Teoria Espectral

1. 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 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

$$\begin{cases} i\partial_t u = -\Delta u + \underbrace{Vu}_{\text{multiplication by a real potential}} = \underbrace{(H_0 + V)}_{\text{symmetric operator}} u, \\ u(0) = \phi \in H^2. \end{cases} \tag{1.1}$$

If the operator were self-adjoint we should show by means of the Spectral Theorem that the IVP (1.1) 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 1.1. *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 1.2. *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 1.3. *Let $\mathcal{H} = L^2(\mathbb{R})$, $A = H_0$ and*

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

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

Indeed, $D(A) = H^2(\mathbb{R}) \subseteq H^1(\mathbb{R}) = D(B)$ implies (i) in Definition 1.1.

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

Using Plancherel's 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

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

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 1.4. *Let A and B be closed linear operators. Suppose that $D(A) \subseteq D(B)$ and $\rho(A) \neq \emptyset$. Then (ii) in Definition 1.1 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 $\phi \in D(A)$

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

□

Exercise 1.5. *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 1.6. *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 1.7.

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

Exercise 1.9. *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 1.10 (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 is 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 first observe that $A = A^*$ implies that $i\lambda \in \rho(A)$, for all $\lambda > 0$.

We write

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

It is sufficient to show that $I+B(A\pm i\lambda)^{-1}$ is surjective. To prove that 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

$$\|B\phi\| \leq \alpha \|\phi\| + \beta \|A\phi\|. \tag{1.2}$$

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

$$\|B(A \pm i\lambda)^{-1}\psi\| = \|B\phi\| \leq \alpha\|\phi\| + \beta \|A\phi\|. \tag{1.3}$$

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,

$$\begin{cases} \|A\phi\| \leq \|\psi\|, \\ \|\phi\| \leq \frac{1}{\lambda} \|\psi\| \end{cases} \tag{1.4}$$

Combining (1.4) with (1.3) 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 1.9, $A \geq M$ yields that $(-\infty, M) \subset \rho(A)$. We would like to find $\widetilde{M}$ so that $(-\infty, \widetilde{M}) \subset \rho(A + B)$. We left this as an exercise. □

Remark 1.11. *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.*

As a consequence of the second part of the Kato-Rellich Theorem we derive

Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be such that $A^* = A$ and let $B : D(B) \subseteq \mathcal{H} \to \mathcal{H}$ be closed linear operator such that $B \subset B^*$.

Definition 1.12. *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 1.13. *We already saw that if B is A-compact, then B is A-bounded.*

Theorem 1.14. *Let $A = A^*$ and let B be an A-compact operator. Then B is A-bounded operator with A-bound equals zero.*

Definition 1.15. *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 1.16 (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 $\sigma_e(A + B) = \sigma_e(A)$.*

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

$$i\hbar\, \partial_t u = -\frac{\hbar^2}{2m}\Delta u + V(x)u \tag{1.5}$$

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

We can normalize the equation (1.5) 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 1.18. *Notice that*

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

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 1.19. *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 1.21 if $R_0(z) = (H_0 - z)^{-1}$ then

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

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

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

and so

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

Next we consider T_{K_1}.

Notice that

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

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 $|V_2(x)| \le \epsilon$ a.e. for $|x| > M_\epsilon$.

Define

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

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

On the other hand,

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

Hence

$$\begin{aligned}\|T_{K_2} - T^\epsilon_{K_2}\| &\le \|V_2 - V_2^\epsilon\|\|(H_0 - z)^{-1}\| \\ &\le \epsilon\,\|(H_0 - z)^{-1}\| \to 0 \quad \text{as} \ \ \epsilon \to 0.\end{aligned}$$

.

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 1.20. *The Coulomb potential* $V(x) = \dfrac{\alpha}{|x|}$, $\alpha > 0$ *belongs to the class in Proposition 1.19.*

Exercise 1.21. *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 $\mathcal{R}_z = \left((|\xi|^2 - z)^{-1}\right)^{\vee}$. *Check that* $R_0(z) \in \mathcal{B}(L^2(\mathbb{R}^n))$*.*

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

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

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).