Faculty of Science

Perturbations of Self-adjoint Operators

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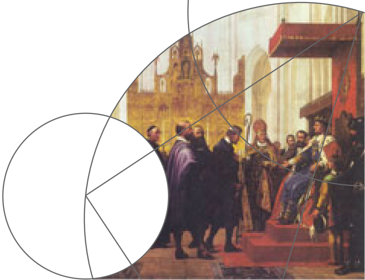

27/10/2011

Introduction

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Focus: Preservation of self-adjointness

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Rigorous meaning?

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Note that the inequality (1) implies

$$\|B\varphi\|^2 \leq a'\|A\varphi\|^2 + b'\|\varphi\|^2. \qquad (2)$$

with $a' = 2a^2$ and $b' = 2b^2$.

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Conversely, (2) implies (1) with $a = \sqrt{a'}$ and $b = \sqrt{b'}$.

The Kato-Rellich Theorem

Theorem (Kato-Rellich)

Let A be self-adjoint and consider a symmetric operator B for which there exists $0 \leq a < 1$ and $b \geq 0$ such that B is (a, b)-bounded with respect to A.

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Then $A + B$ is self-adjoint on $\mathcal{D}(A)$ and essentially self-adjoint on any core of A.

Moreover, if A is bounded below by M, then $A + B$ is bounded below by $M - \max\{\frac{b}{1-a}, a|M| + b\}$.

Proof of the Kato-Rellich Theorem

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$A+B$ is symmetric on the dense domain $\mathcal{D}(A)$ so the self-adjointness of $A+B$ will by [GG,Thm 12.10 and (12.13)] follow if

$$\operatorname{Ran}(A+B\pm i\mu)=\mathcal{H} \quad \text{for some } \mu>0.$$

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$$(A+B+i\mu)\varphi=(1+B(A+i\mu)^{-1})(A+i\mu)\varphi\quad \text{for } \varphi\in\mathcal{D}(A).$$

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[GG,Thm 12.10]: $-i\mu\notin\sigma(A)$ for all $\mu>0$.

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Show: $1 + B(A + i\mu)^{-1}$ is invertible $\mathcal{H} \to \mathcal{H}$ for some $\mu > 0$.

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Choose $\mu > 0$ so that $\|B(A+i\mu)^{-1}\| < 1$.

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closed extension

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- $(A+B)|_{\mathcal{C}} \subset A+B$ so $\overline{(A+B)|_{\mathcal{C}}} \subset A+B$.
- For $\psi \in \mathcal{D}(A)$ we have $(\psi, A\psi) \in \overline{\mathcal{G}\big(A|_{\mathcal{C}}\big)}$ so we can choose a sequence $(\psi_n)_{n\in\mathbb{N}}$ of $\mathcal{C}$-vectors such that

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Then

$$\begin{aligned} &\left\| \overline{(A+B)|_{\mathcal{C}}}\psi_n - (A+B)\psi \right\| \\ &\leq (a+1)\|A\psi_n - A\psi\| + b\|\psi_n - \psi\| \underset{n\to\infty}{\longrightarrow} 0, \end{aligned}$$

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so $(\psi, (A+B)\psi) \in \mathcal{G}\big(\overline{(A+B)|_{\mathcal{C}}}\big)$.
Conclusion: $\overline{(A+B)|_{\mathcal{C}}} \supset A + B$.

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i.e. that for any given $t \in \mathbb{R}$ satisfying

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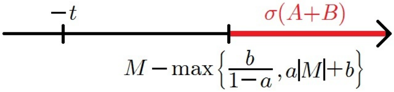
the operator $A + B + t$ has a bounded inverse.



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the operator $A + B + t$ has a bounded inverse. Note that $\inf \sigma(A) \geq M > -t$ so the operator $A + t$ has a bounded inverse and thus

$$(A+B+t)\varphi = (1 + B(A+t)^{-1})(A+t)\varphi \quad \text{for } \varphi \in \mathcal{D}(A).$$

Proof of the Kato-Rellich Theorem

If $A \geq M$ then $A + B \geq M - \max\{\frac{b}{1-a}, a|M| + b\}$:

Under the assumption $A \geq M$ we want to show that

$$\inf \sigma(A+B) \qquad \geq M - \max\left\{\frac{b}{1-a}, a|M| + b\right\}$$

i.e. that for any given $t \in \mathbb{R}$ satisfying

$$-t < M - \max\left\{\frac{b}{1-a}, a|M| + b\right\}$$

the operator $A + B + t$ has a bounded inverse. Note that $\inf \sigma(A) \geq M > -t$ so the operator $A + t$ has a bounded inverse and thus

$$(A + B + t)\varphi = (1 + B(A+t)^{-1})(A+t)\varphi \quad \text{for } \varphi \in \mathcal{D}(A).$$

Show: $1 + B(A+t)^{-1}$ is invertible $\mathcal{H} \to \mathcal{H}$.

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$1 + B(A+t)^{-1}$ is invertible if $-t < M - \max\{\frac{b}{1-a}, a|M| + b\}$:

Proof of the Kato-Rellich Theorem

$\mathbf{1} + \boldsymbol{B}(\boldsymbol{A} + \boldsymbol{t})^{-\mathbf{1}}$ is invertible if $-\boldsymbol{t} < \boldsymbol{M} - \max\{\frac{\boldsymbol{b}}{\mathbf{1}-\boldsymbol{a}}, \boldsymbol{a}|\boldsymbol{M}| + \boldsymbol{b}\}$:

An argument as above gives in the case $t > 0$ that for $\psi \in \mathcal{H}$

$$\begin{aligned} \|A(A+t)^{-1}\psi\|^2 &\leq \|\psi\|^2 - (t^2 + 2tM)\|(A+t)^{-1}\psi\|^2 \\ &\leq \begin{cases} \dfrac{M^2}{(M+t)^2}\|\psi\|^2 & \text{if } t^2 + 2tM \leq 0 \\ \|\psi\|^2 & \text{if } t^2 + 2tM > 0 \end{cases}. \end{aligned}$$

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so $\|B(A+t)^{-1}\psi\|$

$$\leq a\|A(A+t)^{-1}\psi\| + b\|(A+t)^{-1}\psi\|$$
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which means that $\|B(A+t)^{-1}\| < 1$.

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We will consider the case where $d = 3$ and V is in the space

$$L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) = \{V_2 + V_\infty \mid V_2 \in L^2(\mathbb{R}^3) \text{ and } V_\infty \in L^\infty(\mathbb{R}^3)\}.$$

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For $V = V_2 + V_\infty \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\psi \in H^2(\mathbb{R}^3)$ we have

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so $\mathcal{D}(V) \supset \mathcal{D}(-\Delta)$. Thus, the Schrödinger operator $-\Delta + V$ is well defined on the domain $\mathcal{D}(-\Delta) = H^2(\mathbb{R}^3)$.

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In quantum mechanics the self-adjointness of a given Schrödinger operator is essential – we can apply the Kato-Rellich theorem to $-\Delta + V$ in the case where $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ is real-valued if we manage to prove the following Lemma.

Lemma

Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then for any $a > 0$ there exists a $b \geq 0$ such that

$$\|V\psi\|_2 \leq a\| - \Delta\psi\|_2 + b\|\psi\|_2.$$

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Hence, for real $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ the operator $-\Delta + V$ is self-adjoint on the domain $H^2(\mathbb{R}^3)$ and essentially self-adjoint on e.g. $C_c^\infty(\mathbb{R}^3)$.

Proof of Lemma

Note first that for all $\psi \in H^2(\mathbb{R}^3)$

$$\|\psi\|_\infty = (2\pi)^{-3} \sup_{\boldsymbol{x}\in\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \mathrm{e}^{i\boldsymbol{x}\cdot\boldsymbol{p}} \widehat{\psi}(\boldsymbol{p}) \, \mathrm{d}\boldsymbol{p} \right|$$

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Note first that for all $\psi \in H^2(\mathbb{R}^3)$

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&\leq (2\pi)^{-3} \sup_{\boldsymbol{x}\in\mathbb{R}^3} \int_{\mathbb{R}^3} \qquad\qquad \left|\widehat{\psi}(\boldsymbol{p})\right| d\boldsymbol{p}
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&\leq (2\pi)^{-3} \left(\int_{\mathbb{R}^3} (\varepsilon|\boldsymbol{p}|^4 + 1)^{-1}\, \mathrm{d}\boldsymbol{p} \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} (\varepsilon|\boldsymbol{p}|^4 + 1) \left|\widehat{\psi}(\boldsymbol{p})\right|^2 \mathrm{d}\boldsymbol{p} \right)^{\frac{1}{2}}
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$$\int_{\mathbb{R}^3} (\varepsilon|\boldsymbol{p}|^4 + 1)\left|\widehat{\psi}(\boldsymbol{p})\right|^2 \mathrm{d}\boldsymbol{p} = \varepsilon \int_{\mathbb{R}^3} \left||\boldsymbol{p}|^2 \widehat{\psi}(\boldsymbol{p})\right|^2 \mathrm{d}\boldsymbol{p} + \int_{\mathbb{R}^3} \left|\widehat{\psi}(\boldsymbol{p})\right|^2 \mathrm{d}\boldsymbol{p}$$
$$= \varepsilon\| - \Delta\psi\|_2^2 + \|\psi\|_2^2.$$

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\end{aligned}$$

The Hydrogen Atom

Example:

The Hamiltonian $-\Delta - \frac{1}{|\boldsymbol{x}|}$ for the Hydrogen atom is a self-adjoint operator with domain $H^2(\mathbb{R}^3)$ and essentially self-adjoint on e.g. $C_c^\infty(\mathbb{R}^3)$

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$$-\frac{1}{|\boldsymbol{x}|} = -1_{\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|} - 1_{\mathbb{R}^3\setminus\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|},$$

where the function $\boldsymbol{x} \mapsto \left(-1_{\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|}\right)$ is square integrable and $\boldsymbol{x} \mapsto \left(-1_{\mathbb{R}^3\setminus\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|}\right)$ is bounded.

The Hydrogen Atom

Example:

The Hamiltonian $-\Delta - \frac{1}{|\boldsymbol{x}|}$ for the Hydrogen atom is a self-adjoint operator with domain $H^2(\mathbb{R}^3)$ and essentially self-adjoint on e.g. $C_c^\infty(\mathbb{R}^3)$ since

$$-\frac{1}{|\boldsymbol{x}|} = -1_{\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|} - 1_{\mathbb{R}^3\setminus\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|},$$

where the function $\boldsymbol{x} \mapsto \left(-1_{\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|}\right)$ is square integrable and $\boldsymbol{x} \mapsto \left(-1_{\mathbb{R}^3\setminus\mathcal{B}(\mathbf{0},1)}(\boldsymbol{x})\frac{1}{|\boldsymbol{x}|}\right)$ is bounded.

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Note also that $-\Delta$ is bounded from below and so the Kato-Rellich theorem also implies that the Hamiltonian $-\Delta - \frac{1}{|\boldsymbol{x}|}$ is bounded from below: The Hydrogen atom is stable.

Many-body Schrödinger operators

Given $N \in \mathbb{N}$ measurable potentials $V_1, \ldots, V_N : \mathbb{R}^3 \to \mathbb{R}$ consider the many-body Schrödinger operator $-\Delta + \sum_{k=1}^{N} V_k$ formally given by

$$\Big(-\Delta + \sum_{k=1}^{N} V_k\Big)\psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$$

$$= -\Delta\psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) + \sum_{k=1}^{N} V_k(\boldsymbol{x}_k)\psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$$

for (suitable) square integrable functions $\psi : \mathbb{R}^{3N} \to \mathbb{C}$.

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Kato's Theorem

Let $V_1, \dots, V_N \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real. Then $-\Delta + \sum_{k=1}^N V_k$ is self-adjoint on $H^2(\mathbb{R}^{3N})$ and essentially self-adjoint on $C_c^\infty(\mathbb{R}^{3N})$.

Proof of Kato's Theorem

$\sum_{k=1}^{N} V_k$ is (c,d)-bounded wrt. $-\Delta$ for some $c < 1$ and d:

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Let $k \in \{1,\dots,N\}$ and $\psi \in H^2(\mathbb{R}^{3N})$ be arbitrary. Then for all a there exists a b such that

$$\|V_k\psi\|_2^2$$
$$= \int_{\mathbb{R}^3}\cdots\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\cdots\int_{\mathbb{R}^3}\Big(\int_{\mathbb{R}^3}|V_k(\boldsymbol{x}_k)\psi(\boldsymbol{x}_1,\dots,\boldsymbol{x}_N)|^2\mathrm{d}\boldsymbol{x}_k\Big)\mathrm{d}\boldsymbol{x}_1\cdots\mathrm{d}\boldsymbol{x}_{k-1}\mathrm{d}\boldsymbol{x}_{k+1}\cdots\mathrm{d}\boldsymbol{x}_N$$

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$$\begin{aligned}
&\|V_k\psi\|_2^2 \\
&= \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3} |V_k(\boldsymbol{x}_k)\psi(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)|^2 \mathrm{d}\boldsymbol{x}_k\right) \mathrm{d}\boldsymbol{x}_1 \cdots \mathrm{d}\boldsymbol{x}_{k-1} \mathrm{d}\boldsymbol{x}_{k+1} \cdots \mathrm{d}\boldsymbol{x}_N \\
&\leq 2a^2 \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3} |-\Delta_k\psi(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)|^2 \mathrm{d}\boldsymbol{x}_k\right) \mathrm{d}\boldsymbol{x}_1 \cdots \mathrm{d}\boldsymbol{x}_{k-1} \mathrm{d}\boldsymbol{x}_{k+1} \cdots \mathrm{d}\boldsymbol{x}_N \\
&\quad + 2b^2 \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3} |\psi(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)|^2 \mathrm{d}\boldsymbol{x}_k\right) \mathrm{d}\boldsymbol{x}_1 \cdots \mathrm{d}\boldsymbol{x}_{k-1} \mathrm{d}\boldsymbol{x}_{k+1} \cdots \mathrm{d}\boldsymbol{x}_N
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$\sum_{k=1}^{N} V_k$ is (c,d)-bounded wrt. $-\Delta$ for some $c<1$ and d:

Let $k \in \{1,\ldots,N\}$ and $\psi \in H^2(\mathbb{R}^{3N})$ be arbitrary. Then for all a there exists a b such that

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&= 2a^2\|-\Delta_k\psi\|_2^2 + 2b^2\|\psi\|_2^2
\end{aligned}$$

so

$$\|V_k\psi\|_2 \leq \sqrt{2}a\|-\Delta_k\psi\|_2 + \sqrt{2}b\|\psi\|_2.$$

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$\sum_{k=1}^{N} V_k$ is (c,d)-bounded wrt. $-\Delta$ for some $c < 1$ and d:

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$$\Big\|\sum_{k=1}^{N} V_k\psi\Big\|_2 \leq \sum_{k=1}^{N} \|V_k\psi\|_2$$
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and so the desired result follows from the Kato-Rellich Theorem by choosing a such that $\sqrt{2}aN < 1$.

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