Lecture 15

A key question in mathematics is the stability of mathematical properties under perturbation. Here we are concerned with the following question:

If A is s.adj. (or e.s.a) in $\mathcal{H}$ and B is a symmetric operator, is $A+B$ s.adj (or e.s.a.)? The key result here is due to Kato and Rellich.

Definition 196.1

Let A & B be densely defined linear operators in a Hilbert space $\mathcal{H}$. Suppose that

(i) $D(A) \subset D(B)$

(ii) For some a and b in $\mathbb{R}_+$ and all $\varphi \in D(A)$

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \tag{196.2}$$

Then B is A-bounded. The infimum of such a

is called the <u>relative bound</u> of B with respect to A. If the relative bound is zero, we say that B is <u>infinitesimally small</u> wrt A and write $B << A$. We remark that usually b must be chosen large as a is chosen smaller.

Some time it is convenient to replace (ii) with

(iii) For some $\tilde{a}, \tilde{b} \in \mathbb{R}_+$ and all $\varphi \in D(A)$

(197.1) $$\|B\varphi\|^2 \le \tilde{a}^2 \|A\varphi\|^2 + \tilde{b}^2 \|\varphi\|^2$$

Clearly if (197.1) holds, then (196.2) holds with $a = \tilde{a}$, $b = \tilde{b}$. And if (196.1) holds then (197.1) holds with $\tilde{a}^2 = (1+\varepsilon) a^2$ and $\tilde{b}^2 = (1+\varepsilon^{-1}) b^2$. Thus the infimum over all a in (196.2) is equal to the inf. over all $\tilde{a}$ in (197.1). Note that to prove (196.2) or (197.1) it is enough to prove them on a core for A

Th^{m} 198.1 (Kato–Rellich)

Suppose A is s.adj, B is symmetric and B is A-bded with relative bound $a<1$. Then $A+B$ is s.adj. on $D(A)$ and e.s.a. on any core of A. Further, if A is bded below by M, then $A+B$ is bded below by $M - \max\left(\frac{b}{1-a}, a|M|+b\right)$, where a & b are given by (196.2).

Proof: We will show that if A is s.adj then $\mathrm{Ran}(A+B \pm i\mu_0) = \mathcal{H}$ for some $\mu_0>0$. ~~For $\varphi\in D(A)$,~~

~~we have for $\mu>0$,~~

$$\cancel{\|(A+i\mu)\varphi\|^2 = \|A\varphi\|^2 + \mu^2\|\varphi\|^2} \qquad (198.1)$$

~~By the spectral theorem, $\|(A+i\mu)^{-1}\| \le \frac{1}{\mu}$ and~~

~~$\|A(A+i\mu)^{-1}\| \le 1$ (alternatively, for $\varphi = (A+i\mu)^{-1}\psi$ in (198.1)),~~

But the spectral Th^m, for any $\mu > 0$

$$\|A(A+i\mu)^{-1}\| \leq 1 \quad \text{and} \quad \|(A+i\mu)^{-1}\| \leq \frac{1}{\mu}$$

Thus from (196.2), for $\mu > 0$ and any $\psi \in \mathcal{H}$,

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

$$\leq \left(a + \frac{b}{\mu}\right)\|\psi\|$$

Thus for large $\mu = \mu_0$, $C = B(A+i\mu)^{-1}$ has norm < 1,

as $a < 1$. Thus $-1 \notin \sigma(C)$ and

so $\operatorname{Ran}(I+C) = \mathcal{H}$. Since A is s.adj., $\operatorname{Ran}(A+i\mu_0)$

$= \mathcal{H}$, also. Thus the equation

(199.1) $$(A+B+i\mu_0)\varphi = (1+C)(A+i\mu_0)\varphi \quad , \varphi \in D(A)$$

$\Rightarrow \operatorname{Ran}(A+B+i\mu_0) = \mathcal{H}$. The case $\operatorname{Ran}(A+B-i\mu_0) = \mathcal{H}$

is similar. Thus by the fundamental criterion, $A+B$

is s.adj on $D(A)$.

~~Now observe that $A+B$ is closable on any core~~

Let D_0 be a core for A. Then it follows that $\mathrm{Ran}\,(A+i\mu_0)\restriction D_0$ is dense in $\mathcal{H}$. Hence $\mathrm{Ran}\big((1+C)(A+i\mu_0)\big)\restriction D_0$ is dense in $\mathcal{H}$ is $1+C$ is onto. Thus $\mathrm{Ran}\,(A+B+i\mu_0)\restriction D_0$ is dense in $\mathcal{H}$ by (199.1). By the fundamental criterion $A+B$ is e.s.a. on D_0.

Finally we prove the semi-bddness of $A+B$. Suppose $t>0$ and $-t<M$. Then $\mathrm{Ran}\,(A+t)=\mathcal{H}$ and $\|B(A+t)^{-1}\psi\| \le a\,\|A(A+t)^{-1}\psi\| + b\,\|(A+t)^{-1}\psi\|$

Now as $A+t \ge M+t>0$, it follows that if $\lambda\in\sigma(A)$, $\frac{\lambda}{\lambda+t}$ is a smooth monotone function of λ and so
$$\sup_{\lambda\in\sigma(A)}\left|\frac{\lambda}{\lambda+t}\right| \le \max\left(\frac{|M|}{M+t},1\right)$$
Thus $\|B(A+t)^{-1}\psi\| \le a\max\left(\frac{|M|}{M+t},1\right)+\frac{b}{M+t}$

Suppose $\frac{|\mu_1|}{\mu_1+t} > 1$, then

$$a \max\left(\frac{|\mu_1|}{\mu_1+t}, 1\right) + \frac{b}{\mu_1+t} = a\frac{|\mu_1|}{\mu_1+t} + \frac{b}{\mu_1+t}$$

$$= \frac{a|\mu_1|+b}{\mu_1+t}.$$

If $\frac{|\mu_1|}{\mu_1+t} \le 1$, then

$$a \max\left(\left(\frac{|\mu_1|}{\mu_1+t}\right), 1\right) + \frac{b}{\mu_1+t} = a + \frac{b}{\mu_1+t}$$

$$= \frac{a(\mu_1+t)+b}{\mu_1+t}.$$

Thus $\|B(A+t)^{-1}\| < 1$ if

$$a|\mu_1|+b < \mu_1+t$$

and if $a(\mu_1+t)+b < \mu_1+t$ ie $(1-a)(\mu_1+t) > b$.

ie $\frac{b}{1-a} < \mu_1+t$.

Thus $\|B(A+t)^{-1}\| < 1$ if $\max\left(\frac{b}{1-a}, a|\mu_1|+b\right) < \mu_1+t$

ie $-t < \mu_1 - \max\left(\frac{b}{1-a}, a|\mu_1|+b\right) = \mu^*$. For such

t, $(A+B+t) = (1+B(A+t)^{-1})(A+t)$ is a clearly a

bijection and so $-t \in \rho(A+B)$

$\square$

We now prove that the Hamiltonian for the hydrogen atom in $\mathbb{R}^3$

(203.1) $$H = -\Delta - \frac{e^2}{|x|}$$

is self-adjoint of $\mathrm{Dom}(-\Delta) = H^2(\mathbb{R}^3)$

$= \{ f \in L^2 : k^2 \hat{f}(k) \in L^2(\mathbb{R}^3) \}$

Fourier transform of f.

Theorem (Kato)

Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real valued. Then $-\Delta + V(x)$ is e.s.a on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $\mathrm{Dom}(-\Delta)$.

Proof: $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ means $\exists\, V_1 \in L^2$ and $V_2 \in L^\infty$ st $V = V_1 + V_2$. For any $\varphi \in C_0^\infty(\mathbb{R}^3)$ we have for V_1, V_2 as above,

(203.2) $$\|V\varphi\|_2 \le \|V_1\|_2 \|\varphi\|_\infty + \|V_2\|_\infty \|\varphi\|_2$$

So $C_0^\infty(\mathbb{R}^3) \subset D(V) \equiv \{ f \in L^2 : Vf \in L^2 \}$. Now for any $\varphi \in C_0^\infty(\mathbb{R}^3)$, and any $\varepsilon > 0$,

$$|\varphi(x)|^2 = \left| \frac{1}{(2\pi)^{3/2}} \int e^{ix\cdot k}\, \hat{\varphi}(k)\, dk \right|^2$$

$$\leq \frac{1}{(2\pi)^{3/2}} \left(\int |\hat{\varphi}(k)|\, dk \right)^2$$

$$\cancel{= \frac{1}{(2\pi)^{3/2}} \left(\int \frac{1}{(1+\varepsilon^4 k^4)^{\frac{1}{2}}} (1+\varepsilon^4 k^4)^{\frac{1}{2}} \hat{\varphi}(k) \right)^2}$$

$$\cancel{\leq \frac{1}{(2\pi)^{3/2}} \left(\int \frac{1}{(1+\varepsilon^4 k^4)}\, dk \right) \int (1+\varepsilon^4 k^4) |\hat{\varphi}(k)|^2}$$

$$\cancel{= \frac{c}{(2\pi)^{3/2}} \frac{1}{\varepsilon^3} \left(\int \frac{1}{1+t^4}\, t^2\, dt \right)}$$

$$= \frac{1}{(2\pi)^{3/2}} \left(\int \frac{1}{(1+k^2)^2}\, dk \right) \int (1+k^2)^2 |\hat{\varphi}(k)|^2$$

$$\leq \frac{1}{(2\pi)^{3/2}} \left[\varepsilon^{-2} \int \frac{1}{(1+k^2)^2}\, dk + \varepsilon^2 \int (1+k^2)^2 |\hat{\varphi}(k)|^2 \right]$$

As $\displaystyle\int_{\mathbb{R}^3} \frac{1}{(1+k^4)}\, dk = c \int_0^\infty \frac{1}{(1+t^2)^2}\, t^2\, dt < \infty$

we see that for any $a > 0$, no matter how small, $\exists\, b > 0$ st

(204.1) $$|\varphi(x)| \leq a \|\Delta\varphi\|_2 + b \|\varphi\|_2$$

$\forall\, \varphi \in C_0^\infty(\mathbb{R}^3)$. Inserting this inequality into (203.2) we find for $\varphi \in C_0^\infty(\mathbb{R}^3)$

(204.2) $$\|V\varphi\|_2 \leq a \|V_1\|_2 \|-\Delta\varphi\|_2 + (b\|V_1\|_2 + \|V_2\|_\infty) \|\varphi\|_2$$

Thus V is $-\Delta$-bounded with arbitrarily small bound on $C_0^\infty(\mathbb{R}^3)$. Since $-\Delta$ is essentially s.adj on C_0^∞, $-\Delta + V$ is e.s.a on $C_0^\infty(\mathbb{R}^3)$ by the Kato-Rellich Th^m and also $-\Delta+V$ is s.adj on $D(-\Delta) = H^2(\mathbb{R}^3)$. $\square$

Corollary 205.1

The hydrogen Hamiltonian $H = -\Delta - e^2/|x|$ is e.s.a on $C_0^\infty(\mathbb{R}^3)$ and s.adj on $D(-\Delta) = H^2(\mathbb{R}^3)$

Proof
$$\frac{1}{|x|} = \frac{1}{|x|}\chi_{|x|<1} + \frac{1}{|x|}\chi_{|x|\geq 1}.$$
$$= V_1 + V_2$$

as $\displaystyle\int_{|x|<1} \frac{1}{|x|^2}\, d^3x < \infty$, $V_1 \in L^2$. QED.

Theorem 205.2 (Kato's Theorem)

Let $\{V_k\}_{k=1}^m$ be a collection of real-valued functions each of which is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let $V_k(y_k)$

be the mult. oper. in $L^2(\mathbb{R}^{3n})$ obtained by choosing y_k to be "3 orthogonal" coordinates in $\mathbb{R}^{3n}$. Then $-\Delta + \sum_{k=1}^{m} V_k(y_k)$ is e.s.a. on $C_0^\infty(\mathbb{R}^{3n})$, where Δ denotes the Laplacian on $\mathbb{R}^{3n}$.

Proof By choosing $y_k = (y_{k1}, y_{k2}, y_{k3})$ to be "3 orthogonal coordinates in $\mathbb{R}^{3n}$) we mean that if $x_1, \dots, x_{3n}$ are the standard coords in $\mathbb{R}^{3n}$ Then

$$y_{kj} = \sum_{i=1}^{n} A_{ji}^{(k)} \cdot x_i$$

for some $3 \times 3n$ matrix $\{A_{ji}^{(k)}\}$ st the 3 vectors $A_j^{(k)} = (A_{j1}^{(k)}, \dots, A_{j,n}^{(k)}) \in \mathbb{R}^{3n}$ are orthonormal in $\mathbb{R}^{3n}$, $(A_j^{(k)}, A_q^{(k)}) = \delta_{jq}$, $1 \le j, q \le 3$. Then $\exists$ an orthogonal matrix O st $A_j^k O = e_j$, $j = 1, .., 3$ where $e_1 = (1, 0, \dots, 0)$, $e_2 = (0, 1, 0, \dots, 0)$, $e_3 = (0, 0, 1, 0, \dots 0)$

Thus if $u_q = \sum_i O^T_{qi} x_i$, we clearly have $y_{kj} = u_j$, $j = 1, 2, 3$.

As O is orthogonal, Δ is invariant i.e.

$$\sum_{i=1}^{3n} \frac{\partial^2}{\partial x_i^2} = \sum_{i=1}^{3n} \frac{\partial^2}{\partial u_i^2} .$$

and clearly $L^2(\mathbb{R}^{3n})$ and $L^\infty(\mathbb{R}^{3n})$ are also invariant.

Hence for all $\varphi \in C_0^\infty(\mathbb{R}^n)$

$$\int |V_k(y_k)\varphi(x)|^2 \, d^{3n}x.$$

$$= \int |V_k(u_1,u_2,u_3)\, \tilde{\varphi}(u)|^2 \, d^{3n}u \qquad , \qquad \tilde{\varphi}(u) = \varphi(Ou)$$

$$\leq a^2 \int |-\Delta_1 \tilde{\varphi}(u_1, \ldots, u_{3n})|^2 \, du_1 \ldots du_{3n}$$

Laplacian wrt u_1, u_2, u_3

$$+ b^2 \int |\tilde{\varphi}(u_1, \ldots, u_{3n})|^2 \, du_1 \ldots du_{3n}.$$

$$= a^2 \int |(p_1^2 + p_2^2 + p_3^2)\, \hat{\tilde{\varphi}}(p_1, \ldots, p_{3n})|^2 \, dp_1 \ldots dp_{3n}$$

$$+ b^2 \|\tilde{\varphi}\|^2$$

$$\leq a^2 \int \Big|\sum_{i=1}^{3n} p_i^2 \, \hat{\tilde{\varphi}}(p_1, \ldots, p_{3n})\Big|^2 dp_1 \ldots dp_{3n}$$

$$+ b^2 \|\tilde{\varphi}\|^2$$

$$= a^2 \|-\Delta \tilde{\varphi}\|^2 + b^2 \|\tilde{\varphi}\|^2$$

$$= a^2 \|-\Delta \varphi\|^2 + b^2 \|\varphi\|^2 .$$

Thus

$$\left\| \sum_{k=1}^{m} V_k(y_k)\varphi \right\|^2 \le \left(\sum_{k=1}^{m} \| V_k \varphi \| \right)^2$$

$$\le m \sum_{1}^{m} \| V_k \varphi \|^2$$

$$\le m a^2 \| -\Delta \varphi \|^2 + m b^2 \| \varphi \|^2$$

$\forall \varphi \in C_0^\infty(\mathbb{R}^{3n})$. Since a may be chose as small as we like, we conclude that $\sum_{k=1}^{m} V_k(y_k)$ is infinitesimally small wrt $-\Delta$, and the result follows by Kato-Rellich Theorem. □

<u>Corollary</u> <u>(208.1)</u> (<u>atomic</u> <u>Hamiltonian</u>)

Let $x_1, \ldots, x_n$ in $\mathbb{R}^3$ be orthogonal coordinates for $\mathbb{R}^{3n}$. Then

$$H = -\sum_{i=1}^{n} \Delta_i - \sum_{i=1}^{n} \frac{n e^2}{|x_i|} + \sum_{i \ne j} \frac{e^2}{|x_i - x_j|}$$

is e.s.a. on C_0^∞

<u>Proof</u> Note, for example that for $i \ne j$

$$1/|x_i - x_j| = \frac{1}{\sqrt{2}} \left| \frac{x_i}{\sqrt{2}} - \frac{x_j}{\sqrt{2}} \right|$$

and

$$\frac{x_{i1}}{\sqrt{2}} - \frac{x_{j1}}{\sqrt{2}} = \left(\dots, \overbrace{\frac{1}{\sqrt{2}}}^{i}, 0, 0, \dots, \overbrace{-\frac{1}{\sqrt{2}}}^{j}, 0, 0, \dots\right) \cdot (x_{11}, \dots, x_{n3})$$

$$\frac{x_{i2}}{\sqrt{2}} - \frac{x_{j2}}{\sqrt{2}} = \left(\dots, 0, \frac{1}{\sqrt{2}}, 0, \dots, 0, -\frac{1}{\sqrt{2}}, 0, \dots\right) \cdot (x_{11}, \dots, x_{n3})$$

$$\frac{x_{i3}}{\sqrt{2}} - \frac{x_{j3}}{\sqrt{2}} = \left(\dots, 0, 0, \frac{1}{\sqrt{2}}, \dots, 0, 0, -\frac{1}{\sqrt{2}}, \dots\right) \cdot (x_{11}; \dots, x_{n3})$$

are 3 orthogonal co-ordinates in $\mathbb{R}^{3n}$. $\square$.