8 Self-adjoint operators

Definition 17. A densely-defined operator H is said to be *self-adjoint*, if $H = H^*$ (i.e. $\mathrm{Dom}(H) = \mathrm{Dom}(H^*)$).

A self-adjoint operator is symmetric. But a symmetric H may fail to be self-adjoint due to the domain of its adjoint H^* being too large to satisfy the symmetry condition (7.5).

If we take some symmetric $\tilde{H}$ with larger domain than H, then $\tilde{H}^*$ would be a restriction of H^*. We want to achieve

$$H \subset \tilde{H} = \tilde{H}^* \subset H^*,$$

in which case, $\tilde{H}$ would be a *self-adjoint extension* of H. The basic questions are *existence* and *uniqueness* of self-adjoint extensions.

Proposition 8.1. *Let H be a symmetric operator. The following are equivalent.*

1. *H is self-adjoint.*
2. *H is closed and $\ker(H^* \mp i) = 0$.*
3. *$\mathrm{Ran}(H \pm i) = \mathcal{H}$.*

Proof. ((1) $\Rightarrow$ (2).) A self-adjoint $H = H^*$ is closed (Prop. 7.4). Since $H^* = H$ is symmetric, it cannot have $\pm i$ eigenvalues (Exercise 7.3).

((2) $\Rightarrow$ (3).) Suppose H is closed and H^* has no $\pm i$-eigenvalue. By Lemma 7.2,

$$0 = \ker(H^* \mp i) = \mathrm{Range}(H \pm i)^\perp,$$

so $H \pm i$ has dense range.

Let $\xi \in \mathcal{H}$, so by the above density property, ξ can be written as a limit $\xi = \lim_{n\to\infty}(H \pm i)\psi_n$ for some sequence $\psi_n \in \mathrm{Dom}(H)$. Because of the general identity, valid for symmetric H,

$$\begin{aligned} ||(H \pm i)\psi||^2 &= ||H\psi||^2 + \langle H\psi| \pm i\psi\rangle + \langle \pm i\psi|H\psi\rangle + ||\psi||^2 \\ &= ||H\psi||^2 + ||\psi||^2, \qquad \forall\, \psi \in \mathrm{Dom}(H), \end{aligned} \tag{8.1}$$

we deduce that both sequences ψ_n and $H\psi_n$ converge. In other words, $(\psi_n, H\psi_n)$ converges in $\mathcal{H} \oplus \mathcal{H}$. Because H is closed,

$$\lim_{n\to\infty} \psi_n \in \mathrm{Dom}(H), \quad \text{with} \quad H(\lim_{n\to\infty} \psi_n) = \lim_{n\to\infty} H\psi_n.$$

Therefore,

$$\xi = \lim_{n\to\infty} (H \pm i)\psi_n = (H \pm i)(\lim_{n\to\infty} \psi_n) \in \mathrm{Range}(H \pm i).$$

As $\xi \in \mathcal{H}$ was arbitrary, this shows that $\mathrm{Ran}(H \pm i)$ is all of $\mathcal{H}$.

((3) $\Rightarrow$ (1).) Finally, assume that $\mathrm{Range}(H \pm i) = \mathcal{H}$. So, given $\varphi \in \mathrm{Dom}(H^*)$, we can write $(H^* \mp i)\varphi = (H \mp i)\psi_\pm$ for some $\psi_\pm \in \mathrm{Dom}(H)$. As H is symmetric, $\mathrm{Dom}(H) \subset \mathrm{Dom}(H^*)$, we could also write

$$(H^* \mp i)(\varphi - \psi_\mp) = 0.$$

Thus

$$\varphi - \psi_\mp \in \ker(H^* \mp i) \overset{\text{Lemma 7.2}}{=} \mathrm{Range}(H \pm i)^\perp = \mathcal{H}^\perp = 0,$$

so $\varphi = \psi_\mp \in \mathrm{Dom}(H)$. As $\varphi \in \mathrm{Dom}(H^*)$ was arbitrary, we have shown that $\mathrm{Dom}(H^*) \subset \mathrm{Dom}(H)$. As H is symmetric, $\mathrm{Dom}(H) \subset \mathrm{Dom}(H^*)$, this means that $H = H^*$ holds. □

Since self-adjoint operators are closed, when searching for self-adjoint extensions, it is enough to look amongst the *closed* symmetric extensions. The smallest candidate for a closed symmetric extension is the closure.

Lemma 8.2. *A symmetric operator is closable, and its closure is symmetric.*

Proof. Let H be symmetric. By definition, $\mathrm{Dom}(H)$ is dense. As $\mathrm{Dom}(H^*)$ is at least as large $\mathrm{Dom}(H)$, it is also dense. Then Prop. 7.4 guarantees that H is closable. The second statement is left as an exercise. □

Definition 18. A symmetric operator H is *essentially self-adjoint*, if $\overline{H}$ is self-adjoint.

Lemma 8.3. *A symmetric operator H is essentially self-adjoint iff H^* is self-adjoint iff $H^* = \overline{H}$. In this case, H has a unique self-adjoint extension, namely, $\overline{H}$.*

Proof. Let H be symmetric. It is closable by Lemma 8.2, and $\overline{H} = H^{**}$ holds (Prop. 7.4). The essential self-adjointness condition, $\overline{H} = \overline{H}^*$, occurs iff

$$H^{**} = \overline{H} = \overline{H}^* = H^{***} = \overline{H^*} = H^*,$$

iff H^* is self-adjoint, iff $\overline{H} = H^*$.

Let H be essentially self-adjoint, so that $\overline{H} = H^*$. Let T be some other self-adjoint extension of H. In particular, T is a closed extension of H, so

$$T \supset \overline{H}.$$

But T is also self-adjoint, so

$$T = T^* \overset{(7.2)}{\subset} \overline{H}^* = \overline{H}$$

as well. Thus we must have equality, $T = \overline{H} \quad (= H^*)$. □

Usually, H is initially defined on a nice domain $\mathrm{Dom}(H)$ for which the symmetric condition is easily checked. Provided H is known to be essentially self-adjoint on this initial domain, we can simply refer to Lemma 8.3 and work with $\overline{H}$ when we want to utilize the theory of self-adjoint operators. Unfortunately, essential self-adjointness is generally difficult to prove, and often false. Here are some reformulations of essential self-adjointness, based on similar arguments to Prop. 8.1:

Proposition 8.4. *A symmetric operator H is essentially self-adjoint iff* $\ker(H^* \mp i) = 0$ *iff* $\mathrm{Ran}(H \pm i)$ *is dense.*

Proof. Exercise. □

8.1 Self-adjoint position and momentum operators

For an open subset Ω of $\mathbb{R}^d$, we write $C_c^\infty(\Omega)$ for the space of smooth functions $\Omega \to \mathbb{C}$ with compact support. We have

$$C_c^\infty(\mathbb{R}^d) \subset \mathscr{S}(\mathbb{R}^d) \subset L^p(\mathbb{R}^d),$$

and a standard fact is that $C_c^\infty(\mathbb{R}^d)$ is dense in $L^p(\mathbb{R}^d)$, $1 \leq p \leq \infty$.

Definition 19. On $L^2(\mathbb{R})$ (with Lebesgue measure), the *position operator* is

$$\begin{aligned}\mathrm{Dom}(\hat{x}) &= \left\{\psi \in L^2(\mathbb{R}) \,:\, \int_{\mathbb{R}} |x\psi(x)|^2 < \infty\right\}\\ (\hat{x}\psi)(x) &= x\psi(x).\end{aligned}$$

The *momentum operator* is

$$\begin{aligned}\mathrm{Dom}(\hat{p}) &= H^1(\mathbb{R}) \equiv \left\{\psi \in L^2(\mathbb{R}) \,:\, \psi' \in L^2(\mathbb{R})\right\}\\ \hat{p}\psi &= -i\psi',\end{aligned} \tag{8.2}$$

where ψ' means the *weak derivative*.

Remark. Let Ω be an open subset of $\mathbb{R}$. We recall that a locally integrable function $f \in L^1_{\mathrm{loc}}(\Omega)$ has *weak derivative* $f' \in L^1_{\mathrm{loc}}(\Omega)$ if the following holds for all $g \in C_c^\infty(\Omega)$,

$$\int_{\mathbb{R}} f'g = -\int_{\mathbb{R}} f\frac{dg}{dx}.$$

Above, $g \in C_c^\infty(\Omega)$ has an ordinary derivative $\frac{dg}{dx}$. If f is smooth, then f' is its usual derivative $\frac{df}{dx}$. But, for example, the function $f : x \mapsto |x|$ has weak derivative f' being the sign function.

It is conventional to regard weak derivatives as almost-everywhere-equal equivalence classes of functions (so a weak derivative is unique when it exists). The domain $H^1(\mathbb{R})$ of the momentum operator (Eq. (8.2)) is then a subspace of $L^2(\mathbb{R})$. It is an example of a *Sobolev space* — it is actually a Hilbert space when equipped with the inner product

$$\langle\varphi|\psi\rangle_{H^1(\mathbb{R})} = \langle\varphi|\psi\rangle_{L^2(\mathbb{R})} + \langle\varphi'|\psi'\rangle_{L^2(\mathbb{R})}.$$

Another Sobolev space is

$$H^2(\mathbb{R}) = \{\psi \in L^2(\mathbb{R}) \,:\, \psi', \psi'' \in L^2(\mathbb{R})\}. \tag{8.3}$$

Here, we would also add a term $\langle\varphi''|\psi''\rangle_{L^2(\mathbb{R})}$ to get an inner product on $H^2(\mathbb{R})$.

Theorem 8.5. *The position operator $\hat{x}$ and the momentum operator $\hat{p}$ are self-adjoint. Both operators are essentially self-adjoint when restricted to either $C_c^\infty(\mathbb{R})$ or $\mathscr{S}(\mathbb{R})$.*

Proof. Certainly $\hat{x}$ is densely-defined (its domain contains $\mathscr{S}(\mathbb{R})$), and symmetric. By definition,

$$\varphi \in \mathrm{Dom}(\hat{x}^*) \;\Leftrightarrow\; \exists \eta \in L^2(\mathbb{R}) \,:\, \int_{\mathbb{R}} \big(\overline{\varphi(x)}x - \overline{\eta(x)}\big)\psi(x)\,dx = 0 \quad \forall \psi \in \mathrm{Dom}(\hat{x}).$$

As $\mathrm{Dom}(\hat{x})$ is dense, φ lies in the above space iff $x\varphi(x) = \eta(x)$ holds for almost every $x \in \mathbb{R}$, i.e., φ remains square-integrable after applying multiplication-by-x. Thus,

$$\mathrm{Dom}(\hat{x}^*) = \left\{ \varphi \in L^2 \,:\, \int_{\mathbb{R}} |x\varphi(x)|^2 < \infty \right\},$$

which is the same as $\mathrm{Dom}(\hat{x})$, so $\hat{x}$ is self-adjoint.

The restrictions $\hat{x}|_{C_c^\infty(\mathbb{R})}$ or $\hat{x}|_{\mathscr{S}(\mathbb{R})}$ are symmetric, and the same argument as above shows that in each case, their adjoint is the operator $\hat{x}^* = \hat{x}$, which is self-adjoint. By Lemma 8.3, $\hat{x}|_{C_c^\infty(\mathbb{R})}$ and $\hat{x}|_{\mathscr{S}(\mathbb{R})}$ are essentially self-adjoint.

As for $\hat{p}$, let us first consider

$$\hat{p}|_{C_c^\infty(\mathbb{R})},$$

which is easily seen to be symmetric using integration-by-parts. By definition, $\varphi \in \mathrm{Dom}((\hat{p}|_{C_c^\infty(\mathbb{R})})^*)$ iff there exists $\eta \in L^2(\mathbb{R})$ such that

$$\int_{\mathbb{R}} \overline{\eta} \cdot \psi = -i \int_{\mathbb{R}} \overline{\varphi} \frac{d\psi}{dx}, \qquad \forall \psi \in C_c^\infty(\mathbb{R}).$$

This is precisely the statement that φ admits an L^2 weak derivative, η. Thus

$$(\hat{p}|_{C_c^\infty(\mathbb{R})})^* = \hat{p}.$$

Therefore,

$$\ker((\hat{p}|_{C_c^\infty(\mathbb{R})})^* \pm i) = \ker(\hat{p} \pm i) = \{\varphi \in \mathrm{Dom}(\hat{p}) \,:\, -i\varphi' \pm i\varphi = 0\}.$$

The (weak) differential equation $-\varphi' \pm \varphi = 0$ would be solved by $\varphi(x) = e^{\pm x}\cdot$constant, but these solutions do not lie in $\mathrm{Dom}(\hat{p})$ as they are not square-integrable. So $\ker((\hat{p}|_{C_c^\infty(\mathbb{R})})^* \pm i) = 0$. By Prop. 8.4 and Lemma 8.3, $\hat{p}|_{C_c^\infty(\mathbb{R})}$ is essentially self-adjoint, and $\hat{p}$ is its self-adjoint closure.

Similarly,

$$\hat{p}|_{\mathscr{S}(\mathbb{R})}$$

is symmetric, and it follows from

$$\hat{p}|_{C_c^\infty(\mathbb{R})} \subset \hat{p}|_{\mathscr{S}(\mathbb{R})} \subset \hat{p} = (\hat{p}|_{C_c^\infty(\mathbb{R})})^*$$

that $(\hat{p}|_{\mathscr{S}(\mathbb{R})})^* = \hat{p}$ as well. By Lemma 8.3, $\hat{p}|_{\mathscr{S}(\mathbb{R})}$ is essentially self-adjoint. □

8.2 Reality of spectrum

Here is the first important property of self-adjoint operators.

Proposition 8.6. *Let H be a self-adjoint operator. Then $\sigma(H) \subset \mathbb{R}$.*

Proof. We will show that $\mathbb{C} \setminus \mathbb{R} \subset \rho(H)$, which is equivalent to $\sigma(H) \subset \mathbb{R}$. Let $\lambda = a + ib \in \mathbb{C} \setminus \mathbb{R}$, so $b \neq 0$.

- $\mathrm{Ran}(H - \bar{\lambda})$ is a closed subspace of $\mathcal{H}$, by the following argument. Suppose $(H - \bar{\lambda})\psi_n$ is a sequence in $\mathrm{Ran}(H - \bar{\lambda})$ which converges in $\mathcal{H}$. As H is symmetric, the inequality

$$\begin{aligned} ||(H - \bar{\lambda})\psi||^2 &= ||(H - a)\psi||^2 - ib\langle\psi|(H - a)\psi\rangle + ib\langle(H - a)\psi|\psi\rangle + b^2||\psi||^2 \\ &\geq b^2||\psi||^2, \end{aligned} \tag{8.4}$$

  is valid for all $\psi \in \mathrm{Dom}(H)$. Applying (8.4) to $\psi_n \in \mathrm{Dom}(H)$, we see that convergence of $(H - \bar{\lambda})\psi_n$ implies that ψ_n is Cauchy, thus convergent to some $\psi \in \mathcal{H}$. Since H is closed, $\lim \psi_n \in \mathrm{Dom}(H)$ and $\lim((H - \bar{\lambda})\psi_n) = (H - \bar{\lambda})(\lim \psi_n)$ lies in $\mathrm{Ran}(H - \bar{\lambda})$.

  Thus,

$$\begin{aligned} \text{For } \lambda \in \mathbb{C} \setminus \mathbb{R}, \qquad & H - \bar{\lambda} \text{ surjective iff } \mathrm{Ran}(H - \bar{\lambda}) \text{ dense} \\ & \text{iff } \ker(H^* - \lambda) = 0. \quad \text{(Lemma7.2)} \end{aligned} \tag{8.5}$$

- For $\lambda \in \mathbb{C} \setminus \mathbb{R}$, injectivity of $H - \bar{\lambda}$ is automatic, since H is symmetric and can only have real eigenvalues (Exercise 7.3).

- From the above two arguments, we deduce that

$$\text{For } \lambda \in \mathbb{C} \setminus \mathbb{R}, \qquad \bar{\lambda} \in \rho(H) \text{ iff } \ker(H^* - \lambda) = 0. \tag{8.6}$$

Self-adjointness enters here: $H^* = H$ is symmetric, so the right side of (8.6) holds (for $\lambda \in \mathbb{C} \setminus \mathbb{R}$). □

If H is merely a closed symmetric operator, the proof in Prop. 8.6 only works up to (8.6). Indeed, we know from Prop. 8.1 that H^* has imaginary eigenvalues when self-adjointness of H fails. In fact, the spectral situation is even worse.

Theorem 8.7. *Let H be a closed symmetric operator. Then $\lambda \mapsto \dim\ker(H^* - \lambda)$ is constant on the open upper half-plane and the open lower-half plane. Consequently, $\sigma(H)$ is either the closed upper-half plane, closed lower-half plane, all of $\mathbb{C}$, or a (closed) subset of $\mathbb{R}$. The last case occurs iff H is self-adjoint.*

Proof. Let $\lambda = a + ib \in \mathbb{C} \setminus \mathbb{R}$.

- Consider a perturbation $\lambda + \eta$, with $|\eta|$ small enough to ensure that $\lambda + \eta$ remains in the same open half-plane as λ. We argue that

$$\ker(H^* - (\lambda + \eta)) \cap \ker(H^* - \lambda)^\perp = 0, \qquad \forall\, |\eta| \ll |b|. \tag{8.7}$$

  For this, we may assume that $\ker(H^* - (\lambda + \eta)) \neq 0$, and pick some unit vector $\varphi \in \ker(H^* - (\lambda + \eta))$. Suppose, for a contradiction, that $\varphi \in \ker(H^* - \lambda)^\perp$ as well. By Eq. (8.5), there exists $\psi \in \mathrm{Dom}(H)$ such that $\varphi = (H - \overline{\lambda})\psi$. So

$$0 = \langle (\underbrace{H^* - (\lambda + \eta))\varphi}_{0} \,|\psi\rangle = \langle\varphi|\, \underbrace{(H - \overline{\lambda})\psi}_{\varphi}\rangle - \overline{\eta}\langle\varphi|\psi\rangle = \underbrace{||\varphi||^2}_{1} - \overline{\eta}\langle\varphi|\psi\rangle. \tag{8.8}$$

  By Eq. (8.4), we also have

$$||\psi|| \leq \frac{1}{|b|}||(H - \overline{\lambda})\psi|| = \frac{1}{|b|}||\varphi|| = \frac{1}{|b|}.$$

  So when $|\eta| \ll |b|$, we have $||\psi|| \ll \frac{1}{|\eta|}$, and it becomes impossible for the right-side of Eq. (8.8) to vanish (Cauchy–Schwarz).

- Eq. (8.7) implies (Exercise) that

$$\dim\ker(H^* - (\lambda + \eta)) \leq \dim\ker(H^* - \lambda). \qquad \text{(small } \eta\text{)}$$

  By swapping the roles of $\lambda + \eta$ and λ, to get the reverse inequality, we deduce that $\dim\ker(H^* - \lambda)$ is locally constant as λ is varied in the upper/lower half-plane. By connectedness, $\lambda \mapsto \dim\ker(H^* - \lambda)$ is constant on the entire open upper/lower half-planes.

- Putting this last result into (8.6), we learn that the whole upper/lower half plane lies in either $\rho(H)$ or $\sigma(H)$, depending on whether $\ker(H^* \mp i) = 0$ or not. Since $\sigma(H)$ is closed, it can only be one of the four options stated in the Theorem. Furthermore, the fourth option, $\sigma(H) \subset \mathbb{R}$, occurs iff $\ker(H^* \mp i) = 0$, iff H is self-adjoint, by Prop. 8.1.

□

Theorem 8.7 shows why symmetric but non-self-adjoint operators are bad for spectral theory. The next result shows that, furthermore, the real spectrum of a self-adjoint operator is very well-behaved.

Theorem 8.8. *Let $H = H^*$ be a self-adjoint operator. Then $\sigma(H) = \sigma_{\mathrm{ap}}(H)$.*

Proof. Let $\lambda \notin \sigma_{\mathrm{ap}}(H)$.

In particular, λ is not an eigenvalue of H, so $H - \lambda$ is injective. We shall show that $H - \lambda$ is surjective, then $\lambda \in \rho(H)$, and therefore,

$$\sigma(H) = \mathbb{C} \setminus \rho(H) \subseteq \sigma_{\mathrm{ap}}(H) \subseteq \sigma(H),$$

so equality holds.

To show that $H - \lambda$ is surjective, we first check that it has dense range. Suppose otherwise, that there exists a non-zero $\varphi \in \mathrm{Ran}(H - \lambda)^{\perp}$. Then

$$0 = \langle \varphi | (H - \lambda)\psi \rangle = \langle (H^* - \bar{\lambda})\varphi | \psi \rangle, \qquad \forall \psi \in \mathrm{Dom}(H),$$

which means that $\varphi \in \mathrm{Dom}(H^* - \bar{\lambda}) = \mathrm{Dom}(H - \bar{\lambda})$, with $0 = (H^* - \bar{\lambda})\varphi = (H - \bar{\lambda})\varphi$. Thus $\bar{\lambda} \in \sigma_{\mathrm{p}}(H)$. As H is symmetric, we have $\lambda = \bar{\lambda} \in \sigma_{\mathrm{p}}(H) \subset \sigma_{\mathrm{ap}}(H)$, which contradicts the initial assumption $\lambda \notin \sigma_{\mathrm{ap}}(H)$.

So we know that $H - \lambda$ has dense range. The argument that it is surjective is similar to that in Prop. 6.3. For any $\psi \in \mathcal{H}$, we can find a sequence ψ_n in $\mathrm{Dom}(H) = \mathrm{Dom}(H - \lambda)$ such that $(H - \lambda)\psi_n \to \psi$. Also, $\lambda \notin \sigma_{\mathrm{ap}}(H)$ means that $H - \lambda$ is bounded below by some $\alpha > 0$. Thus

$$||\psi_n - \psi_m|| \leq \alpha^{-1} ||(H - \lambda)\psi_n - (H - \lambda)\psi_m|| \to 0.$$

So $\{\psi_n\}$ is Cauchy, and converges to some $\tilde{\psi} \in \mathcal{H}$. As $(H - \lambda)$ is a closed operator, $\tilde{\psi} \in \mathrm{Dom}(H - \lambda)$ and $(H - \lambda)\tilde{\psi} = \psi$. This verifies that $H - \lambda$ is surjective. □

Exercise 8.1. Does the self-adjoint position operator $\hat{x}$ (Definition 19) have any eigenvalues? Compute its spectrum, and check that each spectral value is an approximate eigenvalue.

Exercise 8.2. Give an example of an operator on some $\mathbb{C}^N$ which has eigenvalues lying within $\mathbb{R}$, but whose eigenspaces do not sum up to the identity operator.

8.3 Self-adjoint extensions

Let us give names to the obstructions to (essential) self-adjointness provided in Prop. 8.1–8.4.

Definition 20. Let H be a symmetric operator on $\mathcal{H}$. Its *deficiency subspaces* and *deficiency indices* are

$$\mathcal{H}_\pm := \ker(H^* \mp i), \qquad n_\pm := \dim \mathcal{H}_\pm \in \mathbb{N} \cup \{\infty\}.$$

There is a systematic classification and construction of self-adjoint extensions of (closed) symmetric operators H, due to von Neumann. It is summarized below, and we refer to Reed–Simon's textbook, Theorem X.2, for a proof.

1. A (closed) symmetric operator H admits self-adjoint extensions iff its deficiency indices n_+, n_- are equal.

2. In case H has equal deficiency indices, its self-adjoint extensions are parametrized by unitary maps $U : \mathcal{H}_+ \to \mathcal{H}_-$,

$$\begin{aligned} \mathrm{Dom}(H_U) &:= \{\psi + \psi_+ + U\psi_+ \,:\, \psi \in \mathrm{Dom}(H),\ \psi_+ \in \mathcal{H}_+\}\,, \\ H_U(\psi + \psi_+ + U\psi_+) &:= H\psi + i\psi_+ - iU\psi_+. \end{aligned}$$

Example 8.1. [Anomalous momentum on half-line] Recall our informal discussion of the problematic "momentum operator" $P = -i\frac{d}{dx}$ on the half-line $\mathbb{R}_+ = [0, \infty)$. It is symmetric on the initial domain,

$$\mathrm{Dom}(P) = C_c^\infty(0, \infty),$$

because of the Dirichlet condition at $x = 0$. Let us compute P^*. We have

$$\begin{aligned} \mathrm{Dom}(P^*) &= \left\{ \varphi \in L^2(\mathbb{R}_+) \,:\, \exists \eta \in L^2(\mathbb{R}_+) \text{ with } \int_0^\infty \overline{\eta}\psi = \int_0^\infty \overline{\varphi}\left(-i\tfrac{d\psi}{dx}\right) \ \ \forall \psi \in C_c^\infty(0,\infty) \right\} \\ &= \left\{ \varphi \in L^2(\mathbb{R}_+) \,:\, \varphi' \in L^2(\mathbb{R}_+) \right\}, \end{aligned} \tag{8.9}$$

with $P^*\varphi = -i\varphi'$ (weak derivative). The deficiency subspaces are

$$\mathcal{H}_+ = \mathrm{span}_{\mathbb{C}}\{e^{-x}\}, \qquad \mathcal{H}_- = \{0\}.$$

Since $n_+ \neq 0$, we know from Prop. 8.4 that P is not essentially self-adjoint. In fact, by von Neumann's theory, P does not admit *any* self-adjoint extensions at all.

The last claim can also be understood more explicitly, as follows. First, for the closure $\overline{P} = P^{**}$, we have

$$\mathrm{Dom}(\overline{P}) = \left\{ \xi \in L^2(\mathbb{R}_+) \,:\, \exists \eta \in L^2(\mathbb{R}_+) \text{ with } \int_0^\infty \overline{\eta}\varphi \stackrel{*}{=} \int_0^\infty \overline{\xi}(-i\varphi') \;\; \forall \varphi \in \mathrm{Dom}(P^*) \right\}.$$

Taking $\varphi \in C_c^\infty(0,\infty)$ in $(*)$ above shows that $\xi \in \mathrm{Dom}(\overline{P})$ has L^2 weak derivative, with $\overline{P}\xi = -i\xi'$. But ξ also satisfies $(*)$ for general $\varphi \in \mathrm{Dom}(P^*)$. Recalling from (8.9) that $\varphi \in \mathrm{Dom}(P^*)$ have L^2 weak derivatives, we are in a situation where ξ, φ are both locally absolutely continuous (see, e.g., 10.9 of Ziemer's Modern Real Analysis). We may then integrate by parts,

$$\begin{aligned} \langle \xi | P^* \varphi \rangle &= \int_0^\infty \overline{\xi}(-i\varphi') \\ &= i\overline{\xi}(0)\varphi(0) + \underbrace{i\int_0^\infty \overline{\xi'}\varphi}_{\langle \overline{P}\xi | \varphi \rangle} \qquad \xi \in \mathrm{Dom}(\overline{P}), \varphi \in \mathrm{Dom}(P^*). \end{aligned} \tag{8.10}$$

Since the boundary value $\varphi(0)$ is arbitrary, it follows that $\xi(0) = 0$. To summarize,

$$\mathrm{Dom}(\overline{P}) = \left\{ \xi \in L^2(\mathbb{R}_+) \,:\, \xi' \in L^2(\mathbb{R}_+),\ \xi(0) = 0 \right\}.$$

Now consider some extension $\tilde{P}$ with $\mathrm{Dom}(\tilde{P})$ lying between $\mathrm{Dom}(\overline{P})$ and $\mathrm{Dom}(P^*)$. The integration-by-parts calculation will lead, in particular, to

$$\langle \xi | \tilde{P}\xi \rangle = i|\xi(0)|^2 + \langle \tilde{P}\xi | \xi \rangle, \qquad \xi \in \mathrm{Dom}(\tilde{P}).$$

In order for $\tilde{P}$ to be self-adjoint, it must at least be symmetric, then the above equation says that $\xi(0) = 0$ must be enforced. But this just makes $\mathrm{Dom}(\tilde{P}) = \mathrm{Dom}(\overline{P})$, and we had already seen that $\overline{P}$ is not self-adjoint. We conclude that P does not admit any self-adjoint extension.

Exercise 8.3. Let us return to the problem of defining a self-adjoint momentum operator on the interval $[0, 2\pi]$. The initial domain is $\mathrm{Dom}(P) = C_c^\infty(0, 2\pi)$, on which $P = -i\frac{d}{dx}$ is symmetric. The adjoint P^* is the weak (or almost-everywhere) derivative operator on the domain

$$\mathrm{Dom}(P^*) = \mathrm{AC}[0, 2\pi].$$

- What are the eigenfunctions of P? Do they span all of $L^2[0, 2\pi]$?
- Compute the deficiency indices of P, and deduce that P is not essentially self-adjoint.
- What is the domain of $\overline{P}$?
- Check that for each $\alpha \in \mathrm{U}(1)$,
$$\begin{aligned} \mathrm{Dom}(P_\alpha) &= \{\psi \in \mathrm{AC}[0, 2\pi] \,:\, \psi(2\pi) = \alpha\psi(0)\}, \\ P_\alpha &= P^*|_{\mathrm{Dom}(P_\alpha)}, \end{aligned} \tag{8.11}$$
defines a self-adjoint extension of P.
- Are P_α and $P_{\alpha'}$ unitarily equivalent for distinct α, α'?

Definition 21. An surjective map $C : \mathcal{H} \to \mathcal{H}$ is *antiunitary* if
$$\langle C\varphi | C\psi \rangle = \langle \psi | \varphi \rangle, \qquad \forall \varphi, \psi \in \mathcal{H}.$$

There is an easy sufficient criterion for the existence of self-adjoint extensions.

Exercise 8.4. Let H be a symmetric operator. Suppose there exists an antiunitary C with $C^2 = 1$, such that $C : \mathrm{Dom}(H) \to \mathrm{Dom}(H)$ and $CH = HC$. Deduce that H has equal deficiency indices (thus it admits self-adjoint extensions).

Example 8.2. For the operator $\tilde{p} = -i\frac{d}{dx}$ on $C_c^\infty(\mathbb{R})$, we can consider the conjugation
$$C\psi(x) = \overline{\psi(-x)}, \qquad \psi \in C_c^\infty(\mathbb{R}),$$
and apply Exercise 8.4 to deduce immediately that it admits self-adjoint extensions (the one described in Definition 19). However, this C does not work on $C_c^\infty(\mathbb{R}_+)$ (why?).

For a Hamiltonian of the form $H = -\nabla^2 + V$, where V is a *real*-valued potential, it is easy to see that it is symmetric on the initial domain $C_c^\infty(\mathbb{R}^d)$. If V does not grow too quickly, we can also use $\mathscr{S}(\mathbb{R}^d)$ as the initial domain.

The operators $H = -\nabla^2 + V$ are the non-magnetic Schrödinger operators. Clearly, the operation of pointwise complex-conjugation provides a C such that Exercise 8.4 applies. So $H = -\nabla^2 + V$ admits self-adjoint extensions. However, depending on the nature of V, it may not be *essentially* self-adjoint on the convenient domains $C_c^\infty(\mathbb{R}^d)$ or $\mathscr{S}(\mathbb{R}^d)$. The abstract criterion of Prop. 8.4 is, unfortunately, not easy to use generally, because it requires detailed knowledge of H^*.

8.4 Some sufficient criteria for (essential) self-adjointness

8.4.1 Nelson's criterion

Proposition 8.9. *Let H be a symmetric operator. If there is a Hilbert space basis comprising eigenvectors of H, then H is essentially self-adjoint.*

Proof. Let $\lambda_n, n \in \mathbb{N}$ be the (real) eigenvalues of H. (Counted with multiplicity; there are at most countably many, because $\mathcal{H}$ is separable and the eigenspaces with distinct eigenvalues are orthogonal). The assumption on H is basically the statement that it is unitarily equivalent to the (densely-defined, symmetric) diagonal multiplication T operator on $\ell^2(\mathbb{N})$,

$$\begin{aligned} \mathrm{Dom}(T) &\subset \{s \in \ell^2(\mathbb{N}) \,:\, \sum_{n\in\mathbb{N}} \lambda_n^2 |s_n|^2 < \infty\}, \\ (Ts)_n &= \lambda_n s_n. \end{aligned}$$

We leave it as an exercise to show that T is essentially self-adjoint (i.e., its closure is self-adjoint). □

Example 8.3. The initial domain for the harmonic oscillator Hamiltonian $H_{\mathrm{SHO}} = \frac{1}{2}(-\Delta + X^2)$ is $\mathrm{Dom}(H_{\mathrm{SHO}}) = \mathscr{S}(\mathbb{R})$. We had found that its eigenfunctions are generated from a Gaussian by applying the creation operator repeatedly. The resulting eigenfunctions may be checked to provide a Hilbert space basis. A proof of this basis property could be be given based on general properties of the Fourier transform[15]. Prop. 8.9 may then be applied to deduce that H_{SHO} is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$.

There are two major shortfalls of Prop. 8.9. First, it is extremely difficult to find the eigensystem of a general symmetric operator. Second, there are many essentially self-adjoint operators which do not have any eigenvectors at all. An interesting result of Nelson says that we can replace the eigenvector requirement with a much more general requirement of analyticity:

Definition 22. Let T be an (unbounded) operator on a Hilbert space. An *analytic vector* for T is an element

$$\psi \in \bigcap_{n\in\mathbb{N}} \mathrm{Dom}(T^n) \quad \text{such that} \quad \sum_{n\in\mathbb{N}} \frac{t^n \|T^n\psi\|}{n!} < \infty \ \text{ for some } t > 0.$$

[15] E.g., Chapter 3.6, Prop. 3.90 of Moretti's Spectral Theory and Quantum Mechanics textbook.

The power series

$$e^{itT}\psi \;=\; \sum_{n\in\mathbb{N}} \frac{(itT)^n\psi}{n!}. \tag{8.12}$$

makes sense on analytic vectors, and partially defines e^{itT}. If the analytic vectors for T are dense, we might hope that e^{itT} extends to a well-defined bounded operator on $\mathcal{H}$. We will return to this when studying Stone's Theorem later.

Theorem 8.10 (Nelson's criterion)**.** *A symmetric operator H is essentially self-adjoint if* $\mathrm{Dom}(H)$ *contains a dense set of analytic vectors for H.*

A proof can be found in Reed–Simon Theorem X.39. It uses the spectral theorem (specifically, Stone's theorem), which we have not even stated yet. Applications to quantum field theory can be found there.

Remark. A finite linear combination of analytic vectors is again analytic (check this). So in Theorem 8.10, it is enough to require that $\mathrm{Dom}(H)$ contains a set of analytic vectors for H, whose (algebraic) linear span is dense in $\mathcal{H}$.

An eigenvector of H is an example of an analytic vector for H. So if there is a Hilbert space basis comprising eigenvectors of H, we can apply Nelson's criterion, Theorem 8.10; this yields Prop. 8.9 as a special case.

Example 8.4. On $\psi \in L^1(\mathbb{R}^d)$, the Fourier transform is the function $\widehat{\psi} : \widehat{\mathbb{R}^d} \to \mathbb{C}$ given by

$$\widehat{\psi}(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}} e^{-ip\cdot x}\psi(x)\,dx, \qquad p \in \widehat{\mathbb{R}^d}.$$

Here, we wrote $\widehat{\mathbb{R}^d}$ to distinguish it from $\mathbb{R}^d$. The Fourier transform maps the subspace $\mathscr{S}(\mathbb{R}^d)$ onto $\mathscr{S}(\widehat{\mathbb{R}^d})$, and is in fact an isometry with respect to the L^2-norm. It extends by continuity to a (abstract!) unitary map $\mathscr{F} : L^2(\mathbb{R}^d) \to L^2(\widehat{\mathbb{R}^d})$. More details on the Fourier transform can be found in Chapter 3.6 of Moretti's Spectral Theory and Quantum Mechanics textbook, and Reed–Simon Chapter IX. We may use the Fourier transform to deduce essential self-adjointness of the Euclidean space Laplacian $-\Delta$ on various domains:

- For Schwartz functions, under the Fourier transform, the Laplacian $\Delta = \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2}$ becomes the (symmetric) multiplication operator by

the function $p \mapsto -|p|^2$. As an exercise, we may check that $|p|^2$, thus also $-\Delta$, is essentially self-adjoint on the Schwartz functions, using the criterion of Prop. 8.4.

- Let us argue that $-\Delta$ is already essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$. A preliminary claim is that the domain of the self-adjoint Laplacian, L, is the Sobolev space (cf. (8.3)),

$$\begin{aligned} H^2(\mathbb{R}^d) &= \mathscr{F}^{-1}\big\{\widehat{\psi} \in L^2(\widehat{\mathbb{R}^d}) \,:\, |p|^2 \cdot \widehat{\psi} \in L^2(\widehat{\mathbb{R}^d})\big\} \\ &= \{\psi \in L^2(\mathbb{R}^d) \,:\, L\psi \in L^2(\mathbb{R}^d)\}, \end{aligned}$$

on which L acts as the Laplacian in the sense of distributions (See Reed–Simon Chapter V.3, IX for generalities on distributions).

Recall that $-L\psi \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ means that

$$\int_{\mathbb{R}^d} \overline{(-L\psi)(x)}\varphi(x) = \int_{\mathbb{R}^d} \overline{\psi(x)}(-\Delta\varphi)(x), \qquad \forall\, \varphi \in C_c^\infty(\mathbb{R}^d) = \mathrm{Dom}(-\Delta).$$

In particular, for $\psi \in H^2(\mathbb{R}^d)$, i.e., $-L\psi \in L^2(\mathbb{R}^d)$, we have

$$\langle -L\psi | \varphi\rangle = \langle \psi | -\Delta\varphi\rangle, \qquad \forall\, \varphi \in \mathrm{Dom}(-\Delta),$$

which says that $(-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*\psi = -L\psi \in L^2(\mathbb{R}^d)$; so $H^2(\mathbb{R}^d) \subset \mathrm{Dom}((-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*)$. Conversely, if $\psi \in \mathrm{Dom}((-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*)$, then

$$\langle (-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*\psi | \varphi\rangle = \langle \psi | -\Delta\varphi\rangle, \qquad \forall\, \varphi \in C_c^\infty(\mathbb{R}^d),$$

which says that $(-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*\psi \in L^2(\mathbb{R}^d)$ equals $-L\psi$; so $\mathrm{Dom}((-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*) \subset H^2(\mathbb{R}^d)$. So

$$\mathrm{Dom}((-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*) = H^2(\mathbb{R}^d) = \mathrm{Dom}(-L).$$

Therefore, $(-\Delta|_{C_c^\infty(\mathbb{R}^d)})^*$ coincides with $-L$ on the domain $H^2(\mathbb{R}^d)$.

It is a standard result that Fourier transform still converts $-L$ to the operator of multiplication-by-$|p|^2$. But multiplication-by-$|p|^2$ is *self-adjoint* on $\mathscr{F}(H^2(\mathbb{R}^d)) = \big\{\widehat{\psi} \in L^2(\widehat{\mathbb{R}^d}) \,:\, |p|^2 \cdot \widehat{\psi} \in L^2(\widehat{\mathbb{R}^d})\big\}$. (Exercise.) Undoing the Fourier transform, $-L$ is self-adjoint on $H^2(\mathbb{R}^d)$.

We conclude that $-\Delta|_{C_c^\infty(\mathbb{R}^d)}$ is essentially self-adjoint (with closure being its adjoint operator, $-L$).

- Consider the domain $\mathscr{F}^{-1}(C_c^\infty(\widehat{\mathbb{R}^d}))$. This is contained in $\mathscr{S}(\mathbb{R}^d)$, but does not contain $C_c^\infty(\mathbb{R}^d)$, so we cannot use the previous results to infer essential self-adjointness on this domain. As an exercise, check that elements of $C_c^\infty(\widehat{\mathbb{R}^d})$ are analytic vectors for the multiplication-by-$(|p|^2)$ operator. Then essential self-adjointness follows from Nelson's criterion, Theorem 8.10. Consequently, $-\Delta$ is essentially self-adjoint on $\mathscr{F}^{-1}(C_c^\infty(\widehat{\mathbb{R}^d}))$.

8.4.2 Kato–Rellich

For Schrödinger operators $-\Delta + V$, if the potential function V is bounded, at least in a relative sense with respect to $-\Delta$, we could treat V as a kind of "perturbation" of $-\Delta$. Then perturbation arguments, generally called Kato–Rellich theorems, give us the desired (essential) self-adjointness result for $-\Delta + V$.

Definition 23. Let T be a densely-defined operator. An operator V is *T-bounded* if there exists $a, b \in [0, \infty)$ such that

$$\|V\varphi\| \leq a\|T\varphi\| + b\|\varphi\|, \qquad \forall\, \varphi \in \mathrm{Dom}(T). \tag{8.13}$$

(Implicitly, $\mathrm{Dom}(V) \supset \mathrm{Dom}(T)$ here.) In this case, the *relative bound* of V with respect to T is the infimum of those a such that (8.13) is attainable for some b.

If $V \in L^\infty(\mathbb{R}^d)$, it has relative bound 0 with respect to $-\Delta$. The relative-boundedness concept is important to handle certain *unbounded* potentials, as the following example of a Kato–Rellich theorem indicates. Note, however, that the next result does not apply to the harmonic oscillator potential V (which we handled by another method).

Theorem 8.11 (Kato–Rellich)**.** *Let T be a self-adjoint operator, and let V be a symmetric operator, which is T-bounded with relative bound < 1. Then*

- *$T + V$ is self-adjoint on* $\mathrm{Dom}(T)$*;*
- *$T+V$ is essentially self-adjoint on any domain of essential self-adjointness for T.*

Proof. Note that by definition, $\mathrm{Dom}(T+V) = \mathrm{Dom}(T) \cap \mathrm{Dom}(V) = \mathrm{Dom}(T)$.

- It suffices to show that there exists some $c > 0$ such that

$$\text{Range}(T + V \pm ic) = \mathcal{H}. \tag{8.14}$$

(By a rescaling argument, $\text{Range}(T + V \pm i) = \mathcal{H}$ holds, so Prop. 8.1 gives self-adjointness of $T + V$ on $\text{Dom}(T)$.)

For any $c > 0$, self-adjointness of T implies (Prop. 8.6) that there is a bounded resolvent,

$$(T \pm ic)^{-1} : \mathcal{H} \to \text{Dom}(T).$$

As T is symmetric, we also have the general identity (cf. (8.1)),

$$\|(T + ic)\varphi\|^2 = \|T\varphi\|^2 + c^2\|\varphi\|^2, \qquad \forall\, \varphi \in \text{Dom}(T).$$

As we can rewrite $\varphi \in \text{Dom}(T)$ as $(T \pm ic)^{-1}\psi$ for appropriate $\psi \in \mathcal{H}$, the above norm identity becomes

$$\|\psi\|^2 = \|T(T \pm ic)^{-1}\psi\|^2 + c^2\|(T \pm ic)^{-1}\psi\|^2, \qquad \forall\, \psi \in \mathcal{H},$$

which implies that

$$\|T(T \pm ic)^{-1}\|_{\text{op}} \leq 1, \qquad \|(T \pm ic)^{-1}\|_{\text{op}} \leq c^{-1}.$$

Combining these op-norm bounds with the assumption that V has relative bound $a \in [0, 1)$, we get

$$\begin{aligned} \|V(T \pm ic)^{-1}\psi\| &\leq a\|T(T \pm ic)^{-1}\psi\| + b\|(T \pm ic)^{-1}\psi\| \\ &\leq (a + bc^{-1})\|\psi\|, \qquad\qquad \psi \in \mathcal{H}. \end{aligned}$$

Here, $V(T \pm ic)$ is a bounded operator (Exercise 7.1; replace V by $\overline{V}$.), so it has a finite operator norm. As $a < 1$, we can choose c large enough so that $a + bc^{-1} < 1$, in which case,

$$\|V(T \pm ic)^{-1}\|_{\text{op}} < 1, \qquad c \text{ large}.$$

As spectral radius is bounded by the operator norm, we have $-1 \in \rho(V(T \pm ic))$, therefore,

$$\begin{aligned} \mathcal{H} &= \text{Range}(V(T \pm ic)^{-1} + 1) \\ &= \{(V(T \pm ic)^{-1} + 1)\psi \,:\, \psi \in \mathcal{H}\} \\ &= \{(V(T \pm ic)^{-1} + 1)(T \pm ic)\varphi \,:\, \varphi \in \text{Dom}(T)\} \qquad (T \pm ic \text{ surjective}) \\ &= \{(T + V \pm ic)\varphi \,:\, \varphi \in \text{Dom}(T)\} \\ &\equiv \text{Range}(T + V \pm ic). \end{aligned}$$

This is the claim (8.14).

- Let $\mathcal{D} \subseteq \mathrm{Dom}(T)$ be a domain of essential self-adjointness for T, so

$$\mathrm{Dom}(T) = \mathrm{Dom}(\overline{T|_{\mathcal{D}}}). \tag{8.15}$$

  From the T-boundedness of V, we may deduce the first inclusion below,

$$\mathrm{Dom}(\overline{T|_{\mathcal{D}}}) \subseteq \mathrm{Dom}(\overline{(T+V)|_{\mathcal{D}}}) \subseteq \mathrm{Dom}(\overline{T+V}) = \mathrm{Dom}(T+V) = \mathrm{Dom}(T),$$

  while the second-last equality above is due to self-adjointness of $T+V$ established in the earlier part of the proof. Because of (8.15), we actually have equality throughout; in particular,

$$\mathrm{Dom}(\overline{(T+V)|_{\mathcal{D}}}) = \mathrm{Dom}(T+V).$$

  This says that $(T+V)|_{\mathcal{D}}$ is essentially self-adjoint.

□

Theorem 8.12 (Kato–Rellich′)**.** *Let $d = 1, 2, 3$, and Δ be the Laplacian on $\mathbb{R}^d$. Suppose V is a real-valued potential function with $V = V_2 + V_\infty$ for some $V_2 \in L^2(\mathbb{R}^d)$ and $V_\infty \in L^\infty(\mathbb{R}^d)$. Then $H = -\Delta + V$ is essentially self-adjoint on the domains $C_c^\infty(\mathbb{R}^d)$ and $\mathscr{S}(\mathbb{R}^d)$.*

Proof. We had seen that $-\Delta$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$ and $\mathscr{S}(\mathbb{R}^d)$. The assumptions on V imply that

$$\|V\psi\|_2 \leq \|V_2\|_2 \|\psi\|_\infty + \|V_\infty\|_\infty \|\psi\|_2, \qquad \psi \in C_c^\infty(\mathbb{R}^d).$$

Using a general Lemma 8.13 (later) in the above inequality, we find that $a \in [0, 1)$, there exists $b > 0$ such that

$$\|V\psi\|_2 \leq a\|V_2\|_2 \|\Delta\psi\|_2 + \big(b + \|V_\infty\|_\infty\big)\|\psi\|_2, \qquad \psi \in C_c^\infty(\mathbb{R}^d).$$

Passing to closures, this implies that

- $\mathrm{Dom}(\overline{-\Delta}) \subset \mathrm{Dom}(\overline{V})$;
- $\overline{V}$ is $\overline{-\Delta}$-bounded, with relative bound < 1 (in fact, arbitrarily small).

The assumptions of the Kato–Rellich Theorem 8.11 are satisfied, so we conclude that $-\Delta + V$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$, thus also on $\mathscr{S}(\mathbb{R}^d)$. □

Example 8.5. For $d = 3$, the Coulomb potential is

$$V(x) = -\frac{eQ}{|x|},$$

where $-e < 0$ is the electron charge and $Q > 0$ is the nuclear charge. We may simplify the analysis by considering $V(x) = -\frac{1}{|x|}$. This potential has a blowup at the origin, but locally, it is square integrable near the origin due to $d = 3$. (Note that this fails for $d < 3$.) So we may write $V = V_2 + V^\infty$, as in Theorem 8.12, to deduce that the Schrödinger operator with Coulomb potential is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$, or $\mathscr{S}(\mathbb{R}^3)$.

There is another important physical issue that must be mentioned. As V is unbounded from below, it is unclear whether the spectrum of (the self-adjoint closure of) $H = -\Delta + V$ is bounded from below. If this fails, then the electron would keep lowering its energy state indefinitely. Therefore, it is important that the Kato–Rellich theorems 8.11–8.12 are supplemented by the statement that $\sigma(\overline{-\Delta + V})$ is bounded from below. In fact, in Theorem 8.11, if $\sigma(T)$ is bounded below by $M \in \mathbb{R}$, then $\sigma(\overline{T + V})$ is bounded below by

$$M - \max\Big\{\frac{b}{1-a}, a|M| + b\Big\},$$

where $a \in [0, 1)$, $b \in [0, \infty)$ are the constants such that(8.13) is satisfied. See Reed–Simon Theorem X.12 for a proof.

Lemma 8.13. *Let Δ be the Laplacian on $\mathbb{R}^d$, where $d = 1, 2, 3$. Then, given any $a > 0$, there exists $b > 0$ such that*

$$\|\psi\|_\infty \le a\|\Delta\psi\|_2 + b\|\psi\|_2, \qquad \psi \in C_c^\infty(\mathbb{R}^d).$$

Proof. Let $\psi \in C_c^\infty(\mathbb{R}^d)$. After Fourier transform, ψ becomes an element $\widehat{\psi} \in L^2(\widehat{\mathbb{R}^d})$ (which is very smooth, why?) such that $(p \mapsto -|p|^2 \cdot \widehat{\psi}(p))$ remains square-integrable, i.e.,

$$(1 + |p|^2) \cdot \widehat{\psi} \in L^2(\widehat{\mathbb{R}^d}).$$

Now, as $d \le 3$, we also have $\frac{1}{1+|p|^2} \in L^2(\widehat{\mathbb{R}^d})$. (Use polar coordinates.) So, by Hölder/Cauchy–Schwarz inequality,

$$\widehat{\psi} = (1 + |p|^2) \cdot \widehat{\psi} \cdot \frac{1}{1 + |p|^2} \in L^1(\widehat{\mathbb{R}^d}),$$

and furthermore,

$$\begin{aligned} \|\widehat{\psi}\|_1 &\le c\|(1+|p|^2)\cdot\widehat{\psi}\|_2 \\ &\le c\Big(\big\|\widehat{\Delta\psi}\big\|_2 + \|\widehat{\psi}\|_2\Big), \qquad c = \big\|\tfrac{1}{1+|p|^2}\big\|_2. \end{aligned} \tag{8.16}$$

Eq. (8.16) also applies to the rescaled $\widehat{\psi_r}(p) = r^d\widehat{\psi}(rp)$, which have

$$\|\widehat{\psi_r}\|_1 = \|\widehat{\psi}\|_1, \qquad \|\widehat{\psi_r}\|_2 = r^{d/2}\|\widehat{\psi}\|_2, \qquad \||p|^2\cdot\widehat{\psi_r}\|_2 = r^{d/2-2}\||p|^2\cdot\widehat{\psi}\|_2.$$

So (8.16) may be improved to

$$\|\widehat{\psi}\|_1 \le cr^{d/2-2}\big\|\widehat{\Delta\psi}\big\|_2 + cr^{d/2}\|\widehat{\psi}\|_2, \qquad r>0.$$

Undoing the Fourier transform, it is straightforward to see that $\|\psi\|_\infty \le \|\widehat{\psi}\|_1$. So the last inequality is

$$\|\psi\|_\infty \le cr^{d/2-2}\|\Delta\psi\|_2 + cr^{d/2}\|\psi\|_2, \qquad r>0.$$

Setting r such that $a = cr^{d/2-2}$ gives the result. □