Reed/Simon II

X.2 Perturbations of self-adjoint operators

In this section we will prove several theorems which say that if A is self-adjoint and B is not too large compared to A, then $A + B$ is self-adjoint. These theorems have fundamental applications in quantum mechanics. First we define what we mean by a "small" perturbation.

Definition Let A and B be densely defined linear operators on a Hilbert space $\mathscr{H}$. Suppose that:

(i) $D(B) \supset D(A)$
(ii) For some a and b in $\mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\| \le a\|A\varphi\| + b\|\varphi\| \tag{X.19a}$$

Then B is said to be **A-bounded**. The infimum of such a is called the **relative bound** of B with respect to A. If the relative bound is zero, we say that B is **infinitesimally small** with respect to A and write $B << A$. We remark that usually b must be chosen larger as a is chosen smaller.

Sometimes, it is convenient to replace (ii) in the above definition by

(iii) For some $\tilde{a}, \tilde{b} \in \mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\|^2 \le \tilde{a}^2\|A\varphi\|^2 + \tilde{b}^2\|\varphi\|^2 \tag{X.19b}$$

If (iii) holds, then (ii) holds with $a = \tilde{a}$, $b = \tilde{b}$. And if (ii) holds, we can conclude that (iii) holds with $\tilde{a}^2 = (1 + \varepsilon)a^2$, $\tilde{b}^2 = (1 + \varepsilon^{-1})b^2$ for each $\varepsilon > 0$. Thus, the infimum over all a in (ii) is equal to the infimum over all $\tilde{a}$ in (iii). Note that to prove estimates of the form (ii) or (iii) it is sufficient to prove them on a core for A.

A fundamental perturbation result is:

Theorem X.12 (the Kato–Rellich theorem) Suppose that A is self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A. Further, if A is bounded below by M, then $A + B$ is bounded below by $M - \max\{b/(1 - a), a|M| + b\}$ where a and b are given by (X.19a).

Proof We will show that $\mathrm{Ran}(A + B \pm i\mu_\circ) = \mathscr{H}$ for some $\mu_\circ > 0$. For $\varphi \in D(A)$, we have

$$\|(A + i\mu)\varphi\|^2 = \|A\varphi\|^2 + \mu^2\|\varphi\|^2$$

Letting $\varphi = (A + i\mu)^{-1}\psi$, we conclude from this that $\|A(A + i\mu)^{-1}\| \le 1$ and $\|(A + i\mu)^{-1}\| \le \mu^{-1}$. Therefore, applying (X.19a) with $\varphi = (A + i\mu)^{-1}\psi$, we find that

$$\begin{aligned}\|B(A + i\mu)^{-1}\psi\| &\le a\|A(A + i\mu)^{-1}\psi\| + b\|(A + i\mu)^{-1}\psi\| \\ &\le \left(a + \frac{b}{\mu}\right)\|\psi\|\end{aligned}$$

Thus, for $\mu_\circ$ large, $C = B(A + i\mu_\circ)^{-1}$ has norm less than one, since $a < 1$. This implies that $-1 \notin \sigma(C)$, so $\mathrm{Ran}(I + C) = \mathscr{H}$. Since A is self-adjoint, $\mathrm{Ran}(A + i\mu_\circ) = \mathscr{H}$ also. Thus the equation

$$(I + C)(A + i\mu_\circ)\varphi = (A + B + i\mu_\circ)\varphi \qquad \text{for} \quad \varphi \in D(A)$$

implies that $\mathrm{Ran}(A + B + i\mu_\circ) = \mathscr{H}$. The proof that $\mathrm{Ran}(A + B - i\mu_\circ) = \mathscr{H}$ is the same. Thus, by the fundamental criterion (Theorem VIII.3), $A + B$ is self-adjoint on $D(A)$.

It is a direct consequence of (X.19) that $D(\overline{(A + B) \restriction D_0}) \supset D(\overline{A \restriction D_0})$, so $A + B$ is essentially self-adjoint on any core of A.

Finally we prove the semiboundedness statement. Suppose that $t \in \mathbb{R}$ and $-t < M$. Then $\mathrm{Ran}(A + t) = \mathscr{H}$ and the same estimates as before show that $\|B(A + t)^{-1}\| < 1$ if

$$-t < M - \max\left\{\frac{b}{1 - a}, a|M| + b\right\}$$

Thus for such t, $\mathrm{Ran}(A + B + t) = \mathscr{H}$ and $(A + B + t)^{-1} = (A + t)^{-1} \times (I + C)^{-1}$ which implies that $-t \in \rho(A + B)$. ∎

The following symmetric form of the Kato–Rellich theorem is sometimes useful. For an application, see Example 3 in the Appendix to Section X.1.

Theorem X.13 Let A and C be symmetric operators. Suppose that D is a linear subspace satisfying $D \subseteq D(A)$, $D \subseteq D(C)$, and that

$$\|(A - C)\varphi\| \le a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\|$$

for all $\varphi \in D$, where $a < 1$. Then,

(a) A is essentially self-adjoint on D if and only if C is essentially self-adjoint on D.
(b) $D(\overline{A \restriction D}) = D(\overline{C \restriction D})$.

Proof Let $B = A - C$ with $D(B) = D$ and define $F(\alpha) = C + \alpha B$ for $0 \le \alpha \le 1$. Then $F(0) = C$, $F(1) = A$ and $C\varphi = F(\alpha)\varphi - \alpha B\varphi$, $A\varphi = F(\alpha)\varphi + (1-\alpha)B\varphi$ for all $\varphi \in D$. Thus, the inequality in the hypothesis implies that

$$\begin{aligned}\|B\varphi\| &\le a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\| \\ &\le 2a\|F(\alpha)\varphi\| + a\|B\varphi\| + b\|\varphi\|\end{aligned}$$

or

$$\|B\varphi\| \le \frac{2a}{1-a}\|F(\alpha)\varphi\| + \frac{b}{1-a}\|\varphi\| \tag{X.20}$$

Let $0 \le \alpha' \le 1$. If $2a\alpha'/(1-a) < 1$, (X.20) and Theorem X.12 imply that $F(\alpha + \alpha') = F(\alpha) + \alpha' B$ is essentially self-adjoint on D if and only if $F(\alpha)$ is. Thus, starting with $\alpha = 0$ and applying this result finitely many times, we conclude (a). The reader is asked (Problem 13) to follow similar steps to prove (b). ∎

The following theorem extends Theorem X.12 to the case of relative bound one, but it has a slightly weaker conclusion.

Theorem X.14 (Wüst's theorem) Let A be self-adjoint and B be symmetric with $D(B) \supset D(A)$. Suppose that for some b and all $\varphi \in D(A)$,

$$\|B\varphi\| \le \|A\varphi\| + b\|\varphi\| \tag{X.21a}$$

Then $A + B$ is *essentially* self-adjoint on $D(A)$ or any core for A.

Proof By a simple argument, it is enough to show that $A + B$ is essentially self-adjoint on $D(A)$. Suppose that $(A + B + i)^*h = 0$. For each $t < 1$, $A + tB$ is self-adjoint on $D(A)$ by Theorem X.12. Thus, there exists $\varphi_t \in D(A)$ with $\|\varphi_t\| \le \|h\|$, so that $(A + tB + i)\varphi_t = h$. Define $\psi_t = h - (t-1)B\varphi_t$. Then a short calculation shows that $(\psi_t, h) = 0$. By (X.21a),

$$\begin{aligned}\|A\varphi_t\| &\le \|(A + tB)\varphi_t\| + \|tB\varphi_t\| \\ &\le \|(A + tB)\varphi_t\| + t\|A\varphi_t\| + tb\|\varphi_t\|\end{aligned}$$

so

$$(1-t)\|A\varphi_t\| \le \|(A + tB)\varphi_t\| + tb\|\varphi_t\|$$

Since $\|(A + tB)\varphi_t\|^2 = \|h\|^2 - \|\varphi_t\|^2$, this implies that $(1-t)\|A\varphi_t\|$ is bounded as $t \uparrow 1$. It follows by using (X.21a) again that $(1-t)\|B\varphi_t\|$ and therefore also $\|\psi_t\|$ are bounded as $t \uparrow 1$. Now let $\eta \in D(A)$. Then

$$\lim_{t\uparrow 1}(\psi_t - h, \eta) = \lim_{t\uparrow 1}(t-1)(\varphi_t, B\eta) = 0$$

Since the $\|\psi_t\|$ are uniformly bounded, we conclude that $h = w\text{-}\lim \psi_t$. But then $(h, h) = \lim(h, \psi_t) = 0$ so $h = 0$. We conclude that $\operatorname{Ker}(A + B + i)^* = \{0\}$. The proof that $\operatorname{Ker}(A + B - i)^* = \{0\}$ is similar. ∎

Choosing $A = -B$ shows that "essentially self-adjoint" cannot be replaced by "self-adjoint" in the statement of Theorem X.14. We also note that there are counterexamples which show that the conclusion of the theorem may be false if the relative bound is larger than one. (See Example 4 at the end of this section.) We also note that according to our discussion of (X.19a) and (X.19b), the condition (X.21a) needed to apply Theorem X.14 is itself implied by the condition

$$\|B\varphi\|^2 \le \|A\varphi\|^2 + b^2\|\varphi\|^2 \tag{X.21b}$$

which is equivalent to the operator inequality

$$B^2 \le A^2 + b^2 \tag{X.21c}$$

We come now to Kato's basic application of the Kato–Rellich theorem to atomic Hamiltonians. First, we define some new classes of functions.

Definition Let $\langle M, \mu\rangle$ be a measure space. The set of measurable functions f on M which can be written $f = f_1 + f_2$ where $f_1 \in L^r(M, d\mu)$ and $f_2 \in L^s(M, d\mu)$ will be denoted by $L^r(M, d\mu) + L^s(M, d\mu)$.

Theorem X.15 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $-\Delta + V(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $D(-\Delta)$.

Proof Since V is real-valued, the operator of multiplication by V is self-adjoint on

$$D(V) = \{\varphi \mid \varphi \in L^2(\mathbb{R}^3), V\varphi \in L^2(\mathbb{R}^3)\}$$

Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then

$$\|V\varphi\|_2 \le \|V_1\|_2\|\varphi\|_\infty + \|V_2\|_\infty\|\varphi\|_2 \tag{X.22}$$

so $D(V) \supset C_0^\infty(\mathbb{R}^3)$. By Theorem IX.28, given any $a > 0$, there is a $b > 0$ so that

$$\|\varphi\|_\infty \le a\|\Delta\varphi\|_2 + b\|\varphi\|_2 \tag{X.23}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. This inequality and (X.22) give

$$\|V\varphi\|_2 \le a\|V_1\|_2\|-\Delta\varphi\|_2 + (b + \|V_2\|_\infty)\|\varphi\|_2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. Thus V is $-\Delta$-bounded with arbitrarily small bound on $C_0^\infty(\mathbb{R}^3)$. Since $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, the Kato–Rellich theorem implies that $-\Delta + V$ is also essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 1 Let $V(r) = -e^2/r$ where $r = \sqrt{x^2 + y^2 + z^2}$. Then $-\Delta - e^2/r$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Theorem X.16 (Kato's theorem) Let $\{V_k\}_{k=1}^m$ be a collection of real-valued measurable functions each of which is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let $V_k(\mathbf{y}_k)$ be the multiplication operator on $L^2(\mathbb{R}^{3n})$ obtained by choosing $\mathbf{y}_k$ to be three coordinates of $\mathbb{R}^{3n}$. Then $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$, where Δ denotes the Laplacian on $\mathbb{R}^{3n}$.

Proof First we consider one of the functions V_k separately. By a rotation of variables we may assume the variables in $V_k(\cdot)$ are x_1, x_2, x_3. (This is because $\|\cdot\|_2$, $\|\cdot\|_\infty$, and $-\Delta$ are invariant under rotations of coordinates.) Let Δ_1 denote the Laplacian with respect to x_1, x_2, x_3. By the estimate (X.23), together with the "equivalence" of the bounds (X.19a) and (X.19b), we have for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$,

$$\begin{aligned}
\|V_k\varphi\|^2_{L^2(\mathbb{R}^{3n})} &\le a^2 \int |-\Delta_1\varphi(x_1, \ldots, x_{3n})|^2\, dx_1 \cdots dx_{3n} \\
&\quad + b^2 \int |\varphi(x_1, \ldots, x_{3n})|^2\, dx_1 \cdots dx_{3n} \\
&= a^2 \int \left| \sum_{i=1}^3 p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2\|\varphi\|^2 \\
&\le a^2 \int \left| \sum_{i=1}^n p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2\|\varphi\|^2 \\
&= a^2\|-\Delta\varphi\|^2 + b^2\|\varphi\|^2
\end{aligned}$$

Thus, using the Schwarz inequality, one easily concludes that

$$\left\| \sum_{k=1}^m V_k(\mathbf{y}_k)\varphi \right\|^2 \le m^2a^2\|-\Delta\varphi\|^2 + m^2b^2\|\varphi\|^2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$. Since a may be chosen as small as we like, we conclude that $\sum_{k=1}^m V_k(\mathbf{y}_k)$ is infinitesimally small with respect to $-\Delta$. Thus, by the Kato–Rellich theorem, $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 2 (atomic Hamiltonians) Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$ be orthogonal coordinates for $\mathbb{R}^{3n}$. Then

$$-\sum_{i=1}^n \Delta_i - \sum_{i=1}^n \frac{ne^2}{|\mathbf{x}_i|} + \sum_{i<j}^n \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$.

For an application of the Kato–Rellich theorem to ordinary differential operators, see Problem 7.

There is a form analogue of the Kato–Rellich theorem which can be used when the form $(B\varphi, \varphi)$ is "small" with respect to the form $(A\varphi, \varphi)$ even though B may not be A-bounded. Although the statement of the theorem below is similar to Theorem X.12, the proof is very different.

Theorem X.17 (the KLMN theorem) Let A be a positive self-adjoint operator and suppose that $\beta(\varphi, \psi)$ is a symmetric quadratic form on $Q(A)$ such that

$$|\beta(\varphi, \varphi)| \le a(\varphi, A\varphi) + b(\varphi, \varphi) \qquad \text{all } \varphi \in D(A) \tag{X.24}$$

for some $a < 1$ and $b \in \mathbb{R}$. Then there exists a unique self-adjoint operator C with $Q(C) = Q(A)$ and

$$(\varphi, C\psi) = (\varphi, A\psi) + \beta(\varphi, \psi) \qquad \text{all } \varphi, \psi \in Q(C)$$

C is bounded below by $-b$ and any domain of essential self-adjointness for A is a form core for C.

Proof Define a form $\gamma(\varphi, \psi) = (\varphi, A\psi) + \beta(\varphi; \psi)$ on $Q(A)$. By (X.24),

$$\begin{aligned}
\gamma(\varphi, \varphi) &\ge (1 - a)(\varphi; A\varphi) - b(\varphi, \varphi) \\
&\ge -b(\varphi, \varphi)
\end{aligned}$$

since A is positive. Thus γ is bounded from below by $-b$. Furthermore

$$\begin{aligned}
(1 - a)(\varphi, A\varphi) + (\varphi, \varphi) &\le \gamma(\varphi, \varphi) + (b + 1)(\varphi, \varphi) \\
&\le (1 + a)(\varphi, A\varphi) + (2b + 1)(\varphi, \varphi)
\end{aligned}$$

Thus the $\|\cdot\|_{+1,A}$ and $\|\cdot\|_{+1,\gamma}$ norms are equivalent on $Q(A)$. Since $Q(A)$ is closed under $\|\cdot\|_{+1,A}$, it is closed under $\|\cdot\|_{+1,\gamma}$. Thus γ is a semi-bounded, closed quadratic form on $Q(A)$. The theorem now follows from the statement and proof of Theorem VIII.15. ∎

This theorem suggests that we define:

Definition Let A be a positive self-adjoint operator. Suppose that B is a self-adjoint operator which satisfies:

(i) $Q(B) \supset Q(A)$
(ii) $|(\varphi, B\varphi)| \leq a(\varphi, A\varphi) + b(\varphi, \varphi)$, $\varphi \in Q(A)$

for some $a > 0$ and $b \in \mathbb{R}$. Then B is said to be **relatively form-bounded** with respect to A. If a can be chosen arbitrarily small, B is said to be **infinitesimally form-bounded** with respect to A (written $B \prec\prec A$).

If B is self-adjoint and relatively form-bounded ($a < 1$) with respect to a positive self-adjoint operator A, then the KLMN theorem gives meaning to $A + B$. We emphasize that this definition of "$A + B$" may *differ* from the operator sum. There are examples where B is relatively form-bounded with respect to A even though $D(A) \cap D(B) = \{0\}$. In fact, as the following example shows, the form β in the KLMN theorem need not be a form arising from an operator or even a closable form.

Example 3 Let $A = -d^2/dx^2$ on $\mathbb{R}$ and define $\beta(\varphi, \psi) = \overline{\varphi}(0)\psi(0)$ for $\varphi, \psi \in C_0^\infty(\mathbb{R})$. By Sobolev's lemma, for any $a > 0$, there is a b so that

$$\|\varphi\|_\infty^2 \leq a(\varphi, -\varphi'') + b\|\varphi\|^2$$

Thus we can apply the KLMN theorem to define $-d^2/dx^2 + \delta$! A function $\psi \in Q(-d^2/dx^2) \subset C_\infty(\mathbb{R})$ is in the domain of $-d^2/dx^2 + \delta$ if and only if $-\psi''(x) + \delta(x)\psi(0) \in L^2(\mathbb{R})$ where the derivative is taken in the sense of distributions. For example, if $\psi(x)$ looks like $1 + \frac{1}{2}|x|$ near zero and is C^∞ away from zero with compact support, then $\psi \in D(-d^2/dx^2 + \delta(x))$, since the $\delta(x)\psi(0)$ will just cancel the term $-\delta(x)\psi(x)$ which appears in $-\psi''(x)$. Thus, $D(A + B)$ can contain vectors which are neither in $D(A)$ nor in $D(B)$ but for which there are cancellations in "$A\psi + B\psi$."

The following theorem shows that if B is A-bounded, then B is form-bounded with respect to A.

Theorem X.18 Let A be a positive self-adjoint operator and suppose that B is self-adjoint. Then

(a) If B is A-bounded with relative bound a, then B is form-bounded with respect to A with relative bound a.
(b) $B << A$ implies $B \prec\prec A$.

Proof Let $C^\infty(A) = \bigcap_{n=1}^\infty D(A^n)$, $\mu > 0$, and let $\mathscr{H}_n$ be the closure of $C^\infty(A)$ under the norm $\|\varphi\|_n = \|(A + I)^{n/2}\varphi\|$, $n = 0, \pm 1, \pm 2, \ldots$. Then a map C from $C^\infty(A)$ to $\mathscr{H}$ extends to be a bounded operator from $\mathscr{H}_m$ to $\mathscr{H}_{-n}$ if and only if $(A + I)^{-n/2}C(A + I)^{-m/2}$ is bounded on $C^\infty(A)$ in the usual operator norm.

If B is A-bounded with relative bound a, then $B(A + \mu I)^{-1}$ and $(A + \mu I)^{-1}B$ are bounded by $(a + b/\mu)$. The interpolation argument in Example 3 of the Appendix to Section IX.4 proves that

$$(A + \mu I)^{-1/2}B(A + \mu I)^{-1/2}$$

is also bounded by $a + (b/\mu)$ and it follows immediately that

$$(\varphi, B\varphi) \leq \left(a + \frac{b}{\mu}\right)(\varphi, (A + \mu I)\varphi)$$

for $\varphi \in D_\infty(A)$. Since $\mu > 0$ is arbitrary, parts (a) and (b) follow. ∎

The KLMN theorem can sometimes be used to define Hamiltonians when Rellich's theorem does not apply. To see that the $L^2 + L^\infty$ class of potentials does not include all "reasonable" potentials, we remark that it is venerable physical folklore that potentials of the form $V_\alpha(r) = -r^{-\alpha}$ produce reasonable quantum dynamics as long as $\alpha < 2$. But $V_\alpha \in L^2 + L^\infty$ only if $\alpha < \frac{3}{2}$! Thus we cannot use Rellich's theorem if $\frac{3}{2} \leq \alpha < 2$ (see Problem 14). However, we can use the KLMN theorem. First, we prove an estimate:

Lemma (the uncertainty principle lemma) Let $\psi \in C_0^\infty(\mathbb{R}^3)$. Then

$$\int_{\mathbb{R}^3} \frac{1}{4r^2}\,|\psi(\mathbf{r})|^2\,d\mathbf{r} \leq \int_{\mathbb{R}^3} |\nabla\psi(\mathbf{r})|^2\,d\mathbf{r}$$

Proof We may suppose that ψ is real-valued. Then,

$$\nabla(r^{+1/2}\psi) = r^{1/2}\nabla\psi + \tfrac{1}{2}r^{-3/2}\mathbf{r}\psi$$

Thus, if $r \neq 0$,

$$\begin{aligned}|\nabla\psi|^2 &= |r^{-1/2}\nabla(r^{1/2}\psi) - \tfrac{1}{2}r^{-2}\mathbf{r}\psi|^2 \\ &\geq -r^{-3/2}\psi\frac{\partial}{\partial r}(r^{1/2}\psi) + \frac{1}{4}r^{-2}|\psi|^2 \\ &= -\frac{1}{2r^2}\frac{\partial}{\partial r}(r|\psi|^2) + \frac{1}{4}r^{-2}|\psi|^2\end{aligned}$$

So,

$$\int |\nabla\psi|^2\,d\mathbf{r} \geq \int \frac{1}{4r^2}\,|\psi|^2\,d\mathbf{r} - \frac{1}{2}\int_0^\infty \frac{\partial}{\partial r}\int_{S_2} r|\psi|^2\,d\Omega\,dr$$

$$= \int \frac{1}{4r^2}\,|\psi|^2\,d\mathbf{r} \quad \blacksquare$$

Proposition If $\alpha < 2$, then $-r^{-\alpha} \prec\prec -\Delta$.

Proof Let $\varphi \in C_0^\infty$ and let $a > 0$ be given. Choose $\varepsilon > 0$ so that $1/r^\alpha \leq a/4r^2$ for all $r \leq \varepsilon$. Then

$$\int_{\mathbb{R}^3} \frac{1}{r^\alpha}|\varphi(\mathbf{r})|^2\,d\mathbf{r} = \int_{|\mathbf{r}|\leq\varepsilon} \frac{1}{r^\alpha}\,|\varphi(\mathbf{r})|^2\,d\mathbf{r} + \int_{|\mathbf{r}|>\varepsilon} \frac{1}{r^\alpha}\,|\varphi(\mathbf{r})|^2\,d\mathbf{r}$$

$$\leq a\int_{|\mathbf{r}|\leq\varepsilon} |\nabla\varphi(\mathbf{r})|^2\,d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{|\mathbf{r}|>\varepsilon} |\varphi(\mathbf{r})|^2\,d\mathbf{r}$$

$$\leq a\int_{\mathbb{R}^3} (-\Delta\varphi(\mathbf{r}))\overline{\varphi(\mathbf{r})}\,d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{\mathbb{R}^3} |\varphi(\mathbf{r})|^2\,d\mathbf{r} \quad \blacksquare$$

This proposition shows that for $\frac{3}{2} \leq \alpha < 2$, we can use the KLMN theorem to define $-\Delta - r^{-\alpha}$. $L^2 + L^\infty$ is the natural class of potentials associated with the Kato–Rellich theorem (see Problem 14). There is no completely natural class associated with the KLMN theorem.

Definition A measurable function V on $\mathbb{R}^3$ is called a **Rollnik potential** if

$$\|V\|_R^2 \equiv \int_{\mathbb{R}^3} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\,d^3x\,d^3y < \infty$$

We denote the set of Rollnik potentials by R.

R turns out to be a vector space which is complete under the Rollnik norm $\|\cdot\|_R$. Moreover, by Sobolev's inequality (IX.19), $L^{3/2}(\mathbb{R}^3) \subset R$; in particular $r^{-\alpha} \in R + L^\infty$ if $\alpha < 2$. The analogue of the Kato theorem is:

Theorem X.19

(a) If $V \in R + L^\infty(\mathbb{R}^3)$, then $V \prec\prec -\Delta$

(b) If $V_i(\mathbf{r})$ and $V_{ij}(\mathbf{r})$ are all in $R + L^\infty$ and

$$V = \sum V_i(\mathbf{r}_i) + \sum_{i,j=1}^{N} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

on $\mathbb{R}^{3N}$, then $V \prec\prec -\Delta$.

For the proof, see the references in the Notes or Problem 17. We remind the reader again that the meaning given to $-\Delta + V$ by the KLMN Theorem *may* differ from the operator sum defined on $D(-\Delta) \cap D(V)$.

The problem of determining conditions on a potential on $\mathbb{R}^s$ so that $-\Delta + V$ is essentially self-adjoint has been extensively studied using Rellich's theorem and the KLMN theorem. The proofs of the necessary inequalities often use the L^p-estimates of Section IX.4 and the interpolation theorems and therefore the results are usually dependent on the dimension s. We present two examples below. For other theorems, see Section X.4 and the references in the Notes.

Theorem X.20 Let $s \geq 4$. If $V \in L^p(\mathbb{R}^s)$ for some $p > s/2$, then $V << -\Delta$.

Proof By Theorem IX.27, we know that if $u \in D(-\Delta)$ then

$$(1 + k^2)\hat{u}(k) \in L^2(\mathbb{R}^s)$$

Further, since $p > s/2$, $(1 + k^2)^{-1} \in L^p(\mathbb{R}^s)$, so by the Hölder inequality $\hat{u} \in L^q$ and

$$\|\hat{u}\|_q \leq \|(1 + k^2)^{-1}\|_p\,\|(1 + k^2)\hat{u}\|_2$$

where $q^{-1} = p^{-1} + \frac{1}{2}$. Therefore, by the Hansdorff–Young inequality $u \in L(\mathbb{R}^s)$ where $r^{-1} = \frac{1}{2} - p^{-1}$. Since $V \in L^p$, it follows from the Hölder inequality that $Vu \in L^2$. Thus, $D(V) \supset D(-\Delta)$ and

$$\begin{aligned}\|Vu\|_2 \leq \|V\|_p\,\|u\|_r &\leq \|V\|_p\,\|\hat{u}\|_q \\ &= \|V\|_p\,\|(1 + tk^2)^{-1}(1 + tk^2)\hat{u}\|_q \\ &\leq \|V\|_p\,\|(1 + tk^2)^{-1}\|_p\,\|(1 + tk^2)\hat{u}\|_2 \\ &\leq (\|V\|_p\,\|(1 + k^2)^{-1}\|_p)t^{-s/2p}(\|u\|_2 + t\|-\Delta u\|_2)\end{aligned}$$

Since $p > s/2$. this estimate shows that $V << -\Delta$. $\blacksquare$

The above theorem can be extended to the borderline case $p = s/2$ when $s \geq 5$, but in fact a stronger result is true.

Theorem X.21 (Strichartz's theorem) Let $s \geq 5$ and suppose $V \in L_w^{s/2}$. Then V is Δ-bounded with bound less than or equal to $C\|V\|_{s/2,\,w}$ where C depends only on s.

Proof It is sufficient to show that $\|V(I + \Delta)^{-1}\varphi\|_2 \leq C\|V\|_{s/2,\,w}\|\varphi\|_2$ for all $\varphi \in L^2(\mathbb{R}^s)$. Since $(I + \Delta)^{-1}\varphi = G * \varphi$ where G is the Fourier transform

of $(1+p^2)^{-1}$ on $\mathbb{R}^s$, we need the properties of G established in Problems 49 or 50 of Chapter IX. Since $G(x)$ is exponentially decreasing at ∞ and $\overline{\lim}_{|x|\to 0} |x|^{s-2}|G(x)| < \infty$, we easily find that $\mu\{\mathbf{x} \mid |G(x)| \geq t\}$ is bounded by $c_2 t^{s/s-2}$ for some $c_2 > 0$, where μ is Lebesgue measure. Thus, using the inequality in Problem 39 of Chapter IX, with $p = s/2$ and $q = 2$, we conclude that

$$\|V(G * \varphi)\|_2 \leq C_3 \|V\|_{s/2,\,\mathrm{w}} \|G\|_{s/s-2,\,\mathrm{w}} \|\varphi\|_2 \quad \blacksquare$$

Corollary Let μ denote Lebesgue measure on $\mathbb{R}^s$, $s \geq 5$. If $V(x)$ is a real-valued measurable function and

$$\lim_{t\to\infty} t^{s/2}\mu\{x \mid |V(x)| \geq t\} = 0$$

then $V << -\Delta$. In particular, if $V \in L^{s/2}(\mathbb{R}^s)$, then $V << -\Delta$.

Example 4 Let $s = 5$. From Theorems X.10 and X.11, it follows that $-\Delta + \alpha/r^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -1.25$. Further, $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$. The reader can easily check that $1/r^2 \in L_{\mathrm{w}}^{5/2}(\mathbb{R}^5)$, so by Strichartz' theorem, α/r^2 is $-\Delta$-bounded. Thus, the closure of $-\Delta + \alpha/r^2 \restriction C_0^\infty(\mathbb{R}^5\backslash\{0\})$ contains

$$(-\Delta + \alpha/r^2) \restriction C_0^\infty(\mathbb{R}^5)$$

Therefore, in the case $\alpha < -1.25$, $-\Delta + \alpha/r^2$ is not even essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$.

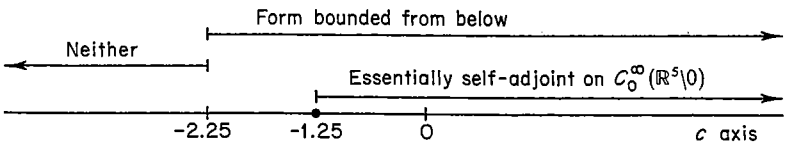

FIGURE X.4 The operator $-\Delta + (c/r^2)$ when $n = 5$.

In Problem 15, the reader is asked to show that $-d^2/dx^2 + c/x^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^+)$ if and only if $c \geq -\frac{1}{4}$. Thus, using the method of Example 4 of the Appendix to Section X.1, we conclude that $-\Delta + \alpha/r^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -2.25$. Therefore, if α is in the range $-2.25 \leq \alpha < -1.25$, we can use the quadratic form techniques of Theorem VIII.15 to define $-\Delta + \alpha/r^2$, even though $-\Delta + \alpha/r^2$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$. See Figure X.4.

Example 5 (Schrödinger operators for systems with magnetic fields) According to the Lagrangian–Hamiltonian theory of classical mechanics, the energy operator written in terms of the coordinate $\mathbf{q}$ and the canonically conjugate momentum $\mathbf{p} = m\dot{\mathbf{q}} + e\mathbf{A}/c$ is

$$E = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}/c)^2 + V(\mathbf{q})$$

where $\mathbf{A}$ is the **magnetic vector potential**, related to $\mathbf{B}$, the **magnetic field** by

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{X.25}$$

Using the correspondence between classical energy functions and quantum-mechanical Hamiltonian operators (Section VIII.11), we see that the Hamiltonian for an n-particle system in the presence of a magnetic field is

$$H = \sum_{j=1}^{n} (2m_j)^{-1}\left(-i\nabla_j - \frac{e_j}{c}\mathbf{A}\right)^2 + V(\mathbf{x}_1, \ldots, \mathbf{x}_n) \tag{X.26}$$

The case

$$A(\mathbf{x}) = \tfrac{1}{2}\mathbf{x} \times \mathbf{B}_0 \tag{X.27}$$

with $\mathbf{B}_0$ constant is especially important for this leads to $\mathbf{B} = \mathbf{B}_0$. This constant field situation is called the Zeeman effect, and its treatment requires special methods (see Section 4) since A grows at infinity. For the present, we note that perturbation methods do allow the treatment of some kinds of magnetic vector potentials. We give a detailed version of the operator perturbation theory result and leave the form result to the reader (Problem 36):

Theorem X.22 Suppose that each component of $\mathbf{A}$ is a real-valued function in $L^4(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, that $\nabla \cdot \mathbf{A} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (in the sense of distributions), and that V is a real-valued function in $L^2 + L^\infty$. For $\varphi \in C_0^\infty(\mathbb{R}^3)$, define

$$H\varphi = -\Delta\varphi + -2i\mathbf{A} \cdot \nabla\varphi - i(\nabla \cdot \mathbf{A})\varphi + V\varphi + A^2\varphi$$

Then H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Proof Integration by parts shows that H is symmetric on $C_0^\infty(\mathbb{R}^3)$ and the hypotheses on V, A^2, and $\nabla \cdot \mathbf{A}$ were chosen so that, by Theorem X.15, we have $V << -\Delta$ and $\nabla \cdot \mathbf{A} << -\Delta$. We will show that $\mathbf{A} \cdot \nabla << -\Delta$,

which implies by Theorem X.12 that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$. Suppose that $A \in L^4(\mathbb{R}^3)$. By the Hölder and Hausdorff–Young inequalities, we have

$$\begin{aligned}\left\| A^{(i)} \frac{\partial}{\partial x_i} \varphi \right\| &\le \|A^{(i)}\|_4 \left\| \frac{\partial}{\partial x_i} \varphi \right\|_4 \\ &\le \|A^{(i)}\|_4 \, \|p_i \hat{\varphi}(p)\|_{4/3} \\ &\le \|A^{(i)}\|_4 \, \|(1+|p|)^{-\alpha}\|_4 \, \|(1+|p|)^{\alpha} p_i \hat{\varphi}(p)\|_2\end{aligned}$$

where we have chosen α to be any fixed number in $(\frac{3}{4}, 1)$. For any $a > 0$, there is a b so that

$$\begin{aligned}\|(1+|p|)^{\alpha} p_i \hat{\varphi}(p)\|_2 &\le \|(b + a|p|^2)\hat{\varphi}(p)\|_2 \\ &\le a\|\Delta\varphi\|_2 + b\|\varphi\|_2\end{aligned}$$

by the Plancherel theorem. Thus $A^{(i)} \partial/\partial x_i << -\Delta$. A separate proof works for the L^∞ part of A. ∎

Perturbation theorems are simple and elegant and are applicable in so many cases that the test of the usefulness of any other self-adjointness method is its applicability to situations that cannot be directly handled by Theorems X.12, X.14, or X.17. One of the simplest physically interesting examples of such a situation is the **anharmonic oscillator Hamiltonian** $-d/dx^2 + x^2 + x^4$, its analogues on $\mathbb{R}^s$, and more generally the operators $-d^2/dx^2 + x^2 + x^{2m}$ $(m = 2, 3, \ldots)$. Both $H_0 = -d^2/dx^2 + x^2$ and $V = x^4$ are essentially self-adjoint on $C_0^\infty(\mathbb{R})$, but neither is a small perturbation of the other. We will use $-d^2/dx^2 + x^2 + x^4$ as a test case for many of the self-adjointness methods which we discuss later; in fact, we present five distinct proofs that $-d^2/dx^2 + x^2 + x^4$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$! All these proofs extend to prove that

$$\sum_{i=1}^{n} a_i \left(-\frac{d^2}{dx_i^2} + \omega_i^2 x_i^2 \right) + \sum_{i,j,k,\ell=1}^{n} b_{ijk\ell} x_i x_j x_k x_\ell$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if $a_1, \ldots, a_n > 0$ and if

$$\sum_{i,j,k,\ell} b_{ijk\ell} x_i x_j x_k x_\ell \ge 0$$

for all x. All but two of them can be extended to treat the x^{2m} operators and their higher dimensional analogues. We note that the limit point–limit circle techniques discussed in the Appendix to Section X.1 can also be used to discuss the *one-dimensional* anharmonic oscillator.

There is one method of using Theorems X.12 and X.14 (the Kato–Rellich and Wüst theorems) in tandem to treat operators which are not directly amenable to perturbation theorems. The method, known as Konrady's trick, will provide our first proof that the anharmonic oscillator Hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R})$. Konrady's trick proves that $X + Y$ is essentially self-adjoint on some set D by a three-step process which is schematically of the following form:

(a) One finds some Z so that $X + Z$ is essentially self-adjoint on $D \subset D(X) \cap D(Z)$. Z is not a small perturbation of X. A typical example is to take Z to be a power of X and $D = C^\infty(X)$.

(b) One proves $X + Z + Y$ is essentially self-adjoint on D. Typically, this is done by proving Y is $(X + Z)$-bounded with bound less than one, so that the Kato–Rellich theorem is applicable. Notice that since Z is not a small perturbation of X, Y can be $(X + Z)$-bounded even if it is not X-bounded.

(c) One proves an estimate $\|Z\psi\| \le \|(X + Y + Z)\psi\| + b\|\psi\|$ for some b and all $\psi \in D$. By Wüst's theorem, $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D. Typically one proves this estimate (which is of the form (X.21a)) by proving the stronger estimate on operators (of the form of (X.21c)): $Z^2 \le (X + Y + Z)^2 + b^2$.

Of course, to apply Konrady's trick, one must choose Z cleverly.

Example 6 (essential self-adjointness of $-d^2/dx^2 + x^2 + x^4$ on $C_0^\infty(\mathbb{R})$; first proof) Let $X = -d^2/dx^2 + x^2$ and $Y = x^4$. Let $Z = cX^2$ where c is a positive constant which we will choose later in the proof. Let $D = C^\infty(X) = \mathscr{S}(\mathbb{R})$. We will prove essential self-adjointness of $X + Y$ on D; the simple argument that allows one to conclude essential self-adjointness on $C_0^\infty(\mathbb{R})$ from this is left to the reader. We know that the Hermite functions (see the Appendix to Section V.3) are a complete orthonormal set for $L^2(-\infty, \infty)$ (Chapter IX, Problems 6 and 7), and that $X\psi_n = (2n + 1)\psi_n$. It follows from the Appendix to Section V.3, that $\mathrm{Ran}(X + 1) = \mathscr{S}(\mathbb{R})$, so we conclude that X is essentially self-adjoint on $\mathscr{S}$. By the spectral theorem, $X + Z$ is essentially self-adjoint on $D = C^\infty(X)$. This completes step (a) in Konrady's trick. In terms of the operators A, $A^\dagger$ introduced in Section V.3, $X = 2A^\dagger A + 1$, and $Y = \frac{1}{4}(A + A^\dagger)^4$. Using the inequality

$$\|A_1^\# \cdots A_n^\# \psi\| \le c_n \|X^{n/2}\psi\| \tag{X.28}$$

(where each $A_i^\#$ is an A or an $A^\dagger$), one proves that $\|Y\psi\| \le d\|X^2\psi\| \le dc^{-1}\|(X + Z)\psi\|$. We thus pick $c = 2d$ and conclude that $X + Y + Z$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ by employing the Kato–Rellich theorem.

This completes step (b) of Konrady's trick. Finally, let us prove that for some constant e,

$$Z^2 \leq (X + Y + Z)^2 + e \tag{X.29}$$

We compute

$$\begin{aligned}(X + Y + Z)^2 &= (X + Y)^2 + Z^2 + Z(X + Y) + (X + Y)Z \\ &= (X + Y)^2 + Z^2 + 2cX^3 + 2cXYX + 2c[X, [X, Y]] \\ &\geq Z^2 + 2cX^3 + 2c[X, [X, Y]]\end{aligned}$$

where we have used $Y \geq 0$, and $[X, [X, Y]] = X^2Y + YX^2 - 2XYX$ together with the fact that all the manipulations we perform are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R})$. Finally we note that $[X, [X, Y]]$ can be written as the sum of 16 monomials of the form $A_1^{\#}A_2^{\#}A_3^{\#}A_4^{\#}$. Thus, using Theorem X.18, (X.28), and the fact that $[X, [X, Y]]$ is symmetric, we conclude

$$-[X, [X, Y]] \leq fX^2 \leq X^3 + (f + 1)$$

This proves (X.29), and thereby, applying Wüst's theorem, we conclude that $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D.

We will use Konrady's trick again in Example 3 of Section X.9. (See also Problem 22.)

X.3 Positivity and self-adjointness I: Quadratic forms

We have already proven several results about positive or semibounded operators; see, for example, Theorems X.12 and X.17. In this section and the next, we exploit two different notions of positivity to prove a variety of self-adjointness theorems. In this section we use the concept of positive operator and quadratic form techniques. In the next, we use the fact that if a Hilbert space is of the form $L^2(M, d\mu)$, which is usual in applications, then it contains the distinguished cone of functions that are nonnegative a.e. Further applications of positivity conditions appear throughout this chapter, for example in Theorem X.55, and in later chapters, for example, in Section XIII.11.

It follows from the first corollary to Theorem X.1 that a semibounded symmetric operator A has equal deficiency indices, and therefore by von

Neumann's theorem, such an operator always has self-adjoint extensions. There is a distinguished extension, called the **Friedrichs extension**, which is obtained from the quadratic form associated to A.

Theorem X.23 (the Friedrichs extension) Let A be a positive symmetric operator and let $q(\varphi, \psi) = (\varphi, A\psi)$ for $\varphi, \psi \in D(A)$. Then q is a closable quadratic form and its closure $\hat{q}$ is the quadratic form of a unique self-adjoint operator $\hat{A}$. $\hat{A}$ is a positive extension of A, and the lower bound of its spectrum is the lower bound of q. Further, $\hat{A}$ is the only self-adjoint extension of A whose domain is contained in the form domain of $\hat{q}$.

Proof Let $(\varphi, \psi)_{+1} = q(\varphi, \psi) + (\varphi, \psi)$. Then $(\cdot, \cdot)_{+1}$ is an inner product on $D(A)$, so we can complete $D(A)$ under $(\cdot, \cdot)_{+1}$ to obtain a Hilbert space $\mathscr{H}_{+1}$. q clearly extends to a closed form $\hat{q}$ on $\mathscr{H}_{+1}$, but to show that $\hat{q}$ is a closed form on $\mathscr{H}$, we must show that $\mathscr{H}_{+1}$ is a subset of $\mathscr{H}$. Let $i: D(A) \to \mathscr{H}$ be the identity map. Since $\|\varphi\| \leq \|\varphi\|_{+1}$, i is bounded and thus extends by the B.L.T. theorem to a bounded map $\hat{i}: \mathscr{H}_{+1} \to \mathscr{H}$ of norm less than or equal to one. To show that $\mathscr{H}_{+1} \subset \mathscr{H}$, we proceed to show that $\hat{i}$ is injective. Suppose that $\hat{i}(\varphi) = 0$. Then, there exist $\varphi_n \in D(A)$ so that $\|\varphi - \varphi_n\|_{+1} \to 0$ and so that $\|\hat{i}(\varphi_n)\| = \|\varphi_n\| \to 0$. Thus

$$\begin{aligned}\|\varphi\|_{+1} &= \lim_{n, m \to \infty} (\varphi_n, \varphi_m)_{+1} \\ &= \lim_{n \to \infty} \lim_{m \to \infty} \{(\varphi_m, A\varphi_n) + (\varphi_m, \varphi_n)\} \\ &= 0\end{aligned}$$

since $\varphi_n \in D(A)$ and $\|\varphi_m\| \to 0$. Thus $\hat{i}$ is injective. Notice that the proof that $\hat{i}$ is well-defined uses only the positivity of q, but the proof that $\hat{i}$ is one to one uses the hypothesis that q arises from an operator.

Since $\hat{q}$ is closed and symmetric, by Theorem VIII.15 there is a unique self-adjoint operator $\hat{A}$ so that $D(\hat{A}) \subset Q(\hat{q})$ and $\hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$ if $\varphi \in Q(\hat{q})$ and $\psi \in D(\hat{A})$. Now, suppose also that $\varphi \in D(A)$. Then by the continuity of $\hat{q}$,

$$(A\varphi, \psi) = \hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$$

Since, this holds for all $\psi \in D(\hat{A})$, we conclude that $\varphi \in D(\hat{A}^*) = D(\hat{A})$ and $\hat{A}^*\varphi = \hat{A}\varphi = A\varphi$. Thus $\hat{A}$ extends A. The same proof shows that if A_e is any symmetric extension of A with $D(A_e) \subset Q(\hat{q})$, then $\hat{A}$ extends A_e. Thus if A_e is self-adjoint $\hat{A} = A_e$.

The easy proof of the statement about the spectrum of A is left to the reader. ∎