^{1/2}} < \frac{s}{s^{1/2}} + \frac{t}{t^{1/2}} = s^{1/2} + t^{1/2}$$

we have

$$\|V\varphi\| \le \left(\alpha^2\|H\varphi\|^2 + b^2\|\varphi\|^2\right)^{1/2}$$

$$\le \alpha\|H\varphi\|^2 + b\|\varphi\| \qquad \forall \varphi \in \mathcal{D}(H).$$

So (1) holds if (2) is true. Moreover, this shows that any α, b which make (2) also make (1), so

$$\alpha_0 := \inf(\alpha \mid (1) \text{ holds})$$

$$\le \inf(\alpha \mid (2) \text{ holds}) =: \alpha_1$$

i.e. $\alpha_0 \le \alpha_1$.

(1) $\Rightarrow$ (2) (and $\alpha_0 \geq \alpha_1$):

Recall $\quad 2cd \le c^2 + d^2$ and for any $\delta > 0$

$$2cd = 2c\delta\frac{d}{\delta} \le (c\delta)^2 + \left(\frac{d}{\delta}\right)^2$$

So if (1) holds, then

$$\|V\varphi\|^2 \le \left(\alpha\|H\varphi\| + b\|\varphi\|\right)^2$$

$$= \alpha^2\|H\varphi\|^2 + \underbrace{2\alpha\|H\varphi\|\,b\|\varphi\|}_{\le (\alpha\delta\|H\varphi\|)^2 + \left(\frac{b}{\delta}\|\varphi\|\right)^2} + b^2\|\varphi\|^2$$

$$\le \alpha^2(1+\delta^2)\|H\varphi\| + b^2(1+\delta^{-2})\|\varphi\|$$

$\Rightarrow$ So if α works for (1) for some b, then

$\alpha(1+\delta^2)^{1/2}$ works for (2) (with $b(1+\delta^{-2})^{1/2}$)

for any $\delta > 0$.

$$\Rightarrow \alpha_1 = \inf(\alpha \mid (2) \text{ holds}) \le \alpha\sqrt{1+\delta^2}$$

$$\Rightarrow \alpha_1 \le \inf(\alpha(1+\delta^2)^{1/2} \mid \alpha \text{ works for } (1)) = \alpha_0\sqrt{1+\delta^2} \quad \forall \delta > 0.$$

Let $\delta \downarrow 0 \Rightarrow \alpha_1 \le \alpha_0$.

So $\alpha_0 = \alpha_1$ $\square$

We also note the nice

Lemma 18 V is relatively H_0-bounded with relative bound α_0 iff

$$\boxed{\lim_{\lambda \to \infty} \| V(H_0 \pm i\lambda)^{-1} \| = \alpha_0}$$

Proof: "$\Leftarrow$":

Let $\varphi \in \mathcal{D}(H_0)$ and $\lambda > 0$. Then

$$\|V\varphi\| = \|V(H_0 \pm i\lambda)^{-1}(H_0 \pm i\lambda)\varphi\|$$

$$\leq \|V(H_0 \pm i\lambda)^{-1}\| \, \|(H_0 \pm i\lambda)\varphi\|$$

$$\leq \underbrace{\|V(H_0 \pm i\lambda)^{-1}\|}_{=\alpha} \|H_0\varphi\| + \underbrace{\|V(H_0 \pm i\lambda)^{-1}\| \lambda}_{=b} \|\varphi\|$$

so

$$\alpha_0 = \inf\{\alpha \mid (1) \text{ holds}\}$$

$$\leq \|V(H_0 \pm i\lambda)^{-1}\| \quad \forall \lambda > 0$$

$$\Rightarrow \quad \alpha_0 \leq \liminf_{\lambda \to \infty} \|V(H_0 \pm i\lambda)^{-1}\|.$$

"$\Rightarrow$": Let $\alpha_0 < \alpha$. Then, by Lemma 17,

for some $b < \infty$ and all $\varphi \in \mathcal{D}(H_0)$ we have

$$\|V\varphi\|^2 \leq \alpha^2 \|H_0\varphi\|^2 + b\|\varphi\|^2$$

$$= \alpha^2 \left(\|H_0\varphi\|^2 + \frac{b^2}{\alpha^2}\|\varphi\|^2\right)$$

$$\leq \alpha^2 \left(\|H_0\varphi\|^2 + \lambda^2\|\varphi\|^2\right) \quad \forall \lambda \geq \frac{b}{\alpha}$$

$$= \alpha^2 \|(H_0 \pm i\lambda)\varphi\|^2$$

So $\|V\varphi\| \leq \alpha \|(H_0 \pm i\lambda)\varphi\|^2 \quad \forall \lambda \geq \frac{b}{\alpha}, \ \varphi \in \mathcal{D}(H_0)$

Choose $\varphi := (H_0 \pm i\lambda)^{-1}\psi$. Then

$$\| V (H_0 \pm i\lambda)^{-1} \psi \| \leq \alpha \, \| \psi \| \quad \forall \psi \in \mathcal{H}, \lambda \geq \frac{b}{\alpha}$$

i.e.,

$$\| V (H_0 \pm i\lambda)^{-1} \| \leq \alpha \quad \forall \lambda \geq \frac{b}{\alpha}, \; \alpha > \alpha_0$$

and

$$\limsup_{\lambda \to \infty} \| V (H_0 \pm i\lambda)^{-1} \| \leq \alpha \quad \forall \alpha > \alpha_0$$

$$\Rightarrow \limsup_{\lambda \to \infty} \| V (H_0 \pm i\lambda)^{-1} \| \leq \alpha_0$$

Altogether,

$$\alpha_0 \leq \liminf_{\lambda \to \infty} \| V (H_0 \pm i\lambda)^{-1} \| \leq \limsup_{\lambda \to \infty} \| V (H_0 \pm i\lambda)^{-1} \| \leq \alpha_0$$

$\boxed{\text{qed}}$

The next result is a perturbative criterion for self-adjointness, known as Kato-Rellich theorem

<u>Theorem 19</u> (Kato-Rellich)

If $H_0 : \mathcal{D}(H_0) \to \mathcal{H}$ is self-adj. and V is symmetric with relative H_0 bound $\alpha_0 < 1$, then $H := H_0 + V$ is self-adjoint on its natural domain $\mathcal{D}(H) := \mathcal{D}(H_0)$.

pf: Recall that V relatively H_0 bounded implies that $\mathcal{D}(H_0) \subset \mathcal{D}(V)$, so $H = H_0 + V$ is certainly defined on $\mathcal{D}(H_0)$ and since H_0 is s.a. and V is symmetric, H is symmetric on $\mathcal{D}(H)$.

According to the basic theorem of self-adj. we have to check that for large enough $\lambda \gg 1$

$$\mathrm{Ran}\,(H \pm i\lambda) = \mathcal{H}$$

(for both $+$ and $-$ signs!).

By Lemma 18

$$\lim_{\lambda \to \infty} \| V (H_0 \pm i\lambda)^{-1} \| = \alpha_0 < 1$$

So $\boxed{\| V (H_0 \pm i\lambda)^{-1} \| < 1 \text{ for all large enough } \lambda !}$

Fix such a λ. To check that

$$\mathrm{Ran}\,(H \pm i\lambda) = \mathcal{H}$$

we have, for a given $\phi \in \mathcal{H}$, find a $\psi \in \mathcal{D}(H)$ $(= \mathcal{D}(H_0))$ with

$$\phi = (H \pm i\lambda)\psi$$

$$= (H_0 \pm i\lambda + V)\psi$$

$$= \underbrace{(\mathbb{1} + V(H_0 \pm i\lambda)^{-1})}_{\substack{\text{also invertible,} \\ \text{(Neumann Series!) since } \|V(H_0 \pm i\lambda)^{-1}\| < 1.}} \underbrace{(H_0 \pm i\lambda)}_{\substack{\text{invertible, since } H_0 \text{ is s.a.} \\ \text{and } \lambda \neq 0}} \psi$$

$\Rightarrow$ $H \pm i\lambda$ is invertible and

$$\psi = \underbrace{(H_0 \pm i\lambda)^{-1}}_{\text{maps } \mathcal{H} \text{ onto } \mathcal{D}(H_0)} \underbrace{(\mathbb{1} + V(H_0 \pm i\lambda)^{-1})^{-1} \phi}_{\in \mathcal{H}}$$

$\in \mathcal{D}(H_0)$. Done. $\boxed{\text{KO}}$