The Kato-Rellich Theorem

Problem. Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ and $B : D(B) \subseteq \mathcal{H} \to \mathcal{H}$ be two linear operators densely defined. Suppose that $A^* = A$ and $B \subseteq B^*$ such that $D(A) \subseteq D(B)$.
In particular, it makes sense to consider $A + B : D(A) \subseteq \mathcal{H} \to \mathcal{H}$.
Moreover, it was proved that

$$A + B \subseteq A^* + B^* \subseteq (A + B)^*.$$

The question that arises is under what conditions it holds that

$$(A + B)^* = A + B.$$

That problem appears for instance in Quantum Mechanics.
The initial value problem (IVP) for the Schrödinger equation is written as

$$\begin{cases} i\partial_t u = -\Delta u + \underbrace{Vu}_{\text{multiplication by a real potential}} = \underbrace{(H_0 + V)}_{\text{symmetric operator}} u, \\ u(0) = \phi \in H^2. \end{cases} \tag{0.1}$$

If the operator were self-adjoint we should show by means of the Spectral Theorem that the IVP (0.1) is well-posed, or in other words, the operator $H_0 + V$ generates a unitary group. In addition, we could obtain information on the spectrum of $H_0 + V$.

In order to do this we need of the following notion.

Definition 1. *Let* $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ *and* $B : D(B) \subseteq \mathcal{H} \to \mathcal{H}$ *be two linear operators. We say that* B *is bounded in relation to* A *(or* B *is* A*-bounded) if*

(i) $D(A) \subseteq D(B)$,

(ii) There exist $\alpha > 0$ *and* $\beta > 0$ *such that*

$$\|B\phi\| \leq \alpha \|\phi\| + \beta \|A\phi\|, \quad \forall \phi \in D(A).$$

The number

$$\beta_0 = \inf\{\beta > 0 : \textit{(ii) holds}\}$$

is called the A*-bound related to* B.

Exercise 1. *If A is a closed linear operator and B is a A-bounded linear operator, show that*

(a) $\mathcal{H}_0 = (D(A), [\cdot, \cdot])$ *is a Hilbert space with inner product*

$$[\phi, \psi] = (\phi, \psi) + (A\phi, A\psi).$$

(b) $B \in \mathcal{B}(\mathcal{H}_0)$.

Example 1. *Let* $\mathcal{H} = L^2(\mathbb{R}^n)$, $A = H_0$ *and*

$$B : H^1(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$$
$$\phi \mapsto \frac{1}{i}\phi',$$

then B *is* A*-bounded with* A*-bound equals zero.*

Indeed, $D(A) = H^2(\mathbb{R}^n) \subseteq H^1(\mathbb{R}^n) = D(B)$ implies (i) in Definition (1).

Let $\epsilon > 0$, then $|\xi| \leq \epsilon|\xi|^2 + \frac{1}{4\epsilon}$.

Using the Plancherel identity we have

$$\begin{aligned} \|B\phi\|^2 = \|\widehat{B\phi}\|^2 &= \int_{\mathbb{R}^n} |\xi\phi(\xi)|^2 \, d\xi \\ &\leq \int_{\mathbb{R}^n} (\epsilon|\xi|^2 + \frac{1}{4\epsilon})^2 |\widehat{\phi}(\xi)|^2 \, d\xi \\ &\leq c\epsilon^2 \int_{\mathbb{R}^n} ||\xi|^2 \widehat{\phi}(\xi)|^2 \, d\xi + c(\epsilon) \int_{\mathbb{R}^n} |\widehat{\phi}(\xi)|^2 \, d\xi. \end{aligned}$$

This implies that

$$\|B\phi\| \leq c\epsilon\|A\phi\| + c(\epsilon)\|\phi\|, \quad \forall \phi \in H^2(\mathbb{R}^n).$$

Since this holds for any $\epsilon > 0$, we deduce that B is A-bounded and the A-bound of B is equal to zero.

Proposition 1. *Let A and B be closed linear operators. Suppose that $D(A) \subseteq D(B)$ and $\rho(A) \neq \emptyset$. Then (ii) in Definition 1 holds.*

Proof. Take $z \in \rho(A)$, then

$$B(A-z)^{-1} : \mathcal{H} \to \mathcal{H}$$

is closed. By the Closed Graph Theorem we get $B(A-z)^{-1} \in \mathcal{B}(\mathcal{H})$. Next, for all $\phi \in D(A)$

$$\begin{aligned} \|B\phi\| &= \|B(A-z)^{-1}(A-z)\| \\ &\leq \|B(A-z)^{-1}\| \|(A-z)\phi\| \\ &\leq c\|A\phi\| + c|z|\|\phi\|. \end{aligned}$$

□

Exercise 2. *If B is a closed linear operator, $\rho(A) \neq \emptyset$, prove that the following statements are equivalent*

1. *B is A-bounded.*
2. *$B(A-z)^{-1} \in \mathcal{B}(\mathcal{H})$ for some $z \in \rho(A)$.*
3. *$B(A-z)^{-1} \in \mathcal{B}(\mathcal{H})$ for all $z \in \rho(A)$.*

Definition 2. *Let A be a linear operator such that $A \subseteq A^*$. We say that A is a positive operator if and only if*

$$(A\phi, \phi) \geq 0 \quad \forall \phi \in D(A).$$

(i.e. a bilinear form

$$b_* : D(A) \times D(A) \to \mathbb{C}$$
$$\phi \mapsto (A\phi, \phi)$$

is positive.)

A is strictly positive if and only if

$$(A\phi, \phi) > 0 \quad \forall \phi \in D(A).$$

Remarks 3.

(i) $A \subseteq A^*$ *implies that*

$$(A\phi, \phi) = (\phi, A\phi) = \overline{(A\phi, \phi)} \quad \forall \phi \in D(A)$$

and so $(A\phi, \phi) \in \mathbb{R}$.

(ii) We can define an order relation on positive symmetric operators as: $A \geq B$ *if and only if* $A - B \geq 0$.

Definition 3. *If there exists $\lambda_0 \in \mathbb{C}$ such that $A \geq \lambda_0$, we say that A is lower bounded.*

Exercise 4. *Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ such that $A = A^*$ and $M \in \mathbb{R}$. Show that $A \geq M$ if and only if $(-\infty, M) \subset \rho(A)$.*

From this we can see that a self-adjoint operator is lower bounded if and only if its spectrum is bounded below.

Theorem 5 (Kato-Rellich Theorem)**.** *Let* $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ *be a linear self-adjoint operator and let* $B : D(B) \subseteq \mathcal{H} \to \mathcal{H}$ *be a linear symmetric operator. Suppose that* B *is* A*-bounded with lower bound* $\beta < 1$*. Then*

$$A + B : D(A) \subseteq \mathcal{H} \to \mathcal{H}$$

is a self-adjoint operator.

In addition, if there exists $M \in \mathbb{R}$ *so that* $A \geq M$*, then there exists* $\widetilde{M} \in \mathbb{R}$ *such that* $A + B \geq \widetilde{M}$*.*

Proof. We divide the proof in two parts.

□

First Part. We use the basic criteria for self-adjointness. We have to prove that there exists $\lambda > 0$ such that

$$R(A + B \pm i\lambda) = \mathcal{H}.$$

We observe first that $A = A^*$ implies that $i\lambda \in \rho(A)$, for all $\lambda > 0$.

Next we write

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

Then it is sufficient to show that $I + B(A \pm i\lambda)^{-1}$ is surjective. To prove this it is enough to show that there exists $\lambda > 0$ such that

$$\|B(A \pm i\lambda)^{-1}\| < 1$$

employing Neumann series.

Let $\phi \in D(A)$. By the hypotheses B is A-bounded with A-bound $\beta_0 < 1$, there exist $0 < \beta < 1$ and $\alpha > 0$ such that

$$\|B\phi\| \leq \alpha \|\phi\| + \beta \|A\phi\|. \tag{0.2}$$

Let $\psi \in \mathcal{H}$, since $(A \pm i\lambda)$ is surjective there exists $\phi \in D(A)$ such that $(A \pm i\lambda)\phi = \psi$. This implies that

$$\|B(A \pm i\lambda)^{-1}\psi\| = \|B\phi\| \leq \alpha\|\phi\| + \beta \|A\phi\|. \tag{0.3}$$

In addition,

$$\|\psi\|^2 = \|(A \pm i\lambda)\phi\|^2 = ((A \pm i\lambda)\phi, (A \pm i\lambda)\phi) = \|A\phi\|^2 + \lambda^2\|\phi\|^2.$$

As a consequence,

$$\begin{cases} \|A\phi\| \leq \|\psi\|, \\ \|\phi\| \leq \frac{1}{\lambda} \|\psi\| \end{cases} \tag{0.4}$$

Combining (0.4) with (0.3) we obtain

$$\|B(A \pm i\lambda)^{-1}\psi\| \leq \left(\frac{\alpha}{\lambda} + \beta\right)\|\psi\| < \|\psi\|$$

whenever λ is chosen sufficiently large.

Second Part. We know that $A = A^*$ and $(A+B)^* = A+B$. From the Exercise 4, $A \geq M$ yields that $(-\infty, M) \subset \rho(A)$. We would like to find $\widetilde{M}$ so that $(-\infty, \widetilde{M}) \subset \rho(A+B)$. (exercise!).

Remark 1. *It is not possible to improve the condition* $\beta_0 < 1$*.*

For instance, if we choose $B = -A$ *then* $\beta_0 = 1$*, where* A *is an unbounded operator. Indeed, we have* $A + B : D(A) \subseteq \mathcal{H} \to \mathcal{H}$*,* $A + B = 0$ *but* $0_{\mathcal{H}} : \mathcal{H} \to \mathcal{H}$ *is symmetric which implies that* $A + B$ *is not maximal symmetric and thus* $A + B$ *is not a self-adjoint operator.*

Definition 4. *B is called relatively compact to A, or B is A-compact, if there exists $z \in \rho(A)$ such that*

$$B(A-z)^{-1} \in \mathcal{K}(\mathcal{H}) = \{L \in \mathcal{B} : L \text{ is a compact operator}\}$$

Remark 2. *We already saw that if B is A-compact, then B is A-bounded.*

Theorem 6. *Let $A = A^*$ and let B be an A-compact operator. Then B is A-bounded operator with A-bound equals zero.*

Definition 5. *Let $A = A^*$ be a linear operator. The* **discrete spectrum** *of A is the set in $\mathbb{C}$ given by*

$$\sigma_d(A) = \{\lambda \in V_p(A) : \lambda \text{ is isolated with finite multiplicity}\}.$$

The **essential spectrum** *of A is the set in $\mathbb{C}$ given by* $\sigma_e(A) = \sigma(A) \backslash \sigma_d(A)$.

Theorem 7 (Theorem of Kato-Rellich (II))**.** *Let $A = A^*$ and $B \subseteq B^*$ such that B is A-compact. Then $A + B$ is a self-adjoint operator and $\sigma_e(A + B) = \sigma_e(A)$.*

Application

A quantum particle of mass m interacting with a potential (real measurable) V in $\mathbb{R}^3$ is described by the the Schrödinger equation,

$$i\hbar\,\partial_t u = -\frac{\hbar^2}{2m}\Delta u + V(x)u \tag{0.5}$$

where $\hbar = \frac{h}{2\pi}$ is the Plank constant and $u(x,t) \in \mathbb{C}$.
The quantity $|u(x,t)|^2$ is a probability density of distribution of the particle at instant t. That is, if $u(x,0) = \phi(x)$ and S is a measurable set in $\mathbb{R}^3$, then

$$P(S) = \frac{1}{\|\phi\|^2}\int_S |u(x,t)|^2\,dx$$

is the probability to find a particle in the set S.

Exercise 8. *Verify that* $\|u(\cdot,t)\| = \|\phi\|$ *for all* $t \in \mathbb{R}$ *holds.*

We can normalize the equation (0.5) and write it in the equivalent form

$$i\partial_t u = Hu$$

where $H = H_0 + V$. H is called the Hamiltonian and H_0 is called the free Hamiltonian.

We will show that $H = H^*$.

Remark 3. *Notice that*

$$\frac{d}{dt}\|u(t)\|^2 = (\partial_t u, u) + (u, \partial u)$$

then

$$-i(u, \partial_t u) = (u, i\partial_t u) = (u, Hu) = (Hu, u)$$

which implies

$$\frac{d}{dt}\|u(t)\|^2 = i(Hu, u) - i(u, Hu) = 0.$$

Proposition 2. *Let* $V : \mathbb{R}^3 \to \mathbb{R}$ *be a measurable, if* $V \in L^2(\mathbb{R}^3) + L^\infty_\infty(\mathbb{R}^3)$*. (i.e. there exist* $V_1 \in L^2(\mathbb{R}^3)$ *and* $V_2 \in L^\infty_\infty$ *with* $V = V_1 + V_2$*), then* V *is* H_0*-compact.*

Above we use the notation

$$L^\infty_\infty(\mathbb{R}^3) = \{f \in L^\infty(\mathbb{R}^3) : \forall \epsilon > 0, \exists M > 0, \text{ such that } |f(x)| \le \epsilon \text{ a.e. } |x| \ge M\}.$$

Proof. We shall show that there exists $z \in \rho(H_0) = \mathbb{C} \backslash [0, \infty)$ such that $V(H_0 - z)^{-1}$ is compact.
From Exercise 9 if $R_0(z) = (H_0 - z)^{-1}$ then

$$R_0(z)f = \frac{1}{4\pi} \frac{e^{i\sqrt{z}|x|}}{|x|} * f, \quad \text{for } n = 3 \;\text{ where }\; \mathrm{Im}\sqrt{z} > 0.$$

Hence

$$V(H_o - z)^{-1} f(x) = V(x) \int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|} f(y)\, dy.$$

Then

$$V(H_0 - z)^{-1} f(x) = \int_{\mathbb{R}^3} \underbrace{V_1(x) \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|}}_{K_1(x,y)} f(y)\, dy$$
$$+ \int_{\mathbb{R}^3} \underbrace{V_2(X) \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|}}_{K_2(x,y)} f(y)\, dy.$$

and so

$$V(H_0 - z)^{-1} f = T_{K_1} f + T_{K_2} f.$$

Next we consider T_{K_1}.
Notice that

$$\begin{aligned}
\|K_1\|^2 &= \int_{\mathbb{R}^3} |V_1(x)|^2 \frac{e^{-2\mathrm{Im}\sqrt{z}|x-y|}}{|x-y|^2}\, dxdy \\
&= \int_{\mathbb{R}^3} |V_1(x)|^2 \Big(\int_{\mathbb{R}^3} \frac{e^{-2\mathrm{Im}\sqrt{z}|\tilde{y}|}}{|\tilde{y}|^2}\, d\tilde{y} \Big)\, dx \\
&= \|V_1\|^2 \omega(S^2) \int_0^\infty e^{-2\mathrm{Im}\sqrt{z}r}\, dr \\
&\le c\, \|V_1\|^2 .
\end{aligned}$$

where we used the change of variable $\tilde{y} = x - y$ and after applying Fubinni's theorem we employed polar coordinates.
We conclude that $K_1 \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Thus T_{K_1} is a Hilbert-Schmidt operator. Therefore it is a compact operator.

Now we study T_{K_2}.
For any $\epsilon > 0$, there exists $M_\epsilon > 0$ such that $|V_2(x)| \leq \epsilon$ a.e. for $|x| > M_\epsilon$.
Define

$$V_2^\epsilon(x) = \begin{cases} V_2(x), & \text{if } |x| \leq M_\epsilon \\ 0, & \text{if } |x| \geq M_\epsilon. \end{cases}$$

It is clear that $V_2^\epsilon(x) \in L^2(\mathbb{R}^3$. Then $T_{K_2}^\epsilon = V_2^\epsilon(H_0 - z)^{-1}$ is a compact operator by using the same analysis for T_{K_1}.
On the other hand,

$$\begin{aligned} \|T_{K_2}f - T_{K_2}^\epsilon f\| &= \|(V_2 - V_2^\epsilon)(H_0 - z)^{-1}f\| \\ &\leq \|V_2 - V_2^\epsilon\|\|(H_0 - z)^{-1}f\| \\ &\leq \|V_2 - V_2^\epsilon\|\|(H_0 - z)^{-1}\|\|f\|. \end{aligned}$$

Hence

$$\begin{aligned} \|T_{K_2}f - T^{\epsilon}_{K_2}\| &\leq \|V_2 - V_2^{\epsilon}\| \|(H_0 - z)^{-1}\| \\ &\leq \epsilon \, \|(H_0 - z)^{-1}\| \to 0 \;\; \text{as} \;\; \epsilon \to 0. \end{aligned}$$

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Thus T_{K_2} is also compact (since $\mathcal{K}(L^2(\mathbb{R}^3))$ is closed). Therefore V is H_0-compact.

Using the Theorem of Kato-Rellich II we deduce then that $H = H^*$.

Example 2. *The Coulomb potential* $V(x) = \frac{\alpha}{|x|}$, $\alpha > 0$ *belongs to the class in Proposition 2.*

Exercise 9. *Let* $H_0 = -\Delta : H^2(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ *be the free Hamiltonian and let* $z \in \rho(H_0) = \mathbb{C} \setminus [0, +\infty)$.

(i) Prove that

$$R_0(z)g := (H_0 - z)^{-1} f = \mathcal{R}_z * g, \ \forall g \in L^2(\mathbb{R}^n)$$

where $\mathcal{R}_z = ((|\xi|^2 - z)^{-1})^{\vee}$. *Check that* $R_0(z) \in \mathcal{B}(L^2(\mathbb{R}^n))$.

(ii) In case $n = 1$, *prove that*

$$\mathcal{R}_z(x) = \frac{e^{i\sqrt{z}|x|}}{2\sqrt{z}}, \quad \text{where } \operatorname{Im}\sqrt{z} > 0.$$

Hint: Use the Residue Theorem.

(iii) If $z = \lambda + i\eta$ *with* $\lambda \geq 0$, *prove that* $\lim_{\eta \to 0} R_0(\lambda + i\eta)$ *does not exist* $\mathcal{B}(L^2(\mathbb{R}^n))$.

References

[1] T. Kato, Perturbation Theory for Linear Operators, Springer-Verlag (1995).