10. Potentials for which $H_0 + V$ is self-adjoint on $D(H_0)$

Suppose A and B are self-adjoint, and $D(A) \subset D(B)$. Then $D(A+B) = D(A) \cap D(B) = D(A)$, and thus $A+B$ is densely defined. It is also obviously symmetric. When is $A+B$ self-adjoint? the following theorem shows that this is the case at least when B is suffiently "small" compared to A.

10.1. Definition: Let A and B be densely defined operators on $\mathcal{H}$. B is said to be A-bounded, if

a) $D(B) \supset D(A)$

b) $\exists\, \varepsilon, c \in \mathbb{R}$ such that

(*) $\quad \forall \psi \in D(A): \; \|B\psi\| \leq \varepsilon \|A\psi\| + c\|\psi\|.$

If B is A-bounded, the infimum ε_0 of all ε for which (*) holds is called the relative bound of B with respect to A, that is,

$$\varepsilon_0 := \inf \{ \varepsilon \in \mathbb{R} \mid \exists c \in \mathbb{R} \text{ s.t. } (*) \text{ holds} \}.$$

* Typical application would be $A = H_0$, $B = V$. To use above result, it is crucial to check that $V\psi \in L^2$ for all $\psi \in D(H_0)$. If V is not bounded, it is important to have some estimates for generic $\psi \in D(H_0)$. For $\mathcal{H} = L^2(\mathbb{R})$, $(d=1)$ in particular, the functions in $D(H_0)$ are quite regular: $D(-i\partial)$ is classified in Ex. 10.3. and $D(H_0)$ in Ex. 11.3. Cases $d \leq 3$ will be discussed in Prop. 10.3. →

10.2. Theorem (Kato-Rellich)

Let A be self-adjoint, S densely defined and symmetric, and suppose S is A-bounded with a relative bound $\varepsilon_0 < 1$.

Then $A+S$ is self-adjoint on $D(A)$, and any core D' of A is also a core of $A+S$.

Proof: Since $D(S) \supset D(A)$, now $D(A+S) = D(A)$ is the natural domain of $A+S$. We will soon prove that $\exists \mu_0 > 0$ s.t. $R(A+S \pm i\mu_0) = \mathcal{H}$.
$\Rightarrow R(\frac{1}{\mu_0}(A+S) \pm i) = \mathcal{H}$. Let $T = \frac{1}{\mu_0}(A+S)$.

Then $D(T) = D(A) \subset D(S) \Rightarrow \forall \phi, \psi \in D(T)$:
$$(\phi, T\psi) = \frac{1}{\mu_0}(\phi, A\psi + S\psi)$$
$$= \frac{1}{\mu_0}[(\phi, A\psi) + (\phi, S\psi)]$$
$$\overset{A,S \text{ symm.}}{=} \frac{1}{\mu_0}(A\phi + S\phi, \psi) = (T\phi, \psi).$$
Thus T is densely defined, and symmetric, with $R(T \pm i) = \mathcal{H}$. $\Rightarrow C_T$ is unitary.
Thus by Lemma 9.10. T is self-adjoint.
$\Rightarrow A+S = \mu_0 T$ is self-adjoint. (on $D(A)$).
[In general, if $\lambda \in \mathbb{C}\setminus\{0\}$ and T is densely def., then $D(\lambda T) = D(T)$ and $(\lambda T)^* = \lambda^* T^*$.
Proof: left as exercise.]

Thus to prove the first stament, we only need to find $\mu_0 > 0$ for which $R(A+S \pm i\mu_0) = \mathcal{H}$.
For any $\mu \in \mathbb{R}, \mu \neq 0$, since A is self-adjoint,

(*) $\|(A+i\mu)\psi\|^2 = \|A\psi\|^2 + \mu^2\|\psi\|^2 \quad \forall \psi \in D(A)$.

$\Rightarrow A + i\mu$ is 1-1 $\Rightarrow \exists T := (A+i\mu)^{-1} : R(A+i\mu) \to D(A)$.
$\Rightarrow AT : R(A+i\mu) \to R(A)$ and we have by (*), $\forall \phi \in D(T)$: $\|\phi\|^2 = \|(A+i\mu)T\phi\|^2$
$= \|AT\phi\|^2 + \mu^2\|T\phi\|^2$.

$\Rightarrow \|AT\phi\| \le \|\phi\|$, $\|T\phi\| \le \frac{1}{|\mu|}\|\phi\| \ \forall \phi \in D(T)$.

$\Rightarrow \|AT\| \le 1$, $\|T\| \le \frac{1}{|\mu|}$.

By assumption, $\exists\, 0 \le \varepsilon < 1$ and $c \in \mathbb{R}$ s.t.

$$\forall \psi \in D(A): \quad \|S\psi\| \le \varepsilon \|A\psi\| + c\|\psi\|$$

$$\overset{\psi = T\phi}{\Rightarrow} \forall \phi \in D(T): \|ST\phi\| \le \varepsilon \|AT\phi\| + c\|T\phi\|$$
$$\le \left(\varepsilon + \frac{c}{|\mu|}\right)\|\phi\|.$$

Thus, if we set μ equal to $\mu_0 > \max\left(0, \frac{c}{1-\varepsilon}\right)$,

we have $\mu_0 > 0$ and $a := \varepsilon + \frac{c}{\mu_0} < 1$.
Let $T_0 = (A + i\mu_0)^{-1}$, when we have proven that $\|ST_0\phi\| \le a\|\phi\|$, with $0 \le a < 1$.
Since A is self-adjoint, $\frac{1}{\mu_0}A$ is also s-a.,

9, 10, $\overset{7}{\Rightarrow} \mathcal{H} = R\left(\frac{1}{\mu_0}A + i\right) = R(A + i\mu_0) = D(T_0)$.

Thus $T_0 : \mathcal{H} \to D(A)$ and $D(ST_0) = \mathcal{H}$.
Therefore, $ST_0 \in \mathcal{B}(\mathcal{H})$ with $\|ST_0\| \le a < 1$.
Let $B = \sum_{n=0}^{\infty} (-ST_0)^n$, which by $\|ST_0\| < 1$

is a norm-convergent sum in $\mathcal{B}(\mathcal{H})$
$\Rightarrow B \in \mathcal{B}(\mathcal{H})$. For any $\phi \in \mathcal{H}$, it is obvious that $ST_0 B\phi = -\sum_{n=1}^{\infty} (-ST_0)^n \phi$
$= -(B\phi - \phi)$

$\Rightarrow \phi = (1 + ST_0)B\phi$. (In fact, $B = (1+ST_0)^{-1}$.)

Thus $R(1 + ST_0) = \mathcal{H}$.
On the other hand, $\forall \psi \in D(A)$,
$(1 + ST_0)(A + i\mu_0)\psi$
$= (A + i\mu_0)\psi + S\psi = (A + S + i\mu_0)\psi$.
Since $R(A + i\mu_0) = \mathcal{H} \Rightarrow R(A + S + i\mu_0)$
$= R(1 + ST_0) = \mathcal{H}$.
The proof, that also $R(A + S - i\mu_0) = \mathcal{H}$, is essentially identical. (Consider $T_0' = (A - i\mu_0)^{-1}$ and use $\|(A - i\mu_0)\psi\|^2 = \|A\psi\|^2 + \mu_0^2\|\psi\|^2$ and $R(A - i\mu_0) = \mathcal{H}$ to prove $\|ST_0'\| \le a < 1$, $R(1 + ST_0') = \mathcal{H} \Rightarrow R(A + S - i\mu_0) = \mathcal{H}$.)
Therefore, we have proven that $A + S$ is self-adjoint.

Suppose then that D' is a core of A.
Then $S' := (A+S)|_{D'}$ is densely defined and symmetric. $\Rightarrow$ $\overline{S'} \subset A+S$.
Suppose $\psi \in D(A+S) \Rightarrow \psi \in D(A) \subset D(S)$.
Since A is closed, and D' is its core,
$\exists$ sequence $\psi_n \in D'$ s.t. $\psi_n \to \psi$ and $A\psi_n \to A\psi$. Then $\forall n$: $\psi - \psi_n \in D(A)$ and

$$\|S(\psi-\psi_n)\| \le \varepsilon\|A\psi - A\psi_n\| + C\|\psi-\psi_n\| \to 0, \text{ when } n\to\infty.$$

and thus $S\psi_n \to S\psi$.
Since $S'\psi_n = A\psi_n + S\psi_n$ $\forall n$,
we have also $S'\psi_n \to A\psi + S\psi$.
Since $\overline{S'}$ is closed, this implies (by (cc))
$\psi \in D(\overline{S'})$ and $\overline{S'}\psi = A\psi + S\psi = (A+S)\psi$.
therefore, $A+S \subset \overline{S'}$ and $\overline{S'} \subset A+S$
$\Rightarrow$ $\overline{S'} = A+S$ and we have proven that D' is a core of $A+S$ $\square$

<u>Remark:</u> For any A, S as in Thm. 10.2. (A self-adj. & S symm.)
It is sufficient to check that $(*)$ holds on some <u>core of A</u>. That is, if D' is a core of A, $D(A) \subset D(S)$ and $\exists \varepsilon, C \in \mathbb{R}$ s.t. $\forall \psi \in D'$

$$(**) \quad \|S\psi\| \le \varepsilon\|A\psi\| + C\|\psi\|,$$

then $(**)$ holds for all $\psi \in D(A)$.

To see this, note that since A is closed,
for any $\psi \in D(A) \Rightarrow \exists \psi_n \in D'$, $\psi_n \to \psi$, $A\psi_n \to A\psi$.
Thus $\|S\psi_n\| \le \varepsilon\|A\psi_n\| + C\|\psi_n\|$ $\forall n$

$$\xrightarrow{n\to\infty} \varepsilon\|A\psi\| + C\|\psi\|$$

Also $\forall \phi \in D(S)$: $(\phi, S\psi_n) = (S\phi, \psi_n)$
$\xrightarrow{n\to\infty} (S\phi, \psi) = (\phi, S\psi)$ since $\psi \in D(S)$.
Since $D(S)$ is dense and $(\|S\psi_n\|)_n$ is bounded
$\Rightarrow$ $\forall \phi \in \mathcal{H}$: $(\phi, S\psi_n) \to (\phi, S\psi)$. [exercise]
$\Rightarrow$ $(S\psi, S\psi_n) \to \|S\psi\|^2$

$$\Rightarrow 0 \le \|S\psi - S\psi_n\|^2 = \|S\psi\|^2 + \|S\psi_n\|^2 - 2\,\mathrm{Re}(S\psi, S\psi_n)$$
$$\le \|S\psi\|^2 - 2\,\mathrm{Re}(S\psi, S\psi_n) + (\varepsilon\|A\psi_n\| + C\|\psi_n\|)^2$$
$$\xrightarrow{n\to\infty} \|S\psi\|^2 - 2\|S\psi\|^2 + (\varepsilon\|A\psi\| + C\|\psi\|)^2$$
$$\Rightarrow \|S\psi\| \le \varepsilon\|A\psi\| + C\|\psi\| \quad \square$$

10.3. Proposition Suppose $d \leq 3$ and $\mathcal{H} = L^2(\mathbb{R}^d)$. Then for all $\varepsilon > 0$ there is $C_\varepsilon \geq 0$ s.t.

$$\|\psi\|_\infty \leq \varepsilon \|H_0 \psi\| + C_\varepsilon \|\psi\| \quad \forall \psi \in D(H_0)$$

where $H_0 = -\frac{1}{2}\nabla^2$ = free Hamiltonian.

Proof. Exercise. □

The following theorem now covers most one-particle potentials which do not grow at infinity.

10.4. Theorem Suppose $d \leq 3$, and

$V_1 \in L^\infty(\mathbb{R}^d)$, $V_2 \in L^2(\mathbb{R}^d)$ are such that $V = V_1 + V_2$ is real-valued.
Then $H = H_0 + V = -\frac{1}{2}\nabla^2 + M_V$ is self-adjoint on $D(-\nabla^2)$ and essentially self-adjoint on $\mathcal{S}$. (and on $\mathcal{D}$)

Proof. Since V is real, M_V is self-adjoint with $D(M_V) = \{V\psi \in L^2\}$.
If $\psi \in L^2$ is such that $\|\psi\|_\infty < \infty$ then

$$\int dx\, |V_1(x)\psi(x)|^2 \leq \|V_1\|_\infty^2 \|\psi\|^2,$$
$$\int dx\, |V_2(x)\psi(x)|^2 \leq \|\psi\|_\infty^2 \|V_2\|_{L^2}^2.$$
$$\Rightarrow V\psi = V_1\psi + V_2\psi \in L^2 \text{ and}$$
$$\|V\psi\| \leq \|V_1\|_\infty \|\psi\| + \|\psi\|_\infty \|V_2\|.$$

By proposition 10.3., if $\psi \in D(H_0)$, then $\|\psi\|_\infty < \infty$. Therefore $D(H_0) \subset D(M_V)$.
In addition, $\forall \varepsilon > 0\ \exists C_\varepsilon \geq 0$ s.t. $\forall \psi \in D(H_0)$

$$\|M_V\psi\| \leq \|V_1\|_\infty \|\psi\| + \|V_2\|_{L^2} (\varepsilon \|H_0\psi\| + C_\varepsilon \|\psi\|)$$
$$= \|V_2\|_{L^2}\, \varepsilon\, \|H_0\psi\| + (\|V_1\|_\infty + C_\varepsilon \|V_2\|_{L^2}) \|\psi\|.$$

This proves that M_V is H_0-bounded with a relative bound 0. In particular, since H_0 and M_V are self-adjoint, we can apply the Kato-Rellich Theorem.

$\Rightarrow$ $H_0 + M_V$ is self-adjoint on $D(H_0) = D(-\Delta) = D(-\nabla^2)$. Since $\mathcal{S}_d$ is a core of $-\nabla^2$ (Properties 6.6.4.), $H_0 + M_V$ is essentially self-adj. on $\mathcal{S}$. $\square$

10.5. Remark Other application of the Kato-Rellich Theorem is to show that the atomic Hamiltonians are self-adjoint on $D(-\Delta)$,

$$\Leftrightarrow \quad H = -\sum_{i=1}^{N} \frac{1}{2} \nabla_{\bar{x}_i}^2 - \sum_{i=1}^{N} \frac{Ze^2}{|\bar{x}_i|} + \sum_{i<j=1}^{N} \frac{e^2}{|\bar{x}_i - \bar{x}_j|}$$

10.6. Remark: The domain is important when looking for eigenvectors of H: $\psi_0 \in \mathcal{H}$ is an eigenvector, if $\psi_0 \in D(H)$ and $\exists \lambda_0 \in \mathbb{C}$ s.t.

$$H\psi_0 = \lambda_0 \psi_0.$$

Their importance lies in the fact that they lead to bound states of the time-evolution:

$$\psi(t) := e^{-itH}\psi_0 = e^{-it\lambda}\psi_0.$$

Since H is self-adj. $\Rightarrow \lambda \in \mathbb{R}$

$\Rightarrow$

$$|\psi(x,t)|^2 = |\psi_0(x)|^2 \quad \forall x, t$$

10.5. Theorem: Suppose $V \in L^1_{loc}(\mathbb{R}^d)$ and there is $M \in \mathbb{R}$ s.t. $V(x) \geq -M$ for Lebesgue a.e. $x \in \mathbb{R}^d$. Let $D(H)$ collect all $\psi \in L^2(\mathbb{R}^d)$ for which $V\psi \in L^1_{loc}(\mathbb{R}^d)$ and $\exists \varphi_\psi \in L^2(\mathbb{R}^d)$ s.t.

$$(f, \varphi_\psi) = (-\tfrac{1}{2}\Delta f, \psi) + \int dx\, f(x)^* (V\psi)(x) \quad \forall f \in \mathcal{D}(\mathbb{R}^d).$$

Then φ_ψ is unique, and setting $H\psi := \varphi_\psi$ for $\psi \in D(H)$ defines a self-adjoint operator on $L^2(\mathbb{R}^d)$.

Proof: Uses quadratic forms, see Reed & Simon: book II, Theorem X.32. $\square$

* For instance, if $V \in C(\mathbb{R}^d)$ and $\inf V \geq -M$, then $\mathcal{D}_d \subset D(H)$ but it can happen that $S_d \not\subset D(H)$: If $\psi \in S_d$ and $\varphi_\psi(x) := -\frac{1}{2}\Delta\psi(x) + V(x)\psi(x)$, then $V\psi \in L^1_{loc}$ and for any $f \in \mathcal{D}$ we have $f^*\varphi_\psi \in L^1$ with $\int dx\, f(x)^* \varphi_\psi(x) = (f, -\frac{1}{2}\Delta\psi) + \int dx\, f^* V\psi$

$= (-\frac{1}{2}\Delta f, \psi) + \int dx\, f^* V\psi.$

Thus if $\psi \in \mathcal{D}_d$ also $\int dx\, |V\psi|^2 \leq \max_{x \in K} |V(x)\psi(x)|^2 \cdot |K| < \infty$, $K = \operatorname{supp}\psi$.

$\Rightarrow \varphi_\psi \in L^2$ and hence $\psi \in D(H)$.

But if V increases too fast at ∞, for instance, exponentially, then $\exists \psi \in S_d$ s.t. $\varphi_\psi \notin L^2$.

* As is usual in quantum mechanics, the "direction" of the potential is important, i.e., the cases "$V \geq -M$" and "$V \leq +M$" can behave very differently.

E.g., if $d = 1$ and $V(x) := x^4 \geq 0$, we have

a) $H_0 + V$ is essentially self-adjoint on $\mathcal{D} := C_c^\infty(\mathbb{R})$.

b) $H_0 - V$ is symmetric but <u>not</u> essentially self-adjoint on $\mathcal{D}$. (See Hall, sec. 9.10.)