1. The Kato-Rellich Theorem

For orientation, consider the formal example

$$-\Delta + V(x)$$

as an operator on $C_c^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. We investigate the problem of extending this operator to a self adjoint operator. We have seen that $-\Delta$ on the domain $C_c^\infty(\mathbb{R}^d)$ is essentially self adjoint, i.e., its closure is self adjoint. We denoted this operator by H_0. By adding the potential $V(x)$, it is far from clear whether this new operator has self adjoint extensions and in particular whether it is essentially self adjoint. We approach this problem first in an abstract way.

Definition 1.1. *Let $A : D(A) \to \mathcal{H}$ be a self adjoint operator and let $B : D(B) \to \mathcal{H}$ be symmetric. We say that B is A-bounded with bound a if $D(A) \subset D(B)$ and if there exists b so that*

$$\|Bf\| \le a\|Af\| + b\|f\|$$

for all $f \in D(A)$.

That this definition is a good one follows from the following theorem that has been discovered by Tosia Kato and independently by Franz Rellich.

Theorem 1.2. *Let $A : D(A) \to \mathcal{H}$ be a self adjoint operator and B with A-bounded with bound $a < 1$. Then $A + B : D(A) \to \mathcal{H}$ is self adjoint.*

Proof. Recall the fundamental theorem on self adjointness, which states that A is self adjoint if and only if $\mathrm{Ran}(A \pm iI) = \mathcal{H}$. A trivial extension of this fact states that A is self adjoint if and only if $\mathrm{Ran}(A \pm i\mu I) = \mathcal{H}$ for some real number μ. Now on $D(A)$ consider the operator $A + B$, which is clearly defined because $D(A) \subset D(B)$.

Let us recall a few simple facts about self adjoint operators. For real $\mu \neq 0$ and $f \in D(A)$,

$$\|(A \pm \mu i I)f\|^2 = \|Af\|^2 + \mu^2\|f\|^2 \ , \tag{1}$$

and (once more) since A is self adjoint we also know that $\mathrm{Ran}(A \pm i\mu I) = \mathcal{H}$. Thus,

$$\|(A \pm \mu i I)^{-1}\| \le \frac{1}{|\mu|} \ . \tag{2}$$

Next, we write

$$A + B + i\mu I = (I + B(A + i\mu I)^{-1})(A + i\mu I)$$

and note that for any $f \in \mathcal{H}$, $(A + i\mu I)^{-1}f \in D(A)$. Moreover,

$$\|B(A + i\mu I)^{-1}f\| \le a\|A(A + i\mu I)^{-1}f\| + b\|(A + i\mu I)^{-1}f\| \ .$$

By (**??**)

$$\|A(A + i\mu I)^{-1}f\| \le \|f\|$$

and by (**??**)

$$\|(A + i\mu I)^{-1}f\| \le \frac{b}{|\mu|}$$

so that

$$\|B(A + i\mu I)^{-1}f\| \le (a + \frac{b}{|\mu|})\|f\| \ .$$

Hence for $|\mu|$ large enough we know that

$$(a + \frac{b}{|\mu|}) < 1$$

and the operator

$$(I + B(A + i\mu I)^{-1})$$

has a bounded inverse on $\mathcal{H}$ by the Neumann series. Since $\mathrm{Ran}(A + i\mu I) = \mathcal{H}$, the range of

$$(I + B(A + i\mu I)^{-1})(A + i\mu I)$$

is the whole Hilbert space H. Since μ can have either sign we learn that $A + B$ with domain $D(A)$ is self adjoint. □

Let us turn to applying this theorem to the Schrödinger equation. We have to decide for which kind of potentials V the inequality

$$\|Vf\| \le a\|H_0 f\| + b\|f\|$$

holds for all $f \in D(H_0)$. This is where some "hard analysis" is needed, meaning that we have to develop some inequalities.

Recall that the domain of H_0 consists of functions in $L^2(\mathbb{R}^d)$ whose Fourier Transformation $\widehat{f}$ satisfies

$$\int_{\mathbb{R}^d} |2\pi k|^4 |\widehat{f}(k)|^2 dk < \infty \ . \tag{3}$$

From now on we shall restrict ourselves to the physical case $d = 3$. One can generalize the following arguments to higher dimensions at the expense of doing a bunch of not very enlightning computations.

Lemma 1.3. *For any function $\widehat{f} \in L^2(\mathbb{R}^3)$ satisfying (**??**) the inequality*

$$\|\widehat{f}\|_1^2 \le C \||2\pi \cdot|^2 \widehat{f}\|_2^{\frac{3}{4}} \|\widehat{f}\|_2^{\frac{1}{4}} \ .$$

Proof. Pick any non-zero number ν and write

$$\|\widehat{f}\|_1 = \int_{\mathbb{R}^3} |\widehat{f}(k)| dk = \int_{\mathbb{R}^3} |\widehat{f}(k)(|2\pi k|^2 + \nu^2)|(|2\pi k|^2 + \nu^2)^{-1} dk \ .$$

Schwarz's inequality yields the bound

$$\int_{\mathbb{R}^3} |\widehat{f}(k)| dk$$

$$\le \left(\int_{\mathbb{R}^3} |\widehat{f}(k)(|2\pi k|^2 + \nu^2)|^2 dk \right)^{1/2} \left(\int_{\mathbb{R}^3} (|2\pi k|^2 + \nu^2)^{-2} dk \right)^{1/2} \ .$$

The integral

$$\int_{\mathbb{R}^3} (|2\pi k|^2 + \nu^2)^{-2} dk$$

is finite and by changing variables $k = \frac{\nu}{2\pi} x$ one obtains

$$\int_{\mathbb{R}^3} (|2\pi k|^2 + \nu^2)^{-2} dk = \int_{\mathbb{R}^3} (|x|^2 + 1)^{-2} dk \left(\frac{2\pi}{\nu} \right) \ .$$

With this,

$$\|\widehat{f}\|_1^2 \le D\|(|2\pi \cdot|^2 + \nu^2)\widehat{f}\|^2 \nu^{-1} \le 2D\||2\pi \cdot|^2 \widehat{f}\|^2 \nu^{-1} + 2D\|\widehat{f}\|^2 \nu^3$$

where D is some constant. Minimizing over ν yields the desired inequality. □

Corollary 1.4. *If f is any function in $D(H_0)$, then f is bounded and*

$$\|f\|_\infty^2 \le C\|H_0 f\|_2^{\frac{3}{4}}\|f\|_2^{\frac{1}{4}} \ .$$

Proof. It follows from the Fourier Iinversion formula

$$f(x) = \int_{\mathbb{R}^3} \widehat{f}(k)e^{2\pi k\cdot x}dk$$

that

$$\|f\|_\infty \le \int_{\mathbb{R}^3} |\widehat{f}(k)|dk \ .$$

□

Theorem 1.5. *Let $V \in L^2 + L^\infty$, i.e., assume that $V = v + w$ where $v \in L^2(\mathbb{R}^3)$ and w is bounded. Then $D(H_0) \subset D(V)$ and for any $a > 0$ there exists $b(a)$ so that*

$$\|Vf\| \le a\|H_0 f\| + b(a)\|f\| \ .$$

Proof. Fix some positive number N and split the function v into v_1 and v_2 where $v_1 = v$ on the set where $v > N$ and $v_2 = v$ on the set where $v \le N$. By the monotone convergence theorem we can choose N large enough so that

$$\|v_1\|_2 \le \varepsilon \ ,$$

for any positive ε. Hence we have written our potential V as

$$V = v_1 + v_2 + w$$

where $\|v_1\|_2 \le \varepsilon$ and

$$\|v_2 + w\|_\infty \le N(\varepsilon) + \|w\|_\infty =: B(\varepsilon) \ .$$

Thus, for any $f \in D(H_0)$ we find by the Corollary

$$\|Vf\| \le \|v_1\|_2\|f\|_\infty + B(\varepsilon)\|f\|_2 \ .$$

By the Corollary

$$\|Vf\| \le C\|v_1\|_2\|H_0 f\|_2^{\frac{3}{4}}\|f\|_2^{\frac{1}{4}} + B(\varepsilon)\|f\|_2 \le C\varepsilon\|H_0 f\|_2 + [B(\varepsilon) + C]\|f\|_2 \ ,$$

where we have used that

$$\|H_0 f\|_2^{\frac{3}{4}}\|f\|_2^{\frac{1}{4}} \le \frac{3}{4}\|H_0 f\|_2 + \frac{1}{4}\|f\|_2 \ .$$

Since ε is arbitrary, this proves the claim. □

By the Kato - Rellich Theorem we have now proved.

Theorem 1.6. *Assume that the potential $V = v + w$ where $v \in L^2(\mathbb{R}^3)$ and w is bounded. Then the operator*

$$H := H_0 + V$$

with domain $D(H) = D(H_0)$ is self adjoint.

It is very easy to see that the Coulomb potential is a potential of this type. Split the potential into two pieces, the part living inside the unit ball and the part outside. Clearly $\frac{1}{|x|}$ is bounded by 1 outside the unit ball and

$$\int_{|x|\le 1} \frac{1}{|x|^2} dx = 4\pi \int_0^1 \frac{1}{r^2} r^2 dr = 4\pi \ .$$

The question lingers whether we have found the only self adjoint extension. The following theorem takes care of that.

Theorem 1.7. *Let $A : D(A) \to \mathcal{H}$ be an essentially self adjoint operator and assume that B is symmetric and A bounded with bound $a < 1$, i.e., $D(A) \subset D(B)$ and*

$$\|Bf\| \le a\|Af\| + b\|f\|$$

for all $f \in D(A)$ where b is some constant. Then $A + B$ on $D(A)$ is also essentially self adjoint and

$$\overline{A+B} = \overline{A} + \overline{B} \ .$$

Proof. The operator $\overline{B}$ is $\overline{A}$ bounded. Let $f \in D(\overline{A})$. Then there exists a sequence $f_n \in D(A)$ so that $f_n \to f$ and $Af_n \to \overline{A}f$. Since

$$\|B(f_n - f_m)\| \le a\|A(f_n - f_m)\| + b\|f_n - f_m\|$$

it follows that Bf_n is a Cauchy sequence. Thus, $f_n \to f$ and $Bf_n \to g$ and since B is closable (it is symmetric) it follows that $g = \overline{B}f$. Hence it follows that $D(\overline{A}) \subset D(\overline{B})$. Further for $f \in D(\overline{A})$

$$\|\overline{B}f\| = \lim_{n\to\infty} \|Bf_n\| \le a \lim_{n\to\infty} \|Af_n\| + b \lim_{n\to\infty} \|f_n\| = a\|\overline{A}f\| + b\|f\| \ .$$

Hence, $\overline{B}$ is $\overline{A}$-bounded with bound $a < 1$. Note that this argument shows that

$$(A + B)f_n \to \overline{A}f + \overline{B}f$$

so that

$$\overline{A+B}f = \overline{A}f + \overline{B}f \ .$$

and therefore

$$\overline{A} + \overline{B} \subset \overline{A+B} \ .$$

It follows from the Kato-Rellich theorem that $\overline{A} + \overline{B}$ is a self adjoint operator and

$$A + B \subset \overline{A} + \overline{B} \ .$$

This means that $\overline{A} + \overline{B}$ is a closed extension of $A + B$ and hence

$$\overline{A+B} \subset \overline{A} + \overline{B}$$

which means that

$$\overline{A+B} = \overline{A} + \overline{B} \ ,$$

and the theorem is proved. □

As a consequence we can consider the operator

$$-\Delta + V(x)$$

where $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and define this operator on $\mathcal{C}_c^\infty(\mathbb{R}^3)$. Because we know that $-\Delta$ is essentially self adjoint on $\mathcal{C}_c^\infty(\mathbb{R}^3)$ and V is $-\Delta$ bounded with bound $a < 1$, it follows that $-\Delta + V(x)$ on $\mathcal{C}_c^\infty(\mathbb{R}^3)$ is essentially self adjoint, i.e., $\overline{-\Delta + V(x)}$ is self adjoint.