Chapter 6

Kato-Rellich Theorem

In this and the next chapters, the preservation of self-adjointness under hermitian perturbations are considered. The classical application of Rellich's theorem by Kato to a hydrogen atom hamiltonian is discussed in detail. Examples, the virial and KLMN theorems and an outstanding Kato distributional inequality are also presented in this chapter.

6.1 Relatively Bounded Perturbations

Self-adjointness is a delicate property. It may not be preserved by a sum of operators. For instance, if T, S are self-adjoint operators in $\mathcal{H}$, then $\mathrm{dom}\, T \cap \mathrm{dom}\, S$ is the subspace on which $T + S$ is a priori defined. However, this intersection may be too small for $T + B$ be self-adjoint (e.g., both $C_0^\infty(\mathbb{R})$ and the set of simple functions are both dense in $\mathrm{L}^2(\mathbb{R})$, but their intersection contains only the null vector; see a specific instance in Exercise 6.2.25). It may also happen that such an intersection is dense but $T + S$ is not self-adjoint.

If T is self-adjoint and B is hermitian, under which conditions is $T + B$ self-adjoint? This is the general question to be addressed now. Although the main interest is in perturbations of the free Schrödinger operators H_0 acting in $\mathrm{L}^2(\Lambda), \Lambda \subset \mathbb{R}^n$, by potentials V, it is useful to deal with abstract hermitian perturbations B of a general self-adjoint operator T.

The motivation for the next results is the following. Let T be hermitian; then T is self-adjoint iff λT is self-adjoint for some (and so any) $0 \neq \lambda \in \mathbb{R}$. It is known (Proposition 2.2.4) that a hermitian T is self-adjoint iff $\mathrm{rng}\,(T \pm i\mathbf{1}) = \mathcal{H}$. One has

$$\begin{aligned} T + B \pm i\lambda\mathbf{1} &= (BR_{\pm i\lambda}(T) + \mathbf{1})(T \pm i\lambda\mathbf{1}) \\ &= \lambda(BR_{\pm i\lambda}(T) + \mathbf{1}) \left(\frac{1}{\lambda} T \pm i\mathbf{1}\right), \end{aligned}$$

so that if for some real λ one has $\|BR_{\pm i\lambda}(T)\| < 1$, then $(BR_{\pm i\lambda}(T) + \mathbf{1})$ has also a bounded inverse in $\mathrm{B}(\mathcal{H})$ and so $\operatorname{rng}(BR_{\pm i\lambda}(T) + \mathbf{1}) = \mathcal{H}$. If T is self-adjoint $\operatorname{rng}(T \pm i\lambda\mathbf{1}) = \lambda \operatorname{rng}(T/\lambda \pm i\mathbf{1}) = \mathcal{H}$, and the above relation implies

$$\operatorname{rng}(T + B \pm i\lambda\mathbf{1}) = \mathcal{H},$$

so that $(T + B)$ would also be self-adjoint. We now explore some details of these ideas.

Definition 6.1.1. Let $T : \operatorname{dom} T \sqsubseteq \mathcal{H} \to \mathcal{H}$ and $B : \operatorname{dom} B \sqsubseteq \mathcal{H} \to \mathcal{H}$ be linear operators. Then B is *T-bounded* (or *relatively bounded with respect to T*) if $\operatorname{dom} B \supset \operatorname{dom} T$ and there exist $a, b \geq 0$ so that

$$\|B\xi\| \leq a\|T\xi\| + b\|\xi\|, \qquad \forall \xi \in \operatorname{dom} T.$$

The *T-bound* of B is the infimum $N_T(B)$ of the admissible a's in this inequality.

Remark 6.1.2. An equivalent definition is $\operatorname{dom} B \supset \operatorname{dom} T$ and there exist $c, d \geq 0$ so that

$$\|B\xi\|^2 \leq c^2\|T\xi\|^2 + d^2\|\xi\|^2, \qquad \forall \xi \in \operatorname{dom} T.$$

Further, $N_T(B)$ coincides with the infimum of the admissible c's. Therefore, both formulations will be freely used.

Proof. If the latter relation holds, then

$$\begin{aligned}\|B\xi\|^2 &\leq c^2\|T\xi\|^2 + d^2\|\xi\|^2 + 2cd\,\|T\xi\|\,\|\xi\| \\ &\leq \left(c\|T\xi\| + d\|x\|\right)^2,\end{aligned}$$

and one can take $a = c$ and $b = d$. For the other inequality, consider the following

Lemma 6.1.3. *Let $\xi, \eta \in \mathcal{H}$ and $s, t > 0$. Then, for all $r > 0$ one has*

$$2st\|\eta\|\,\|\xi\| \leq r^2 s^2\,\|\eta\|^2 + \frac{t^2}{r^2}\|\xi\|^2.$$

Proof. It is enough to expand $0 \leq \left(rs\|\eta\| - \frac{t}{r}\|\xi\|\right)^2$. □

Suppose then that $\|B\xi\| \leq a\|T\xi\| + b\|\xi\|$. By Lemma 6.1.3 it follows that

$$\|B\xi\|^2 \leq \left(a\|T\xi\| + b\|\xi\|\right)^2 \leq a^2\left(1 + r^2\right)\|T\xi\|^2 + b^2\left(1 + \frac{1}{r^2}\right)\|\xi\|^2$$

and the second relation holds with $c^2 = a^2(1 + r^2)$ and $d^2 = b^2(1 + 1/r^2)$. By taking $r \to 0$ it is found that the same value of $N_T(B)$ is obtained from both relations. □

Lemma 6.1.4. *Let T be a linear operator in $\mathcal{H}$ with $\rho(T) \neq \emptyset$ and B a closed operator with* $\operatorname{dom} T \subset \operatorname{dom} B$. *Then B is T-bounded and $N_T(B) \leq \|BR_z(T)\|$, $\forall z \in \rho(T)$.*

Proof. If $z \in \rho(T)$, then $BR_z(T) : \mathcal{H} \hookleftarrow$ is a closed operator (check this!) and, by the closed graph theorem, it is bounded. Thus, for $\xi \in \operatorname{dom} T$ and $z \in \rho(T)$ one has

$$\|B\xi\| = \|BR_z(T)(T - z\mathbf{1})\xi\| \leq \|BR_z(T)\| \left(\|T\xi\| + |z|\|\xi\|\right),$$

and B is T-bounded. □

Proposition 6.1.5. *If T is self-adjoint and* $\operatorname{dom} T \subset \operatorname{dom} B$*, then B is T-bounded iff $BR_z(T) \in \mathrm{B}(\mathcal{H})$ for some $z \in \rho(T)$; in this case $BR_z(T) \in \mathrm{B}(\mathcal{H})$, $\forall z \in \rho(T)$, and* $N_T(B) = \lim_{|\lambda|\to\infty} \|BR_{i\lambda}(T)\|$ *($\lambda \in \mathbb{R}$).*

Proof. If $BR_z(T)$ is a bounded operator for some $z \in \rho(T)$, then by the proof of Lemma 6.1.4 it follows that B is T-bounded and $N_T(B) \leq \|BR_z(T)\|$; moreover, by the first resolvent identity,

$$BR_y(T) = BR_z(T) + (y - z)BR_z(T)R_y(T),$$

so that $BR_y(T)$ is bounded for all $y \in \rho(T)$. Hence, since T is self-adjoint one can consider $z = \pm i\lambda$, with $0 \neq \lambda \in \mathbb{R}$, which belongs to $\rho(T)$.

Suppose now that B is T-bounded, so that there are $a, b \geq 0$ obeying, for all $\xi \in \mathcal{H}$,

$$\|BR_{i\lambda}(T)\xi\| \leq a\|TR_{i\lambda}(T)\xi\| + b\|R_{i\lambda}(T)\xi\|,$$

and since $\|T\eta - i\lambda\eta\|^2 = \|T\eta\|^2 + \lambda^2\|\eta\|^2 \geq \|T\eta\|^2$, one has, with $\eta = R_{i\lambda}(T)\xi$,

$$\begin{aligned}\|BR_{i\lambda}(T)\xi\| &\leq a\|(T - i\lambda\mathbf{1})R_{i\lambda}(T)\xi\| + b\|R_{i\lambda}(T)\|\,\|\xi\| \\ &\leq \left(a + \frac{b}{|\lambda|}\right)\|\xi\|,\end{aligned}$$

and $BR_{i\lambda}(T)$ is bounded (Theorem 2.2.17 was employed). Together with the inequality at the beginning of this proof,

$$N_T(B) \leq \|BR_{i\lambda}(T)\| \leq a + \frac{b}{|\lambda|}.$$

From the definition of $N_T(B)$ it then follows that

$$N_T(B) = \lim_{|\lambda|\to\infty} \|BR_{i\lambda}(T)\|.$$

Thereby the proof is complete. □

Exercise 6.1.6. If T is a self-adjoint operator, show that $\|TR_{i\lambda}(T)\| \leq 1$, $\forall 0 \neq \lambda \in \mathbb{R}$.

Exercise 6.1.7. Let $T \geq \beta\mathbf{1}$ be self-adjoint, $\beta \in \mathbb{R}$. Inspect the proof of Proposition 6.1.5 and check that for $\lambda < 0$, $|\lambda|$ large enough, $\|TR_\lambda(T)\| < 1$, and that $N_T(B) = \lim_{\lambda\to-\infty} \|BR_\lambda(T)\|$.

Theorem 6.1.8 (Rellich or Kato-Rellich). *Let T be self-adjoint and B hermitian. If B is T-bounded with $N_T(B) < 1$, then the operator*

$$\text{dom } (T+B) = \text{dom } T, \qquad (T+B)\xi := T\xi + B\xi, \qquad \forall \xi \in \text{dom } T,$$

is self-adjoint.

Proof. Clearly $(T+B)$ is hermitian. Since $N_T(B) < 1$, by Proposition 6.1.5 there exists $\lambda_0 > 0$ so that $\|BR_{i\lambda_0}(T)\| < 1$. Thus, $(\mathbf{1} + BR_{\pm i\lambda_0}(T))$ is invertible in $\mathrm{B}(\mathcal{H})$ and onto. Hence,

$$\begin{aligned}(T+B) \pm i\lambda_0\mathbf{1} &= B + (T \pm i\lambda_0\mathbf{1}) \\ &= (BR_{\pm i\lambda_0}(T) + \mathbf{1})\,(T \pm i\lambda_0\mathbf{1})\end{aligned}$$

and so rng $(T+B \pm i\lambda_0) = \mathcal{H}$. By Proposition 2.2.4 (see also the discussion at the beginning of this section), (T+B) is self-adjoint. ☐

Corollary 6.1.9. *Let T and B be as in Theorem 6.1.8. If $\mathcal{D} \subset \text{dom } T$ is a core of T, then $\mathcal{D}$ is a core of $(T+B)$.*

Proof. Take λ_0 as in the proof of Thm. 6.1.8. Then the operator $(\mathbf{1}+BR_{\pm i\lambda_0}(T))$ is a homeomorphism onto $\mathcal{H}$. Thus, if $(T \pm i\lambda_0\mathbf{1})\mathcal{D}$ is dense in $\mathcal{H}$, then $(T+B\pm i\lambda_0\mathbf{1})\mathcal{D}$ is also dense in $\mathcal{H}$. Therefore the deficiency indices of $(T+B)|_{\mathcal{D}}$ are both zero (see Theorem 2.2.11), consequently $\mathcal{D}$ is a core of $(T+B)$. ☐

Example 6.1.10. In $\mathrm{L}^2(\mathbb{R}^n)$ the momentum operators $P_j = -i\partial_j$, $1 \le j \le n$, are H_0-bounded with $N_{H_0}(P_j) = 0$; thus the operator

$$H\psi = H_0\psi - i\lambda \sum_j \partial_j \psi$$

is self-adjoint in the domain $\mathcal{H}^2(\mathbb{R}^n)$, $\forall \lambda \in \mathbb{R}$. In fact, for $\psi \in \mathcal{H}^2(\mathbb{R}^n) \subset \text{dom } P_j$, $\|P_j\psi\|_2 = \|p_j\hat{\psi}(p)\|_2$, and given $a > 0$ there is $b \ge 0$ so that $|p_j| \le (ap^2 + b)$, and so (assume that $\lambda \ne 0$)

$$\|\lambda P_j \psi\|_2 \le a\,|\lambda|\,\|p^2\hat{\psi}(p)\|_2 + b\,|\lambda|\,\|\hat{\psi}(p)\|_2 = a\,|\lambda|\,\|H_0\psi\|_2 + b\,|\lambda|\,\|\psi\|_2.$$

Since $a > 0$ was arbitrary, the result follows by Theorem 6.1.8.

Exercise 6.1.11. Let T and B be self-adjoint operators in $\mathcal{H}$. If $B \in \mathrm{B}(\mathcal{H})$, verify that

a) $N_T(B) = 0$.
b) $T+B$ is self-adjoint with dom $(T+B) = \text{dom } T$.
c) Every core of T is also a core of $T+B$.

Exercise 6.1.12.

a) If B is T-bounded with $N_T(B) < 1$, show that B is also $(T+B)$-bounded.
b) If T is self-adjoint and B hermitian and T-bounded with $N_T(B) < 1/2$, show that $(T+2B)$ is also self-adjoint.

Exercise 6.1.13. Let T be closed and B a T-bounded operator with T-bound $N_T(B) < 1$. Show that $T + B$ with domain dom T is closed. If $N_T(B) = 1$ take $B = -T$ and conclude that $T + B$ can be nonclosed.

6.1.1 KLMN Theorem

This theorem is a partial counterpart for sesquilinear forms of the Kato-Rellich theorem, and it was dubbed KLMN by J.T. Cannon in 1968 from the initials of Kato, Lions, Lax, Milgram and Nelson. In this subsection b_1 and b_2 denote two (densely defined) hermitian sesquilinear forms in $\mathcal{H}$, with b_1 lower bounded $b_1 \geq \beta$. The domain of $b_1 + b_2$ is dom $b_1 \cap$ dom b_2.

Definition 6.1.14. b_2 is b_1-bounded if dom $b_1 \subset$ dom b_2 and there are $a \geq 0, c \geq 0$ so that

$$|b_2(\xi)| \leq a\,|b_1(\xi)| + c\|\xi\|^2, \qquad \forall \xi \in \text{dom } b_1.$$

The infimum of the admissible $a's$ in this inequality is called the b_1-*bound* of b_2.

Exercise 6.1.15. Show that the b_1-bound of b_2 coincides with the $(b_1 + \alpha)$-bound of b_2 for any $\alpha \in \mathbb{R}$.

By Exercise 6.1.15 there is no loss if it is assumed that $b_1 \geq 0$, i.e., that b_1 is positive.

Lemma 6.1.16. *Suppose that $b_1 \geq 0$ and b_2 is b_1-bounded with b_1-bound < 1, that is, the inequality in Definition* 6.1.14 *holds for some $0 \leq a < 1$ and $0 \leq c \in \mathbb{R}$. Then:*

i) *$b_1 + b_2 \geq -c$, that is, $b_1 + b_2$ is also lower bounded.*
ii) *$b_1 + b_2$ is closed iff b_1 is closed.*

Proof. For all $\xi \in$ dom $b_1 =$ dom $(b_1 + b_2)$,

$$\begin{aligned} -c\|\xi\|^2 &\leq -c\|\xi\|^2 + (1-a)b_1(\xi) = -\left(c\|\xi\|^2 + a\,b_1(\xi)\right) + b_1(\xi) \\ &\leq b_2(\xi) + b_1(\xi) = (b_1 + b_2)(\xi) \leq a\,b_1(\xi) + c\|\xi\|^2 + b_1(\xi) \\ &= (1+a)\,b_1(\xi) + c\|\xi\|^2. \end{aligned}$$

Then i) follows at once. By adding $(1+c)\|\xi\|^2$ to the terms in the above chain of inequalities, one gets

$$\begin{aligned} (1-a)(b_1(\xi) + \|\xi\|^2) &\leq (1-a)b_1(\xi) + \|\xi\|^2 \\ &\leq (b_1 + b_2)(\xi) + (1+c)\|\xi\|^2 \\ &\leq (1+a)b_1(\xi) + (1+2c)\|\xi\|^2 \\ &\leq A\left(b_1(\xi) + \|\xi\|^2\right), \qquad A = \max\{1+a, 1+2c\}; \end{aligned}$$

thus the norms $\xi \mapsto \sqrt{b_1(\xi) + \|\xi\|^2}$ and $\xi \mapsto \sqrt{(b_1 + b_2)(\xi) + (1+c)\|\xi\|^2}$ are equivalent on dom b_1 and ii) follows (see Lemma 4.1.9). ☐

Theorem 6.1.17 (KLMN). *Suppose that $b_1 \geq 0$ and b_2 is b_1-bounded with b_1-bound < 1. Then there exists a unique self-adjoint operator T with* dom $T \sqsubseteq$ dom b_1, *whose form domain is* dom b_1, *and*

$$\langle \xi, T\eta \rangle = b_1(\xi,\eta) + b_2(\xi,\eta), \qquad \forall \xi \in \text{dom } b_1, \eta \in \text{dom } T.$$

Further, T is lower bounded and dom T *is a core of $b_1 + b_2$.*

Proof. By Lemma 6.1.16, $b_1 + b_2$ is closed and lower bounded. The operator T is the one associated with $b_1 + b_2$ as in Definition 4.2.5. The other statements follow by Theorem 4.2.6. □

Although the hypotheses of KLMN are weaker than those of Kato-Rellich, in the latter the domain of the operator sum is explicitly found. Be aware that in concrete situations it can be a nontrivial task to decide if such theorems are applicable.

Typical applications of Theorem 6.1.17 involve the definition of the sum of two hermitian operators $T_1 \geq \beta \mathbf{1}$ and T_2 via $b^{T_1} + b^{T_2}$ (see Example 4.1.11), in particular when Kato-Rellich does not apply, as in Example 6.2.15, and cases of forms not directly related to a potential, as in Examples 6.2.16 and 6.2.19.

One can roughly think of the KLMN theorem as a definition of an adequate quantum observable from the addition of expectation values.

6.2 Applications

6.2.1 H-Atom and Virial Theorem

Now the Kato-Rellich Theorem is applied to perturbations of the free particle hamiltonian

$$\text{dom } H_0 = \mathcal{H}^2(\mathbb{R}^n), \qquad H_0\psi = -\Delta\psi,$$

discussed in Section 3.4. Recall that, by Proposition 3.4.1, $C_0^\infty(\mathbb{R}^n)$ is a core of H_0. Besides the Sobolev embedding theorem, the next result gives valuable information on elements of the Sobolev space $\mathcal{H}^2(\mathbb{R}^n)$, $n \leq 3$.

Lemma 6.2.1. *If $n \leq 3$, then $\mathcal{H}^2(\mathbb{R}^n) \subset C(\mathbb{R}^n) \cap \mathrm{L}^\infty(\mathbb{R}^n)$ and for each $a > 0$ there exists $b > 0$ so that*

$$\|\psi\|_\infty \leq a\|H_0\psi\| + b\|\psi\|, \qquad \forall \psi \in \mathcal{H}^2(\mathbb{R}^n).$$

Proof. Technically, the point of the argument is that for $n \leq 3$ the function $p \mapsto (1+p^2)^{-1} \in \mathrm{L}^2(\mathbb{R}^n)$, and also $(1+p^2)\hat{\psi}(p) = \mathcal{F}(\psi + H_0\psi)$.

If $\psi \in$ dom H_0, by Cauchy-Schwarz,

$$\left(\int_{\mathbb{R}^n} |\hat{\psi}(p)|\, dp \right)^2 \leq \int_{\mathbb{R}^n} (1+p^2)^2 |\hat{\psi}(p)|^2\, dp \int_{\mathbb{R}^n} \frac{dp}{(1+p^2)^2} < \infty,$$

and so $\hat{\psi} \in \mathrm{L}^1(\mathbb{R}^n)$. By Lemma 3.2.8 it follows that $\psi \in C(\mathbb{R}^n) \cap \mathrm{L}^\infty(\mathbb{R}^n)$. Note that since $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and is continuous, then $\lim_{|x|\to\infty} \psi(x) = 0$.

Let $\lambda > 1$ and $\kappa = \|(1+p^2)^{-1}\|_2/(2\pi)^{\frac{n}{2}}$. Then, for $\psi \in \mathrm{dom}\, H_0$, again by Cauchy-Schwarz,

$$\begin{aligned}
|\psi(x)| &= \frac{1}{(2\pi)^{n/2}} \left| \int_{\mathbb{R}^n} (\lambda^2 + p^2) e^{ipx}\, \hat{\psi}(p)\, \frac{dp}{(\lambda^2+p^2)} \right| \\
&\le \frac{1}{(2\pi)^{n/2}} \left\| (\lambda^2+p^2)\, \hat{\psi}(p) \right\|_2 \left\| \frac{1}{(\lambda^2+p^2)} \right\|_2 \\
&\le \frac{\kappa}{\lambda^{2-\frac{n}{2}}} \left(\lambda^2 \left\| \hat{\psi}(p) \right\|_2 + \left\| p^2 \hat{\psi}(p) \right\|_2 \right) \\
&= \frac{\kappa}{\lambda^{2-\frac{n}{2}}} \|H_0\psi\|_2 + \kappa \lambda^{\frac{n}{2}} \|\psi\|_2,
\end{aligned}$$

since the Fourier transform is a unitary operator. Now take λ large enough. □

For the potential $V : \mathbb{R}^n \to \mathbb{R}$ in $\mathrm{L}^\infty(\mathbb{R}^n)$, one associates a bounded self-adjoint multiplication operator $V = \mathcal{M}_V$, and so

$$H := H_0 + V, \qquad \mathrm{dom}\, H := \mathrm{dom}\, H_0,$$

is self-adjoint (see Exercise 6.1.11). This situation can be generalized to some unbounded potentials V.

The notation $V \in \mathrm{L}^r_\mu + \mathrm{L}^s_\mu$ means that the function $V = V_r + V_s$ with $V_r \in \mathrm{L}^r_\mu$ and $V_s \in \mathrm{L}^s_\mu$, and it has already been incorporated into the main stream of Schrödinger operator theory.

Theorem 6.2.2 (Kato). *If $n \le 3$ and $V \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$ is a real-valued function, then V is H_0-bounded with $N_{H_0}(V) = 0$, the operator*

$$H := H_0 + V, \qquad \mathrm{dom}\, H = \mathrm{dom}\, H_0,$$

is self-adjoint and $C_0^\infty(\mathbb{R}^n)$ is a core of H.

Proof. By hypothesis $V = V_2 + V_\infty$ with $V_2 \in \mathrm{L}^2(\mathbb{R}^n)$ and $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^n)$. Thus, by Lemma 6.2.1, for all $a > 0$ there is $b \ge 0$ so that, for all $\psi \in \mathrm{dom}\, H_0$,

$$\begin{aligned}
\|V\psi\|_2 &\le \|V_2\psi\|_2 + \|V_\infty\psi\|_2 \le \|V_2\|_2\, \|\psi\|_\infty + \|V_\infty\|_\infty\, \|\psi\|_2 \\
&\le \|V_2\|_2\, (a\|H_0\psi\|_2 + b\|\psi\|_2) + \|V_\infty\|_\infty\, \|\psi\|_2 \\
&= (a\|V_2\|_2)\, \|H_0\psi\|_2 + (b\|V_2\|_2 + \|V_\infty\|_\infty)\, \|\psi\|_2.
\end{aligned}$$

Since $a > 0$ is arbitrary, it follows that $N_{H_0}(V) = 0$. To finish the proof apply Theorem 6.1.8 and Corollary 6.1.9. □

Example 6.2.3. Consider the class of negative power potentials in $\mathbb{R}^3$,

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad \kappa \in \mathbb{R},\ 0 < \alpha < 3/2.$$

Fix $R > 0$; then $V = V_2 + V_\infty$, with

$$V_2(x) = V(x)\chi_{[0,R)}(|x|), \qquad V_\infty(x) = V(x)\chi_{[R,\infty)}(|x|),$$

where χ_A denotes the characteristic function of the set A. Since $V_2 \in \mathrm{L}^2(\mathbb{R}^3)$ and $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^3)$, it follows that the Schrödinger operator

$$H = H_0 - \frac{\kappa}{|x|^\alpha}, \qquad \mathrm{dom}\ H = \mathcal{H}^2(\mathbb{R}^3),$$

is self-adjoint and $C_0^\infty(\mathbb{R}^3)$ is a core of H (recall $0 < \alpha < 3/2$).

The very important Coulomb potential $\alpha = 1$ gives rise to 3D hydrogenic atoms; if also $\kappa > 0$, it is briefly referred to as an *H-atom* Schrödinger operator H_H (see Remark 6.2.6); as discussed on page 295, this operator is lower bounded (see also Remark 11.4.9). The unidimensional version of the H-atom presents additional technical issues and is addressed in Subsection 7.4.1.

Example 6.2.4. The same conclusions of Example 6.2.3 hold for the "generalized Yukawa-like potential" in $\mathbb{R}^3$,

$$V_Y(x) = -\frac{\kappa}{|x|^\alpha} e^{-a|x|}, \qquad \kappa \in \mathbb{R},\ 0 < \alpha < 3/2,\ a > 0,$$

since $V_Y \in \mathrm{L}^2(\mathbb{R}^3)$. Hence the Schrödinger operator $H = H_0 + V_Y$ with dom $H = \mathcal{H}^2(\mathbb{R}^3)$ is self-adjoint. The genuine *Yukawa potential* is obtained for $\kappa > 0$ and $\alpha = 1$.

Exercise 6.2.5. Apply the Kato-Rellich theorem to the Schrödinger operators of Example 6.2.3, but in dimensions 1 and 2, i.e., for the cases of Hilbert spaces $\mathrm{L}^2(\mathbb{R})$ and $\mathrm{L}^2(\mathbb{R}^2)$, respectively. For which values of $\alpha > 0$ are self-adjoint operators H obtained?

Remark 6.2.6. The expression for the Coulomb potential above describes the electrostatic interaction between two charged particles, and one of them is supposed to be at rest at the origin, so heavy with respect to the other that this approximation is taken. For a hydrogenic atom, that is, with just one electron of mass m and charge $-e$ ($e > 0$), and nuclear mass M and charge Ze, with $M \gg m$ and Z a positive integer indicating the total number of protons in the nucleus, the corresponding Schrödinger operator with all physical constants made explicit is

$$H_H = -\frac{\hbar^2}{2\mu}\Delta - \frac{KZe^2}{|x|},$$

with K indicating the electrostatic constant, $\mu = mM/(m+M)$ the so-called reduced mass, and x corresponding to the relative position between the electron and the nucleus. Note that in the limit of a fixed nucleus, represented here by the condition $M \to \infty$, one has $\mu \to m$. Throughout this discussion the center of mass has been "removed" [Will03], so that only the relative motion remains.

Remark 6.2.7. For $\mathbb{R}^n$, $n \geq 4$, the Kato Theorem 6.2.2 holds for $V \in \mathrm{L}^p(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$, with $p > 2$ if $n = 4$ and $p \geq n/2$ if $n \geq 5$.

By using the Virial Theorem 6.2.8, with relatively little effort it is possible to say something about the spectrum of the H-atom Schrödinger operator. Let $U_d(s)$ be the strongly continuous dilation unitary evolution group discussed in Example 5.4.8, adapted to $\mathbb{R}^n$,

$$(U_d(s)\psi)(x) = e^{-ns/2}\psi(e^{-s}x), \qquad s \in \mathbb{R}, \psi \in \mathrm{L}^2(\mathbb{R}^n).$$

Assume that V is an H_0-bounded potential with $N_{H_0}(V) < 1$, so that $H := H_0 + V$ with dom $H = \mathcal{H}^2(\mathbb{R}^n)$ is self-adjoint.

Theorem 6.2.8 (Virial). *Let V be an H_0-bounded potential with $N_{H_0}(V) < 1$. Suppose there exists $0 \neq \alpha \in \mathbb{R}$ so that*

$$U_d(-s)VU_d(s) = e^{-\alpha s}V.$$

If λ is an eigenvalue of H and ψ_λ the subsequent normalized eigenvector, i.e., $H\psi_\lambda = \lambda\psi_\lambda$, $\|\psi_\lambda\| = 1$, then

$$\langle\psi_\lambda, H_0\psi_\lambda\rangle = -\frac{\alpha}{2}\langle\psi_\lambda, V\psi_\lambda\rangle$$

and

$$\lambda = \left(1 - \frac{2}{\alpha}\right)\langle\psi_\lambda, H_0\psi_\lambda\rangle = \left(1 - \frac{\alpha}{2}\right)\langle\psi_\lambda, V\psi_\lambda\rangle.$$

Proof. Note that $U_d(-s)H_0U_d(s) = e^{-2s}H_0$. Since $\psi_\lambda \in \mathrm{dom}\, H_0 = \mathrm{dom}\, H$ and $U_d(s)\mathrm{dom}\, H_0 = \mathrm{dom}\, H_0$, $\forall s \in \mathbb{R}$, one has

$$\begin{aligned} 0 &= \langle U_d(-s)\psi_\lambda, \lambda\psi_\lambda\rangle - \langle U_d(-s)\lambda\psi_\lambda, \psi_\lambda\rangle \\ &= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle U_d(-s)H\psi_\lambda, \psi_\lambda\rangle \\ &= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle H\psi_\lambda, U_d(s)\psi_\lambda\rangle \\ &= \langle U_d(-s)\psi_\lambda, H\psi_\lambda\rangle - \langle U_d(-s)\psi_\lambda, U_d(-s)HU_d(s)\psi_\lambda\rangle \\ &= \langle U_d(-s)\psi_\lambda, [H - U_d(-s)HU_d(s)]\,\psi_\lambda\rangle, \qquad \forall s \in \mathbb{R}. \end{aligned}$$

Write out $H = H_0 + V$ in the above expression and use the hypothesis on V to get

$$\begin{aligned} 0 &= \lim_{s\to 0}\left\langle U_d(-s)\psi_\lambda, \frac{1}{s}\left[H - U_d(-s)HU_d(s)\right]\psi_\lambda\right\rangle \\ &= \langle\psi_\lambda 2H_0\psi_\lambda + \alpha V\psi_\lambda\rangle\,, \end{aligned}$$

so that

$$\langle\psi_\lambda, H_0\psi_\lambda\rangle = -\frac{\alpha}{2}\langle\psi_\lambda, V\psi_\lambda\rangle,$$

which is the first equality in the theorem. Since

$$\lambda = \langle\psi_\lambda, (H_0 + V)\psi_\lambda\rangle = \langle\psi_\lambda, H_0\psi_\lambda\rangle + \langle\psi_\lambda, V\psi_\lambda\rangle,$$

the other equality follows. □

Corollary 6.2.9. *Let V and α be as in the virial theorem.*

a) *If $\alpha < 2$, then all eigenvalues of H are negative and, if also $V \geq 0$, then H has no eigenvalues.*

b) *The Schrödinger operator $H_0 + V$ with the negative power potential (Example 6.2.3)*

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad 0 < \alpha < 3/2,$$

in $\mathrm{L}^2(\mathbb{R}^3)$ has no eigenvalues if $\kappa < 0$ and all its eigenvalues are negative if $\kappa > 0$ (note that the H-atom is a particular case).

Proof. It is enough to recall that H_0 is a positive operator, to note that

$$U_d(-s)VU_d(s) = e^{-\alpha s}V$$

and apply the conclusions of Theorem 6.2.8. For instance, if $\alpha < 2$ and λ is an eigenvalue of H, then the relation

$$\lambda = \left(1 - \frac{2}{\alpha}\right)\langle\psi_\lambda, H_0\psi_\lambda\rangle$$

implies $\lambda < 0$. □

Exercise 6.2.10. Look for an eigenfunction of the hydrogen atom hamiltonian in the form $\psi(x) = e^{-a|x|}$, for some $a > 0$. Find the corresponding eigenvalue, which is the lowest possible energy value ("ground level" in the physicists' nomenclature) of the electron (see, for instance, [Will03]).

Exercise 6.2.11. Verify the relation $U_d(-s)H_0U_d(s) = e^{-2s}H_0$, and that

$$U_d(s)\mathrm{dom}\; H_0 = \mathrm{dom}\; H_0, \quad \forall\, s \in \mathbb{R}.$$

Exercise 6.2.12. Consider the energy expectation value (see the discussion in Section 14.1)

$$\mathcal{E}^\psi = \langle\psi, H_0\psi\rangle + \langle\psi, V\psi\rangle, \qquad \psi \in C_0^\infty(\mathbb{R}^n),$$

and let $\psi(s) = U_d(s)\psi$. By taking appropriate values of s, show that

$$\inf_{\|\psi\|=1} \mathcal{E}^\psi = -\infty$$

in case $V(x) = -1/|x|^\alpha$ and $\alpha > 2$. Comment on the physical meaning of this result – see Remark 11.4.9.

Example 6.2.13. The condition $U_d(-s)VU_d(s) = e^{-\alpha s}V$ in the virial theorem is not strictly necessary. Consider the bounded potential

$$V_a(x) = -\frac{\kappa}{|x| + a}, \qquad a > 0,$$

acting on $L^2(\mathbb{R})$. Then $U_d(-s)V_aU_d(s) = e^{-s}V_{e^{-s}a}$; if $H\psi_\lambda = \lambda\psi_\lambda$, by following the proof of Theorem 6.2.8 one gets

$$0 \le \langle \psi_\lambda, H_0\psi_\lambda \rangle = \frac{1}{2\kappa}\langle \psi_\lambda, |x|V_a^2\psi_\lambda \rangle,$$

and if $\kappa < 0$ the operator $H = H_0 + V_a$ has no eigenvalues.

Exercise 6.2.14. Present the missing details in Example 6.2.13.

The virial theorem is closely related to its version in classical mechanics. Both relate averages of the potential energy and kinetic energy, and was originally considered by Clausius in the investigation of problems in molecular physics (recall that average kinetic energy is directly related to temperature in equilibrium statistical mechanics). Restricting to dimension 1, Clausius considered the classical quantity $G = xp$, the so-called *virial*; note that in the quantum version this quantity corresponds to the infinitesimal generator of $U_d(s)$ – see Example 5.4.8. Some domain issues are avoided by working directly with the unitary group $U_d(s)$ (as in the virial theorem above) instead of its infinitesimal generator. It has applications to thermodynamics and astrophysics, among others. For several aspects of the quantum virial theorem the reader is referred to [GeoG99].

6.2.2 KLMN: Applications

Let b^{H_0} be the (closed and positive) form generated by the free hamiltonian $H_0 = -\Delta$ in $L^2(\mathbb{R}^n)$, so that

$$b^{H_0}(\psi, \phi) = \langle \psi, -\Delta\phi \rangle, \qquad \forall\psi \in \operatorname{dom} b^{H_0}, \forall\phi \in \operatorname{dom} H_0.$$

According to Examples 4.2.11 and 9.3.9, $\operatorname{dom} b^{H_0} = \mathcal{H}^1(\mathbb{R}^n)$ and

$$b^{H_0}(\psi, \phi) = \langle \nabla\psi, \nabla\phi \rangle, \qquad \forall\psi, \phi \in \operatorname{dom} b^{H_0}.$$

The following three examples consider form perturbations of b^{H_0}.

Example 6.2.15. In $L^2(\mathbb{R}^3)$ the Kato-Rellich theorem allows the definition of a self-adjoint realization of $H_0 + V$ for

$$V(x) = -\frac{\kappa}{|x|^\alpha}, \qquad 0 < \alpha < 3/2,$$

since such potential belongs to $L^2 + L^\infty$. The KLMN theorem can be used to give meaning also for $3/2 \le \alpha < 2$.

Let b_α be the form generated by $|x|^{-\alpha}$. Fix $0 < \alpha < 2$ and note that $\operatorname{dom} b_\alpha \supset \operatorname{dom} b^{H_0}$ in this case; given $a > 0$, choose $\varepsilon > 0$ so that $|x|^{-\alpha} \le a|x|^{-2}/4$ for all

$|x| \le \varepsilon$. By Hardy's Inequality 4.4.16, for all $\psi \in \text{dom } b^{H_0} = \mathcal{H}^1(\mathbb{R}^3)$,

$$\begin{aligned} b_\alpha(\psi) &= \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx = \int_{|x|\le\varepsilon} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx + \int_{|x|>\varepsilon} \frac{|\psi(x)|^2}{|x|^\alpha}\,dx \\ &\le a \int_{|x|\le\varepsilon} \frac{|\psi(x)|^2}{4|x|^2}\,dx + \frac{1}{\varepsilon^\alpha} \int_{|x|>\varepsilon} |\psi(x)|^2\,dx \\ &\le a \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{4|x|^2}\,dx + \frac{1}{\varepsilon^\alpha} \int_{\mathbb{R}^3} |\psi(x)|^2\,dx \\ &\le a \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx + \frac{1}{\varepsilon^\alpha} \int_{\mathbb{R}^3} |\psi(x)|^2\,dx \\ &= a\, b^{H_0}(\psi) + \frac{1}{\varepsilon^\alpha}\|\psi\|^2. \end{aligned}$$

Since $a > 0$ was arbitrary in the above inequality, the b^{H_0}-bound of b_α is zero. Hence the KLMN Theorem 6.1.17 defines a self-adjoint realization of $H_0 - \kappa/|x|^\alpha$ in $L^2(\mathbb{R}^3)$, $0 < \alpha < 2$, given by the operator associated with $b^{H_0} + b_\alpha$.

Example 6.2.16 (Delta-function potential in $\mathbb{R}$). In $L^2(\mathbb{R})$, perturb the free form $b^{H_0}(\psi, \phi) = \langle \psi', \phi' \rangle$ by the nonclosable form $b_\delta(\psi, \phi) = \overline{\psi(0)}\,\phi(0)$ of Example 4.1.15, which simulates a Dirac delta interaction at the origin. Here dom $b_\delta =$ dom $b^{H_0} = \mathcal{H}^1(\mathbb{R})$. The KLMN theorem permits the association of a self-adjoint operator with the form

$$b^{H_0} + \alpha b_\delta, \qquad \alpha \in \mathbb{R},$$

with domain $\mathcal{H}^1(\mathbb{R})$; see also Example 4.4.9.

In fact, if $\psi \in \mathcal{H}^1(\mathbb{R})$ one has $\psi(x) \to 0$ as $|x| \to \infty$, and by using Lemma 6.1.3 with $s = t = 1, \varepsilon = r^2$, for all $M > 0$,

$$\begin{aligned} |b_\delta(\psi)| &= |\psi(0)|^2 \le \big||\psi(0)|^2 - |\psi(M)|^2\big| + |\psi(M)|^2 \\ &= \left| \int_0^M \frac{d}{dx} |\psi(x)|^2\,dx \right| + |\psi(M)|^2 \\ &= \left| \int_0^M \left(\overline{\psi'(x)}\,\psi(x) + \overline{\psi(x)}\,\psi'(x) \right) dx \right| + |\psi(M)|^2 \\ &\le |\psi(M)|^2 + 2\|\psi'\|\,\|\psi\| \le |\psi(M)|^2 + \varepsilon\,\|\psi'\|^2 + \frac{1}{\varepsilon}\,\|\psi\|^2 \\ &\xrightarrow{M\to\infty} \varepsilon\,\|\psi'\|^2 + \frac{1}{\varepsilon}\,\|\psi\|^2 = \varepsilon\, b^{H_0}(\psi) + \frac{1}{\varepsilon}\,\|\psi\|^2. \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, it follows that the b^{H_0}-bound of αb_δ is zero for all $\alpha \in \mathbb{R}$. By KLMN theorem, there is a unique self-adjoint operator T_α with dom $T_\alpha \sqsubseteq \mathcal{H}^1(\mathbb{R})$, whose form domain is $\mathcal{H}^1(\mathbb{R})$, and

$$\langle \psi, T_\alpha \phi \rangle = \langle \psi', \phi' \rangle + \alpha \overline{\psi(0)} \phi(0), \qquad \forall \psi \in \mathcal{H}^1(\mathbb{R}), \phi \in \text{dom } T_\alpha.$$

Further, T_α is lower bounded.

Exercise 6.2.17. If $\alpha < 0$, verify that $e^{\alpha|x|/2}$ is an eigenvector of T_α in Example 6.2.16, whose corresponding eigenvalue is $-\alpha^2/4$.

Remark 6.2.18. In the KLMN theorem it is strictly necessary that $a < 1$. In fact, one has $|-b^{H_0}| \le b^{H_0} + b_\delta$ (so $a = 1$) but the "perturbed" form $(b^{H_0} + b_\delta) - b^{H_0} = b_\delta$ is not closable.

Example 6.2.19. Let ν be a positive Radon measure in $\mathbb{R}^n$, that is, a Borel, finite on compact sets and regular measure. Under suitable conditions, the KLMN theorem will be used to give meaning to the operator

$$H = H_0 + \alpha\nu,$$

that is, the interaction potential is ruled by the measure ν with intensity $\alpha \in \mathbb{R}$, as proposed in [BraEK94]. The "interaction" form $b^{\alpha,\nu}$ associated with this "potential" is introduced by the expression

$$b^{\alpha,\nu}(\psi, \phi) = \alpha \int_{\mathbb{R}^n} \overline{\psi(x)}\phi(x)\, d\nu(x).$$

Singular (with respect to Lebesgue measure) ν are the most interesting cases, but in view of the KLMN theorem one faces the difficulty of getting $\operatorname{dom} b^{\alpha,\nu} \supset \operatorname{dom} b^{H_0} = \mathcal{H}^1(\mathbb{R}^n)$, since the elements of $\mathcal{H}^1(\mathbb{R}^n)$ are not necessarily continuous and the restriction to the support of ν can be meaningless. The idea is to define $b^{\alpha,\nu}$ as above initially on $C_0^\infty(\mathbb{R}^n)$, and assume that ν is such that there are $0 \le a < 1$ and $c \ge 0$ so that (see Remark 6.2.20)

$$(1 + |\alpha|) \int_{\mathbb{R}^n} |\psi(x)|^2\, d\nu(x) \le a \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\, dx + c \int_{\mathbb{R}^n} |\psi(x)|^2\, dx$$

for all $\psi \in C_0^\infty(\mathbb{R}^n)$. Since $C_0^\infty(\mathbb{R}^n)$ is dense in $\mathcal{H}^1(\mathbb{R}^n)$, the map $J : C_0^\infty(\mathbb{R}^n) \to \mathrm{L}^2_\nu(\mathbb{R}^n)$, $J\psi = \psi$, has a unique extension to a continuous linear map (also denoted by J; note that ψ is being used to denote elements in both equivalence classes $\mathrm{L}^2(\mathbb{R}^n)$ and $\mathrm{L}^2_\nu(\mathbb{R}^n)$)

$$J : \mathcal{H}^1(\mathbb{R}^n) \to \mathrm{L}^2_\nu(\mathbb{R}^n),$$

and, by continuity, the above inequality holds for all $\psi \in \mathcal{H}^1(\mathbb{R}^n)$, that is,

$$(1 + |\alpha|) \int_{\mathbb{R}^n} |J\psi(x)|^2\, d\nu(x) \le a \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\, dx + c \int_{\mathbb{R}^n} |\psi(x)|^2\, dx.$$

Finally, the precise definition of the interaction form $b^{\alpha,\nu}$ is presented: $\operatorname{dom} b^{\alpha,\nu} = \mathcal{H}^1(\mathbb{R}^n)$ and for $\psi, \phi \in \operatorname{dom} b^{\alpha,\nu}$,

$$b^{\alpha,\nu}(\psi, \phi) := \alpha \int_{\mathbb{R}^n} \overline{J\psi(x)}\, J\phi(x)\, d\nu(x).$$

For $\psi \in \mathcal{H}^1(\mathbb{R}^n)$, one then has

$$\begin{aligned} |b^{\alpha,\nu}(\psi)| &= |\alpha| \int_{\mathbb{R}^n} |J\psi(x)|^2 \, d\nu(x) \\ &\le \frac{a|\alpha|}{1+|\alpha|} \int_{\mathbb{R}^n} |\nabla\psi(x)|^2 \, dx + \frac{c|\alpha|}{1+|\alpha|} \int_{\mathbb{R}^n} |\psi(x)|^2 \, dx \\ &= \frac{a|\alpha|}{1+|\alpha|} b^{H_0}(\psi) + \frac{c|\alpha|}{1+|\alpha|} \|\psi\|^2. \end{aligned}$$

Since $a|\alpha|/(1+|\alpha|) < 1$, for such measures ν the KLMN Theorem 6.1.17 provides a self-adjoint realization of $H_0 + \alpha\nu$ rigorously defined by the operator associated with $b^{H_0} + b^{\alpha,\nu}$.

Remark 6.2.20. Sufficient conditions for the above inequality to be valid for positive Radon measures ν in $\mathbb{R}^n$ appear in [StoV96]: e.g., all finite measures over $\mathbb{R}$,

$$\lim_{\varepsilon\downarrow 0} \sup_{x\in\mathbb{R}^2} \int_{B(x;\varepsilon)} |\ln|x-y|| \, d\nu(y) = 0, \qquad n = 2,$$

and

$$\lim_{\varepsilon\downarrow 0} \sup_{x\in\mathbb{R}^n} \int_{B(x;\varepsilon)} \frac{1}{|x-y|^{n-2}} \, d\nu(y) = 0, \qquad n \ge 3.$$

Particular interesting cases are $\nu = \mu^{\mathcal{C}}$, that is, a measure concentrated on the ternary Cantor set in $\mathbb{R}$ (see Example 12.2.13), and when ν is supported by smooth curves and other manifolds in $\mathbb{R}^n$, which is part of the set of so-called *leaky quantum graphs*.

6.2.3 Some $\mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ Potentials

Theorem 6.2.21. *Let $V : \mathbb{R}^n \to \mathbb{R}$ be a measurable potential and $\overline{B}_x = \overline{B}(x;1)$ denote the closed ball of center $x \in \mathbb{R}^n$ and radius 1.*

a) *If* $\mathrm{dom}\, H_0 \subset \mathrm{dom}\, V$*, then*

$$d(V) := \sup_{x\in\mathbb{R}^n} \int_{\overline{B}_x} |V(y)|^2 \, dy < \infty,$$

in particular $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$.

b) *If* $\mathrm{dom}\, H_0 \subset \mathrm{dom}\, V$ *and* $\limsup_{|x|\to\infty} |V(x)| = s < \infty$*, then $V \in \mathrm{L}^2(\mathbb{R}^n) + \mathrm{L}^\infty(\mathbb{R}^n)$.*

Proof. a) Since V is a closed operator and $\rho(H_0) \neq \emptyset$, by Lemma 6.1.4 there is $c > 0$ so that

$$\|V\psi\|^2 \le c\left(\|H_0\psi\|^2 + \|\psi\|^2\right), \qquad \forall \psi \in \mathrm{dom}\, H_0.$$

If $x \in \mathbb{R}^n$, pick $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\phi(y) = 1$ for $y \in \overline{B}_0$, and set $\phi_x(y) = \phi(y-x)$. Thus,

$$\int_{\overline{B}_x} |V(y)|^2\, dy \le \|V\phi_x\|^2 \le c\left(\|H_0\phi_x\|^2 + \|\phi_x\|^2\right)$$
$$= c\left(\|H_0\phi\|^2 + \|\phi\|^2\right) < \infty,$$

and note that this upper bound does not depend on x. Hence $d(V) < \infty$.

b) Let $E_s = \{x \in \mathbb{R}^n : |V(x)| \le 2s\}$, $V_\infty = V\chi_{E_s}$ and $V_2 = V\chi_{E_s^c}$, with $E_s^c = \mathbb{R}^n \setminus E_s$. Then $V = V_2 + V_\infty$, $V_\infty \in \mathrm{L}^\infty(\mathbb{R}^n)$ and, by the definition of s, there exists $R > 0$ so that $V_2(x) = 0$ if $x \notin \overline{B}(0;R)$. Pick $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\phi(x) = 1$ for $x \in \overline{B}(0;R)$; then $\phi \in \mathrm{dom}\, H_0 \subset \mathrm{dom}\, \mathcal{M}_V$ and

$$\|V_2\|^2 = \int_{\mathbb{R}^n} |V_2(x)|^2\, |\phi(x)|^2\, dx = \|V_2\phi\|^2 \le \|V\phi\|^2 < \infty,$$

so that $V_2 \in \mathrm{L}^2(\mathbb{R}^n)$. □

Exercise 6.2.22. Show that if $\limsup_{|x|\to\infty} |V(x)| = 0$ in Theorem 6.2.21, then the $\mathrm{L}^\infty(\mathbb{R}^n)$ part of V can be chosen with arbitrarily small L^∞ norm.

Theorem 6.2.23. *Let V and $d(V)$ be as in Theorem* 6.2.21*. Then for $n = 1$, i.e., in* $\mathrm{L}^2(\mathbb{R})$*, the following assertions are equivalent:*

a) $\mathrm{dom}\, H_0 \subset \mathrm{dom}\, V$.
b) $d(V) < \infty$.
c) *V is H_0-bounded.*
d) *V is H_0-bounded with $N_{H_0}(V) = 0$.*

Proof. The implications a) ⇒ c) ⇒ b) were already discussed in the proof of Theorem 6.2.21. d) ⇒ a) is clear. It is only needed to show that b) ⇒ d).

Assume that b) holds. If $\psi \in \mathrm{dom}\, H_0 = \mathcal{H}^2(\mathbb{R})$, then ψ is continuous and continuously differentiable. Assume first that ψ is real valued. By using an idea in Lemma 6.1.3, given $\varepsilon > 0$ for $z, y \in \overline{B}_x$, one has

$$\psi(y)^2 - \psi(z)^2 = \int_z^y \left(\psi(t)^2\right)'\, dt = 2\int_z^y \psi(t)\,\psi'(t)\, dt$$
$$\le \frac{1}{\varepsilon}\int_{\overline{B}_x} \psi(t)^2\, dt + \varepsilon \int_{\overline{B}_x} \psi'(t)^2\, dt.$$

By the mean value theorem, choose $z \in \overline{B}_x$ so that $\psi(z)^2 = \int_{\overline{B}_x} \psi(t)^2\, dt$, thus

$$\psi(y)^2 \le \left(1 + \frac{1}{\varepsilon}\right)\int_{\overline{B}_x} \psi(t)^2\, dt + \varepsilon \int_{\overline{B}_x} \psi'(t)^2\, dt.$$

For complex $\psi \in \mathcal{H}^2(\mathbb{R})$ one gets, for all $\varepsilon > 0$ and all $x \in \mathbb{R}$,

$$|\psi(y)|^2 \le \left(1 + \frac{1}{\varepsilon}\right)\int_{\overline{B}_x} |\psi(t)|^2\, dt + \varepsilon \int_{\overline{B}_x} |\psi'(t)|^2\, dt.$$

Hence,

$$\int_{\overline{B}_x} |V(y)\psi(y)|^2\,dy \le d(V)\left(1+\frac{1}{\varepsilon}\right)\int_{\overline{B}_x} |\psi(t)|^2\,dt + d(V)\varepsilon\int_{\overline{B}_x} |\psi'(t)|^2\,dt,$$

and so (denote the set of even integers by $2\mathbb{Z}$)

$$\begin{aligned}\|V\psi\|^2 = \int_{\mathbb{R}} |V(y)\psi(y)|^2\,dy &= \sum_{x\in 2\mathbb{Z}}\int_{\overline{B}_x} |V(y)\psi(y)|^2\,dy \\ &\le d(V)\left(1+\frac{1}{\varepsilon}\right)\int_{\mathbb{R}} |\psi(t)|^2\,dt + d(V)\varepsilon\int_{\mathbb{R}} |\psi'(t)|^2\,dt, \\ &\le d(V)\left(1+\frac{1}{\varepsilon}\right)\|\psi\|^2\,dt + d(V)\varepsilon\|\psi'\|^2.\end{aligned}$$

Since $0 \le (p^2-1)^2$ it follows that $p^2 \le (p^4+1)/2 < (p^4+1)$, and then

$$\begin{aligned}\|\psi'\|^2 = \|p\hat{\psi}(p)\|^2 &= \int_{\mathbb{R}} p^2|\hat{\psi}(p)|^2\,dp \\ &\le \|p^2\hat{\psi}(p)\|^2 + \|\hat{\psi}\|^2 = \|H_0\psi\|^2 + \|\psi\|^2,\end{aligned}$$

and one obtains

$$\|V\psi\|^2 \le \varepsilon\, d(V)\,\|H_0\psi\|^2 + \left(\varepsilon + 1 + \frac{1}{\varepsilon}\right) d(V)\,\|\psi\|^2.$$

Since this holds for all $\varepsilon > 0$, d) follows. □

Hence, in order to apply the Kato-Rellich theorem to conclude that $H := H_0 + V$, with $\operatorname{dom} H = \operatorname{dom} H_0$, is self-adjoint and $C_0^\infty(\mathbb{R}^n)$ is a core of H, it is necessary that $d(V) < \infty$, and for $n = 1$ this condition is also sufficient.

Example 6.2.24. Let $V_e(x) = e^{|x|}$ and $V_\alpha(x) = |x|^\alpha$, $0 < \alpha < 1/2$, $x \in \mathbb{R}$; then $d(V_e) = \infty$ while $d(V_\alpha) < \infty$. Thus, by Theorem 6.2.23, the operator $H_\alpha := H_0 + V_\alpha$ with domain $\mathcal{H}^2(\mathbb{R})$ is self-adjoint and $C_0^\infty(\mathbb{R})$ is a core of it; however, $H_e := H_0 + V_e$ can not be defined on $\mathcal{H}^2(\mathbb{R})$, although $C_0^\infty(\mathbb{R})$ is a core of H_e by Corollary 6.3.5.

Exercise 6.2.25. For $x \in \mathbb{R}$, let

$$\phi(x) = \begin{cases} 1/\sqrt{|x|}, & \text{if } |x| \le 1 \\ 0, & \text{if } |x| > 1 \end{cases}.$$

Consider the enumeration of rational numbers $\mathbb{Q} = (r_j)_{j=1}^\infty$ and the potential $V(x) := \sum_{j=1}^\infty \phi(x - r_j)/2^j$. Show that:

a) $V \in \mathrm{L}^1(\mathbb{R})$ and V is not L^2 over any open interval in $\mathbb{R}$.
b) If $\psi \in (\operatorname{dom} V \cap C(\mathbb{R}))$, show that $\psi \equiv 0$.

Conclude then that $\operatorname{dom} H_0 \cap \operatorname{dom} V = \{0\}$.

Exercise 6.2.26. Discuss for which dimensions n (i.e., spaces $\mathrm{L}^2(\mathbb{R}^n)$) each of the potentials $V_m(x) = |x|$, $V_l(x) = \ln|x|$ and $V_c(x) = -|x|^{-1}$ have $d(V) < \infty$.

Remark 6.2.27. Note that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ is the minimum requirement for $V\psi$ to be an element of $\mathrm{L}^2(\mathbb{R}^n)$ with $\psi \in C_0^\infty(\mathbb{R}^n)$. It is shown in Section 6.3 that if $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ and is bounded from below $V(x) \geq \beta$, then the operator $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

6.3 Kato's Inequality and Pointwise Positivity

An outstanding distributional inequality due to Kato will be discussed (the original reference is [Kat72]; see also [Sim79]). It involves functions and here applications are restricted to standard hamiltonians in the Hilbert space $\mathrm{L}^2(\mathbb{R}^n)$. It will be used to show that lower bounded $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ leads to essentially self-adjoint hamiltonians $-\Delta + V$ with domain $C_0^\infty(\mathbb{R}^n)$. See Subsection 9.3.1 for other applications. In this section a.e. refers to Lebesgue measure.

Definition 6.3.1. A distribution u in $\mathbb{R}^n$ is *positive* if $u(\phi) \geq 0$ for all test functions $\phi \in C_0^\infty(\mathbb{R}^n)$ with $\phi(x) \geq 0$, $\forall x \in \mathbb{R}^n$. This fact will be denoted by $u \geq 0$ and $u \geq v$ will indicate $(u - v) \geq 0$.

Example 6.3.2.

a) If $F : \mathbb{R}^n \to [0, \infty)$ is continuous, then the distribution $u_F(\phi) = \int F(x)\phi(x)dx$, $\phi \in C_0^\infty(\mathbb{R}^n)$, is positive.
b) If $u_n \geq 0$, $\forall n$, and $u_n \to u$ in the distributional sense (i.e., $u_n(\phi) \to u(\phi)$, $\forall \phi \in C_0^\infty$), then $u \geq 0$.

If $\psi \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, define the function $(\operatorname{sgn}\psi)(x) := 0$ if $\psi(x) = 0$, otherwise set

$$(\operatorname{sgn}\psi)(x) := \frac{\overline{\psi(x)}}{|\psi(x)|},$$

which belongs to $\mathrm{L}^\infty(\mathbb{R}^n)$ and $|\psi(x)| = \psi(x)(\operatorname{sgn}\psi)(x)$ (this is the motivation for introducing the function sgn). Given $\varepsilon > 0$, denote $\psi_\varepsilon(x) := \left(|\psi(x)|^2 + \varepsilon^2\right)^{1/2}$, which converges $\psi_\varepsilon(x) \to |\psi(x)|$ pointwise as $\varepsilon \to 0$. Denote also $\operatorname{sgn}_\varepsilon \psi(x) := \overline{\psi(x)}/\psi_\varepsilon(x)$. In the following, the derivatives of $\mathrm{L}^1_{\mathrm{loc}}$ functions mean distributional derivatives.

Theorem 6.3.3 (Kato's Inequality). *If both $u, \Delta u$ are elements of $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, then $(\operatorname{sgn} u)\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, so it defines a distribution, and*

$$\Delta((\operatorname{sgn} u)u) = \Delta|u| \geq \operatorname{Re}\,((\operatorname{sgn} u)\Delta u),$$

that is to say,

$$\int_{\mathbb{R}^n} |u(x)|\Delta\phi(x)\,dx \geq \int_{\mathbb{R}^n} ((\operatorname{sgn} u)\Delta u(x))\,\phi(x)\,dx$$

for all $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$.

Example 6.3.4. It is instructive to play with some standard functions $u : \mathbb{R} \to \mathbb{C}$ in this inequality. For instance:

1. If $u(x) = e^{ax+ibx}$, $a, b \in \mathbb{R}$, then a straight computation shows that Kato's inequality reads $a^2 e^{ax} \geq (a^2 - b^2)e^{ax}$.
2. If $u(x) = x$, then Kato's inequality expresses that the Dirac delta distribution is positive, i.e., $\delta(x) \geq 0$.
3. If $u(x) = x^3$, then it turns into an equality $6|x| = 6|x|$.

We leave it as an exercise to check details in the above statements.

A very important consequence of this inequality implies that some standard Schrödinger operators in $\mathrm{L}^2(\mathbb{R}^n)$ are well posed; recall $H_0 = -\Delta$.

Corollary 6.3.5. *If there is $\beta \in \mathbb{R}$ so that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ satisfies $V(x) \geq \beta$, $\forall x \in \mathbb{R}^n$, then the operator*

$$H\psi := H_0\psi + V\psi, \qquad \psi \in \mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n),$$

is essentially self-adjoint.

Remark 6.3.6. The domain and action of the unique self-adjoint extension of H in Corollary 6.3.5 are described in Corollary 9.3.17, and its domain can be strictly smaller than dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$, even for $n = 1$; see Example 6.2.24.

Example 6.3.7. a) The operator $H_0 + \kappa/|x|$, $\kappa > 0$, with domain $C_0^\infty(\mathbb{R}^3)$ is essentially self-adjoint. Compare with Example 6.2.3 where negative κ is allowed.

b) The operator $H_0 + \kappa/|x|^j$, $j, \kappa > 0$, with domain $C_0^\infty(\mathbb{R}^n)$ is essentially self-adjoint if $n \geq 2j + 1$.

Remark 6.3.8. Note the great generality of Corollary 6.3.5, since the operator sum $H = -\Delta + V$ is defined on $C_0^\infty(\mathbb{R}^n)$ iff $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$; hence, if V is bounded from below, then H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ iff it is defined (as a sum of operators)!

Before proceeding to proofs, a rough idea and figurative arguments of how Theorem 6.3.3 can be used to get Corollary 6.3.5 are presented. Let $\lambda \in \mathbb{R}$ obeying $\lambda + \beta > 0$; so $V + \lambda > 0$. By Proposition 2.2.4iii), to show that the deficiency index $n_\pm(H) = 0$, it will suffice to show that the solution of

$$(H_0 + V + \lambda\mathbf{1})^*\, u = 0, \qquad u \in \mathrm{L}^2(\mathbb{R}^n) \subset \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n),$$

is solely $u = 0$ (recall that $(\mathrm{rng}\ T)^\perp = \mathrm{N}(T^*)$). Since H_0 is a positive operator, one could guess that $H_0|u| \geq 0$; the positivity of $V + \lambda$ and Kato's inequality will imply $H_0|u| \leq 0$, so that $H_0|u| = 0$ and, since $u \in \mathrm{L}^2$, $u = 0$. Now the proofs.

An important step in the proof of Kato's inequality is first to prove it when u is smooth, and then use the so-called mollifiers to create sequences of smooth functions, via convolutions, approximating certain distributions and nonsmooth functions.

Let $m \in C_0^\infty(\mathbb{R}^n)$, $m(x) \geq 0, \forall x$, with $\int_{\mathbb{R}^n} m(x)\, dx = 1$ (i.e., m is normalized). Given $r \neq 0$ (usually $r > 0$) set

$$m_r(x) := \frac{1}{r^n} m\left(\frac{x}{r}\right), \qquad u^{(r)} := u * m_r,$$

where $*$ denotes the convolution, which was recalled in Section 3.1. The family $r \mapsto m_r$ is called a *mollifier* and m a *mollifier generator*. The standard example of mollifier a generator is

$$m(x) = C \exp\left(-\frac{1}{1-x^2}\right), \qquad |x| < 1,$$

and $m(x) = 0$ for $|x| \geq 1$; C is just a normalization constant. Thus, $\int m_r(x) dx = 1$, $u^{(r)} \in C^\infty(\mathbb{R}^n)$ for all $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, $r \neq 0$, and, by Lemma 6.3.9,

$$\Delta (u^{(r)})_\varepsilon \, \geq \, \mathrm{Re} \, \left(\mathrm{sgn}_\varepsilon (u^{(r)}) \, \Delta u^{(r)}\right).$$

Lemma 6.3.9. *For any $v \in C^\infty(\mathbb{R}^n)$ one has, pointwise and in the distributional sense,*

$$\Delta v_\varepsilon \, \geq \, \mathrm{Re} \, \left(\mathrm{sgn}_\varepsilon (v) \, \Delta v\right).$$

Proof. Clearly $|v_\varepsilon| \geq |v|$. On differentiating $v_\varepsilon^2 = |v|^2 + \varepsilon^2$ one gets $2 v_\varepsilon \nabla v_\varepsilon = \overline{v} \nabla v + v \nabla \overline{v} = 2\mathrm{Re} \, (\overline{v} \, \nabla v)$. This expression will derive two relations. The first one is obtained by taking the divergence of it:

$$|\nabla v_\varepsilon|^2 + v_\varepsilon \, \Delta v_\varepsilon = \mathrm{Re} \, (\overline{v} \, \Delta v) + |\nabla v|^2.$$

The second one is

$$|\nabla v_\varepsilon| = \frac{|\mathrm{Re} \, (\overline{v} \, \nabla v)|}{|v_\varepsilon|} \leq \frac{|\overline{v} \, \nabla v|}{|v|} \leq |\nabla v|.$$

Combine these two relations to get

$$v_\varepsilon \, \Delta v_\varepsilon \geq \mathrm{Re} \, (\overline{v} \, \Delta v) \Longrightarrow \Delta v_\varepsilon \geq \mathrm{Re} \, \left((\mathrm{sgn}_\varepsilon v) \Delta v\right)$$

pointwise; thus, for every $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} v_\varepsilon \Delta \phi \, dx = \int_{\mathbb{R}^n} \Delta v_\varepsilon \, \phi \, dx \geq \mathrm{Re} \, \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon (v) \, \Delta v) \, \phi \, dx,$$

and the inequality also holds in the distributional sense. □

Exercise 6.3.10. If $\phi \in C_0^\infty(\mathbb{R}^n)$, write

$$\phi(x) - \phi^{(r)}(x) = \int_{\mathbb{R}^n} \left(\phi(x) - \phi(x-y)\right) \, m_r(y) \, dy,$$

for a fixed mollifier generator m, and use the uniform continuity of ϕ to show that $\lim_{r \downarrow 0} \|\phi^{(r)} - \phi\|_\infty = 0$.

Lemma 6.3.11.

a) *For any* $r > 0$ *the linear map* $\mathrm{L}^p(\mathbb{R}^n) \mapsto \mathrm{L}^p(\mathbb{R}^n)$, $u \mapsto u^{(r)}$, *is bounded and with norm* ≤ 1, *for all* $1 \leq p < \infty$.

b) *If* $u \in \mathrm{L}^p(\mathbb{R}^n)$, $1 \leq p < \infty$, *then* $\lim_{r\downarrow 0} \|u^{(r)} - u\|_p = 0$.

c) *If* $u \in \mathrm{L}^p(\mathbb{R}^n)$, $1 \leq p < \infty$, *then* $\Delta u^{(r)} \in \mathrm{L}^p(\mathbb{R}^n)$, $\forall r > 0$ (*the laplacian can be replaced by any derivative*).

d) *If* $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, *then* $u^{(r)} \to u$ *in the distributional sense as* $r \downarrow 0$.

Proof. a) Since $m_r \in \mathrm{L}^1(\mathbb{R}^n)$, for $u \in \mathrm{L}^p(\mathbb{R}^n)$ it follows by Young's inequality (Proposition 3.1.9) that (take "$r = p$" in Young's inequality)

$$\|u^{(r)}\|_p = \|u * m_r\|_p \leq \|u\|_p \|m_r\|_1 = \|u\|_p.$$

b) If $\phi \in C_0^\infty(\mathbb{R}^n)$ and Ω_ϕ is the support of ϕ, one has

$$\|\phi^{(r)} - \phi\|_p \leq \|\phi^{(r)} - \phi\|_\infty \, \ell(\Omega_\phi)^{\frac{1}{p}},$$

where $\ell(\cdot)$ denotes Lebesgue measure over $\mathbb{R}^n$. Hence $\|\phi^{(r)} - \phi\|_p \to 0$ as $r \to 0$ (see Exercise 6.3.10). Now take $u \in \mathrm{L}^p(\mathbb{R}^n)$. Given $\varepsilon > 0$, choose $\phi \in C_0^\infty(\mathbb{R}^n)$ so that $\|u - \phi\|_p < \varepsilon$. By triangle inequality and a), for r small enough,

$$\begin{aligned}\|u^{(r)} - u\|_p &\leq \|u^{(r)} - \phi^{(r)}\|_p + \|\phi^{(r)} - \phi\|_p + \|\phi - u\|_p \\ &< \|u - \phi\|_p + \varepsilon + \varepsilon < 3\varepsilon.\end{aligned}$$

Item b) follows.

c) It is a consequence of

$$\frac{\partial}{\partial x_j} u^{(r)} = \frac{\partial}{\partial x_j}(u * m_r) = u * \frac{\partial}{\partial x_j} m_r$$

and Young's inequality, i.e.,

$$\left\| \frac{\partial}{\partial x_j} u^{(r)} \right\|_p \leq \|u\|_p \left\| \frac{\partial}{\partial x_j} m_r \right\|_1.$$

d) Since $u^{(r)} \in C^\infty(\mathbb{R}^n)$ it also defines a distribution. If $\phi \in C_0^\infty(\mathbb{R}^n)$ and Ω_ϕ is the support of ϕ, a change of variable and Fubini's theorem lead to

$$u^{(r)}(\phi) = \int_{\mathbb{R}^n} u^{(r)}(x)\, \phi(x)\, dx = \int_{\mathbb{R}^n} (-1)^n u(x) \phi^{(-r)}(x)\, dx = (-1)^n u(\phi^{(-r)}),$$

and so

$$\left| u(\phi) - u^{(r)}(\phi) \right| = \left| u\left(\phi - (-1)^n \phi^{(-r)}\right) \right| \leq \left\| \phi - (-1)^n \phi^{(-r)} \right\|_\infty \int_{\Omega_\phi} |u(x)|\, dx.$$

Note that $(-1)^n \phi^{(-r)} = \phi * \tilde{m}_r$, where $\tilde{m}(x) := m(-x)$ also satisfies the assumptions required for $\tilde{m}_r$ to be a mollifier; so $\|\phi - (-1)^n \phi^{(-r)}\|_\infty$ vanishes as $r \to 0$ by Exercise 6.3.10. Therefore, $u^{(r)} \to u$ in the distributional sense. □

Other properties needed to complete the proof of Corollary 6.3.5 will be collected in the following proposition.

Proposition 6.3.12. *Let $u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ and $r \downarrow 0$. Then:*

i) *There exists a subsequence $u^{(r)}(x)$ obeying $u^{(r)}(x) \to u(x)$ a.e., and so also $(\operatorname{sgn}_\varepsilon u^{(r)})(x) \to \operatorname{sgn}_\varepsilon u(x)$ a.e.*

ii) *$\Delta u^{(r)} = (\Delta u)^{(r)}$ and, if also $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, one has $\Delta u^{(r)} \to \Delta u$ in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ (that is, $\int_K |u^{(r)} - u|\, dx \to 0$ for every compact $K \subset \mathbb{R}^n$) and a.e. as well.*

Proof. i) Let m be a mollifier generator with support Ω_m. Let K be a compact subset of $\mathbb{R}^n$ and χ_K its characteristic function. By the definition of convolution and Fubini,

$$\left\|(u^{(r)} - u)\chi_K\right\|_1 \le \int_{\Omega_m} m(y)\, \|(u(x) - u(x - ry))\chi_K\|_1\, dy.$$

It turns out that $\|(u(x) - u(x - ry))\chi_K\|_1$ vanishes as $r \to 0$ (see the proof of Lemma 13.3.2), and so $\left\|(u^{(r)} - u)\chi_K\right\|_1 \to 0$. Thus, $u^{(r)} \to u$ in $\mathrm{L}^1(K)$, for any compact K. Hence there is a subsequence with a.e. convergence.

ii) After an interchange of integration and differentiation (by dominated convergence), it is simple to verify that $\Delta u^{(r)} = (\Delta u)^{(r)}$. By hypothesis $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}$; so the convergences stated in ii) follow by i). □

Proof. [**Corollary 6.3.5**] Pick λ so that $\lambda + \beta > 0$ and $u \in \operatorname{dom} H^* \subset \mathrm{L}^2(\mathbb{R}^n)$ a solution of $(H + \lambda\mathbf{1})^* u = 0$, which amounts to

$$0 = \langle (H + \lambda\mathbf{1})^* u, \phi\rangle = \langle u, (H + \lambda\mathbf{1})\phi\rangle, \qquad \forall \phi \in C_0^\infty(\mathbb{R}^n),$$

and since $H + \lambda\mathbf{1} = -\Delta + V + \lambda\mathbf{1}$ one finds that, in the distributional sense,

$$0 = -\Delta u + (V + \lambda\mathbf{1})u.$$

Since $u, Vu \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, it follows that $\Delta u = (V + \lambda\mathbf{1})u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ and Theorem 6.3.3 implies

$$\Delta|u| \ge \operatorname{Re}((\operatorname{sgn} u)\, \Delta u) = \operatorname{Re}((\operatorname{sgn} u)\,(V + \lambda\mathbf{1})u) = (V + \lambda\mathbf{1})|u| \ge 0.$$

However, $|u|$ is not ensured to belong to $\operatorname{dom} \Delta$, and a "regularization process" is necessary. Thus, for any $r > 0$, $\Delta|u|^{(r)} = \Delta|u| * m_r \ge 0$ pointwise and in the distributional sense; also, by Lemma 6.3.11c), $\Delta|u|^{(r)} \in \mathrm{L}^2(\mathbb{R}^n)$ and so

$$\left\langle |u|^{(r)}, \Delta|u|^{(r)}\right\rangle = \int_{\mathbb{R}^n} |u|^{(r)} \Delta|u|^{(r)}\, dx \ge 0.$$

On the other hand, again by Lemma 6.3.11c), $\partial|u|^{(r)}/\partial x_j, \Delta|u|^{(r)} \in \mathrm{L}^2(\mathbb{R}^n)$, consequently $|u|^{(r)} \in \mathcal{H}^2(\mathbb{R}^n) = \operatorname{dom} H_0$ (see Section 3.2); hence (recall $H_0 \ge 0$)

$$\left\langle |u|^{(r)}, \Delta|u|^{(r)}\right\rangle \le 0.$$

Combining with the other inequality one finds $\langle |u|^{(r)}, \Delta |u|^{(r)}\rangle = 0$, and thus $|u|^{(r)} = 0$. Since $u \in \mathrm{L}^2(\mathbb{R}^n)$, by Lemma 6.3.11b) one can consider a subsequence and assume that $|u|^{(r)} \to |u|$ a.e. as $r \downarrow 0$, so that $u = 0$. By Proposition 2.2.4, the deficiency indices of H are null. The corollary is proved. □

Exercise 6.3.13. Use results of Section 3.4 to show that if $\psi \in \mathrm{dom}\, H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and $\langle \psi, H_0\psi\rangle = 0$, then $\psi = 0$. This was used in the proof of Corollary 6.3.5.

Proof. [**Theorem 6.3.3**] Let $u, \Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$. Thus, $u^{(r)} \in C^\infty(\mathbb{R}^n)$ and, by Lemma 6.3.9,

$$\Delta (u^{(r)})_\varepsilon \geq \mathrm{Re}\, \left(\mathrm{sgn}_\varepsilon (u^{(r)})\, \Delta u^{(r)}\right), \qquad \forall \varepsilon, r > 0,$$

that is, for every $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} u_\varepsilon^{(r)}\, \Delta\phi\, dx \geq \mathrm{Re}\, \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)})\, \Delta u^{(r)} \phi\, dx.$$

The point now is to take the limit $r \downarrow 0$ in both terms of this inequality. Since $u, \Delta u \in \mathrm{L}^1_{\mathrm{loc}}$, by Lemma 6.3.11c), d) and Proposition 6.3.12ii), $u^{(r)} \to u$ and $\Delta u^{(r)} = (\Delta u)^{(r)} \to \Delta u$ in $\mathrm{L}^1_{\mathrm{loc}}$ and in the distributional sense. By passing to a subsequence one can suppose that $u^{(r)} \to u$ and $\Delta u^{(r)} = (\Delta u)^{(r)} \to \Delta u$ a.e. Together with the inequality

$$\begin{aligned} |u_\varepsilon^{(r)} - u_\varepsilon| &= \left| \left(|u^{(r)}|^2 + \varepsilon^2\right)^{1/2} - \left(|u|^2 + \varepsilon^2\right)^{1/2} \right| \\ &= \frac{\left| |u^{(r)}|^2 - |u|^2 \right|}{\left(|u^{(r)}|^2 + \varepsilon^2\right)^{1/2} + \left(|u|^2 + \varepsilon^2\right)^{1/2}} \\ &\leq \left| |u^{(r)}| - |u| \right| \leq \left| u^{(r)} - u \right| \end{aligned}$$

the convergence $u^{(r)} \to u$ implies that $u_\varepsilon^{(r)} \to u_\varepsilon$ in $\mathrm{L}^1_{\mathrm{loc}}$ and a.e. as $r \downarrow 0$ (for a subsequence), and so

$$\int_{\mathbb{R}^n} u_\varepsilon^{(r)}\, \Delta\phi\, dx \to \int_{\mathbb{R}^n} u_\varepsilon\, \Delta\phi\, dx.$$

Taking into account the uniform boundedness of $\mathrm{sgn}_\varepsilon u^{(r)}$ (that is, $|\mathrm{sgn}_\varepsilon u^{(r)}| \leq 1$) and $\Delta u^{(r)} \to \Delta u$, in a similar way it is found that (for a subsequence)

$$\mathrm{sgn}_\varepsilon (u^{(r)})\, \left(\Delta u^{(r)} - \Delta u\right) \to 0,$$

in the distributional sense as $r \downarrow 0$. By dominated convergence

$$\int_{\mathbb{R}^n} \mathrm{sgn}_\varepsilon (u^{(r)}) \Delta u\, \phi\, dx \to \int_{\mathbb{R}^n} \mathrm{sgn}_\varepsilon (u) \Delta u\, \phi\, dx, \qquad r \to 0.$$

By collecting these convergences and taking the appropriate subsequence $r \downarrow 0$, for $0 \leq \phi \in C_0^\infty(\mathbb{R}^n)$,

$$\begin{aligned}\mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)})\, \Delta u^{(r)} \phi \, dx &= \mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)}) \left(\Delta u^{(r)} - \Delta u\right) \phi \, dx \\ &\quad + \mathrm{Re} \int_{\mathbb{R}^n} (\mathrm{sgn}_\varepsilon u^{(r)})\, \Delta u \phi \, dx \\ &\quad \to \int_{\mathbb{R}^n} \mathrm{sgn}_\varepsilon(u) \Delta u \, \phi \, dx\end{aligned}$$

as $r \downarrow 0$, that is,

$$\int_{\mathbb{R}^n} u_\varepsilon \, \Delta\phi \, dx \geq \mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}_\varepsilon u)\, \Delta u) \phi \, dx,$$

which is equivalent to the distributional inequality

$$\Delta u_\varepsilon \geq \mathrm{Re}\, ((\mathrm{sgn}_\varepsilon u)\, \Delta u).$$

Since $u_\varepsilon \to |u|$ uniformly as $\varepsilon \to 0$, the left-hand side in the above integral inequality converges to $\int |u| \, \Delta\phi \, dx$. Now $\mathrm{sgn}_\varepsilon u \to \mathrm{sgn}\, u$ as $\varepsilon \to 0$ and since $|\mathrm{sgn}_\varepsilon \Delta u| \leq |\Delta u|$ and $\Delta u \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$, one can apply dominated convergence on the right-hand side of the above integral inequality to get

$$\mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}_\varepsilon u)\, \Delta u) \phi \, dx \to \mathrm{Re} \int_{\mathbb{R}^n} ((\mathrm{sgn}\, u)\, \Delta u) \phi \, dx$$

as $\varepsilon \to 0$. Therefore, the final result, i.e., Kato's inequality, follows by taking the limit $\varepsilon \to 0$ in the latter distributional inequality. □

Remark 6.3.14. In [LeiS81] there is a generalization of Corollary 6.3.5 that includes magnetic fields; for an introduction to Schrödinger operators with magnetic fields see Sections 10.5 and 12.4. The Leinfelder-Simader proof also makes use of Kato's inequality and their theorem reads as follows: Let $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ be bounded from below, the components of the magnetic vector potential $A_j \in \mathrm{L}^4_{\mathrm{loc}}(\mathbb{R}^n)$, $j = 1, \ldots, n$, and the distributional divergent $(\sum_j \partial_j A_j) \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$; then the Schrödinger operator with magnetic field

$$H = \sum_{j=1}^{n} \left(-i \frac{\partial}{\partial x_j} - \frac{e}{c} A_j \right)^2 + V, \qquad \mathrm{dom}\, H = C_0^\infty(\mathbb{R}^n),$$

is essentially self-adjoint.