9

Unbounded Self-Adjoint Operators

9.1 Introduction

Recall that most of the operators of quantum mechanics, including those representing position, momentum, and energy, are not defined on the entirety of the relevant Hilbert space, but only on a dense subspace thereof. In the case of the position operator, for example, given $\psi \in L^2(\mathbb{R})$, the function $X\psi(x) = x\psi(x)$ could easily fail to be in $L^2(\mathbb{R})$. Nevertheless, the space of ψ's in $L^2(\mathbb{R})$ for which $x\psi(x)$ is again in $L^2(\mathbb{R})$ is a dense subspace of $L^2(\mathbb{R})$. A closely related property of these operators is that they are not bounded, meaning that there is no constant C such that

$$\|A\psi\| \leq C\,\|\psi\|$$

for all ψ for which A is defined. Because our operators are unbounded, we cannot use the BLT (bounded linear transformation) theorem to extend them to the whole Hilbert space.

In this chapter and the following one, we are going to study unbounded operators defined on dense subspaces of a Hilbert space $\mathbf{H}$. We will introduce the "correct" notion of self-adjointness for unbounded operators, namely the one for which the spectral theorem holds. As it turns out, the obvious candidate for a definition of self-adjointness, namely that $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all ϕ and ψ in the domain of A, is *not* the correct one. Rather, for any unbounded operator A, we will define another unbounded operator A^*, the adjoint of A, with its own naturally defined domain. Then A is

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said to be self-adjoint if A^* and A are the same operators *with the same domain*.

In the present chapter, we give the definition of an unbounded self-adjoint operator, along with conditions for self-adjointness and several examples and counterexamples. We defer a discussion of the spectral theorem itself until Chap. 10. The statement of the spectral theorem (either in terms of projection-valued measures or in terms of direct integrals) is essentially the same as in the bounded case, with only a few modifications to deal with the domain of the operator.

Although this chapter is rather technical, a reader who is willing to accept some things on faith may wish simply to read the definitions of self-adjoint and essentially self-adjoint operators in Sect. 9.2, and then skip to the statements of Theorem 9.21 and Corollary 9.22 in Sect. 9.5. As in previous chapters, $\mathbf{H}$ will denote a separable Hilbert space over $\mathbb{C}$.

9.2 Adjoint and Closure of an Unbounded Operator

Recall that we briefly introduced unbounded operators in Sect. 3.2. According to Definition 3.1, an *unbounded operator* A on $\mathbf{H}$ is a linear map of some dense subspace $\mathrm{Dom}(A) \subset \mathbf{H}$ (the domain of A) into $\mathbf{H}$. As in Sect. 3.2, "unbounded" means "not necessarily bounded," meaning that we permit the case in which $\mathrm{Dom}(A) = \mathbf{H}$ and A is bounded.

Now, if A *is* bounded, then for any ϕ, the linear functional

$$\langle \phi, A\cdot \rangle$$

is bounded. Thus, by the Riesz theorem (Theorem A.52), there is a unique χ such that

$$\langle \phi, A\cdot \rangle = \langle \chi, \cdot \rangle .$$

We then define the adjoint A^* of A by setting $A^*\phi$ equal to χ. (See Sect. A.4.)

If A is unbounded, then $\langle \phi, A\cdot \rangle$ is not *necessarily* bounded, but may be bounded for certain vectors ϕ. If $\langle \phi, A\cdot \rangle$ does happen to be bounded, for some $\phi \in \mathbf{H}$, then the BLT theorem (Theorem A.36) says that this linear functional has a unique bounded extension from $\mathrm{Dom}(A)$ to all $\mathbf{H}$. The Riesz theorem then tells us that there is a unique χ such that this linear functional is "inner product with χ." This line of reasoning leads to the following definition, which was already introduced briefly in Sect. 3.2.

Definition 9.1 *Suppose A is an operator defined on a dense subspace* $\mathrm{Dom}(A) \subset \mathbf{H}$. *Let* $\mathrm{Dom}(A^*)$ *to be the space of all $\phi \in \mathbf{H}$ for which the linear functional*

$$\psi \mapsto \langle \phi, A\psi \rangle , \quad \psi \in \mathrm{Dom}(A),$$

is bounded. For $\phi \in \mathrm{Dom}(A^*)$*, define* $A^*\phi$ *to be the unique vector such that* $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$ *for all* $\psi \in \mathrm{Dom}(A)$.

Saying that $\langle \phi, A\cdot \rangle$ is bounded means, explicitly, that there exists a constant C such that $|\langle \phi, A\psi \rangle| \leq C \|\psi\|$ for all $\psi \in \mathrm{Dom}(A)$. As in the bounded case, the operator A^* is linear on its domain, and is called the *adjoint* of A.

Another way to think about the definition of A^* is as follows. Given a vector ϕ, if there exists a vector χ such that $\langle \phi, A\psi \rangle = \langle \chi, \psi \rangle$ for all $\psi \in \mathrm{Dom}(A)$, then ϕ belongs to $\mathrm{Dom}(A^*)$ and $A^*\phi = \chi$. By the Riesz theorem, such a χ will exist if and only if $\langle \phi, A\cdot \rangle$ is bounded, which means this way of thinking about A^* is equivalent to Definition 9.1.

Given a densely defined operator A, the adjoint A^* of A could fail to be densely defined. This situation, however, is a pathology that does not usually occur for operators of interest in applications.

Definition 9.2 *An unbounded operator* A *on* $\mathbf{H}$ *is* ***symmetric*** *if*

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle \tag{9.1}$$

for all $\phi, \psi \in \mathrm{Dom}(A)$.

As we will see shortly, if A is symmetric, then A^* is an extension of A, in the sense of the following definition.

Definition 9.3 *An unbounded operator* A *is an* ***extension*** *of an unbounded operator* B *if* $\mathrm{Dom}(A) \supset \mathrm{Dom}(B)$ *and* $A = B$ *on* $\mathrm{Dom}(B)$.

If A is an extension of B, then very likely A is given by the same "formula" as B. If $\mathbf{H} = L^2(\mathbb{R})$, for example, both operators might be given by the formula $-i\hbar\, d/dx$ on their respective domains. Nevertheless, if $\mathrm{Dom}(A) \neq \mathrm{Dom}(B)$, then A is still a different operator from B.

Proposition 9.4 *An unbounded operator* A *is symmetric if and only if* A^* *is an extension of* A.

Proof. If A is symmetric, then for all $\phi \in \mathrm{Dom}(A)$, (9.1) and the Cauchy–Schwarz inequality show that

$$|\langle \phi, A\psi \rangle| \leq \|A\phi\| \, \|\psi\| \,,$$

showing that $\phi \in \mathrm{Dom}(A^*)$. In that case, (9.1) shows that the unique vector $A^*\phi$ for which $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$ is nothing but $A\phi$, which means that A^* agrees with A on $\mathrm{Dom}(A)$.

In the other direction, if A^* is an extension of A, then for each $\phi \in \mathrm{Dom}(A)$, we have

$$\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle = \langle A\phi, \psi \rangle \,,$$

for all $\psi \in \mathrm{Dom}(A)$, which shows that A is symmetric. ∎

We come now to the key definition of this section, that of self-adjointness. This notion constitutes the hypothesis of the spectral theorem for unbounded operators.

Definition 9.5 *An unbounded operator A on $\mathbf{H}$ is* ***self-adjoint*** *if*

$$\mathrm{Dom}(A^*) = \mathrm{Dom}(A)$$

and $A^*\phi = A\phi$ for all $\phi \in \mathrm{Dom}(A)$.

We may reformulate the definition of self-adjointness by saying that A is self-adjoint if A^* is equal to A, provided that equality of unbounded operators is understood to include *equality of domains*. Every self-adjoint operator is symmetric (by Proposition 9.4), but there exist many operators that are symmetric without being self-adjoint. In light of Proposition 9.4, a symmetric operator is self-adjoint if and only if $\mathrm{Dom}(A^*) = \mathrm{Dom}(A)$. In trying to show that a symmetric operator is self-adjoint, the difficulty lies in showing that $\mathrm{Dom}(A^*)$ is no bigger than $\mathrm{Dom}(A)$.

Definition 9.6 *An unbounded operator A on $\mathbf{H}$ is said to be* ***closed*** *if the graph of A is a closed subset of $\mathbf{H} \times \mathbf{H}$. An unbounded operator A on $\mathbf{H}$ is said to be* ***closable*** *if the closure in $\mathbf{H} \times \mathbf{H}$ of the graph of A is the graph of a function. If A is closable, then the closure A^{cl} of A is the operator with graph equal to the closure of the graph of A.*

To be more explicit, an operator A is closed if and only if the following condition holds: Suppose a sequence ψ_n belongs to $\mathrm{Dom}(A)$ and suppose that there exist vectors ψ and ϕ in $\mathbf{H}$ with $\psi_n \to \psi$ and $A\psi_n \to \phi$. Then ψ belongs to $\mathrm{Dom}(A)$ and $A\psi = \phi$. Regarding closability, an operator A is *not* closable if there exist two elements in the closure of the graph of A of the form (ϕ, ψ) and (ϕ, χ), with $\psi \neq \chi$. Another way of putting it is to say that an operator A is closable if there exists some closed extension of it, in which case the closure of A is the smallest closed extension of A.

The notion of the closure of a (closable) operator is useful because it sweeps away some of the arbitrariness in the choice of a domain of an operator. If we consider, for example, the operator $A = -i\hbar\, d/dx$ as an unbounded operator on $L^2(\mathbb{R})$, there are many different reasonable choices for $\mathrm{Dom}(A)$, including (1) the space of C^∞ functions of compact support, (2) the Schwartz space (Definition A.15), and (3) the space of continuously differentiable functions ψ for which both ψ and ψ' belong to $L^2(\mathbb{R})$. As it turns out, each of these three choices for $\mathrm{Dom}(A)$ leads to the same operator A^{cl}. Note that we are not claiming that *every* choice for $\mathrm{Dom}(A)$ leads to the same closure; nevertheless, it is often the case that *many* reasonable choices do lead to the same closure.

Definition 9.7 *An unbounded operator A on $\mathbf{H}$ is said to be* ***essentially self-adjoint*** *if A is symmetric and closable and A^{cl} is self-adjoint.*

Actually, as we shall see in the next section, a symmetric operator is always closable. Many symmetric operators fail to be even essentially self-adjoint. We will see examples of such operators in Sects. 9.6 and 9.10. Section 9.5 gives some reasonably simple criteria for determining when a symmetric operator is essentially self-adjoint.

9.3 Elementary Properties of Adjoints and Closed Operators

In this section, we spell out some of the most basic and useful properties of adjoints and closures of unbounded operators. In Sect. 9.5, we will draw on these results to prove some more substantial results. In what follows, if we say that two operators "coincide," it means that they *have the same domain* and that they are equal on that common domain.

Proposition 9.8 *1. If A is an unbounded operator on* $\mathbf{H}$*, then the graph of the operator A^* (which may or may not be densely defined) is closed in* $\mathbf{H}\times\mathbf{H}$*.*

2. A symmetric operator is always closable.

Proof. Suppose ψ_n is a sequence in the domain of A^* that converges to some $\psi\in\mathbf{H}$. Suppose also that $A^*\psi_n$ converges to some $\phi\in\mathbf{H}$. Then $\langle\psi_n, A\cdot\rangle = \langle A^*\psi_n, \cdot\rangle$ and for any $\chi\in\mathrm{Dom}(A)$, we have

$$\langle\psi, A\chi\rangle = \lim_{n\to\infty}\langle\psi_n, A\chi\rangle = \lim_{n\to\infty}\langle A^*\psi_n, \chi\rangle = \langle\phi,\chi\rangle\,.$$

This shows that ψ belongs to the domain of A^* and that $A^*\psi=\phi$, establishing that the graph of A^* is closed.

If A is symmetric, A^* is an extension of A. Since, as we have just proved, A^* is closed, A has a closed extension and is therefore closable. ■

Corollary 9.9 *If A is a symmetric operator with* $\mathrm{Dom}(A)=\mathbf{H}$*, then A is bounded.*

Proof. Since A is symmetric, it is closable by Proposition 9.8. But since the domain of A is already all of $\mathbf{H}$, the closure of A must coincide with A itself. (The closure of A always agrees with A on $\mathrm{Dom}(A)$, which in this case is all of $\mathbf{H}$.) Thus, A is a closed operator defined on all of $\mathbf{H}$, and the closed graph theorem (Theorem A.39) implies that A is bounded. ■

Proposition 9.10 *If A is a closable operator on* $\mathbf{H}$*, then the adjoint of A^{cl} coincides with the adjoint of A.*

Proof. Suppose that for some $\psi\in\mathbf{H}$ there exists a ϕ such that $\left\langle\psi, A^{cl}\chi\right\rangle = \langle\phi,\chi\rangle$ for all $\chi\in\mathrm{Dom}(A^{cl})$. Since A^{cl} is an extension of A, it follows that $\langle\psi, A\chi\rangle = \langle\phi, \chi\rangle$ for all $\chi \in \mathrm{Dom}(A)$. This shows that $\mathrm{Dom}(A^*) \supset \mathrm{Dom}((A^{cl})^*)$ and that A^* agrees with $(A^{cl})^*$ on $\mathrm{Dom}((A^{cl})^*)$.

In the other direction, suppose for some $\psi \in \mathbf{H}$ there exists a ϕ such that $\langle\psi, A\chi\rangle = \langle\phi, \chi\rangle$ for all $\chi \in \mathrm{Dom}(A)$. Suppose now $\xi \in \mathrm{Dom}(A^{cl})$ with $A^{cl}\xi = \eta$. Then there exists a sequence χ_n in $\mathrm{Dom}(A)$ with $\chi_n \to \xi$ and $A\chi_n \to \eta$, and we have

$$\langle\psi, A\chi_n\rangle = \langle\phi, \chi_n\rangle$$

for all n. Letting n tend to infinity, we obtain $\langle\psi, \eta\rangle = \langle\phi, \xi\rangle$, or $\left\langle\psi, A^{cl}\xi\right\rangle = \langle\phi, \xi\rangle$. This shows that $\psi \in \mathrm{Dom}((A^{cl})^*)$ and $A^{cl}\psi = \phi$. Thus, $\mathrm{Dom}(A^*) \subset \mathrm{Dom}((A^{cl})^*)$. ■

Proposition 9.11 *If A is essentially self-adjoint, then A^{cl} is the* unique *self-adjoint extension of A.*

Proof. Suppose B is a self-adjoint extension of A. Since $B = B^*$, B is closed and is, therefore, an extension of A^{cl}. It then follows from the definition of the adjoint that $\mathrm{Dom}(B^*) \subset \mathrm{Dom}(A^{cl})$. Thus, we have

$$\mathrm{Dom}(B^*) \subset \mathrm{Dom}(A^{cl}) \subset \mathrm{Dom}(B).$$

Since B is self-adjoint, all three of the above sets must be equal, so actually $B = A^{cl}$. ■

Proposition 9.12 *If A is an unbounded operator on $\mathbf{H}$, then*

$$(\mathrm{Range}(A))^{\perp} = \ker(A^*).$$

Proof. First assume that $\psi \in (\mathrm{Range}(A))^{\perp}$. Then for all $\phi \in \mathrm{Dom}(A)$ we have

$$\langle\psi, A\phi\rangle = 0.$$

That is to say, the linear functional $\langle\psi, A\cdot\rangle$ is bounded—in fact, zero—on $\mathrm{Dom}(A)$. Thus, from the definition of the adjoint, we conclude that $\psi \in \mathrm{Dom}(A^*)$ and $A^*\psi = 0$.

Meanwhile, suppose that ψ is in $\mathrm{Dom}(A^*)$ and that $A^*\psi = 0$. The only way this can happen is if the linear functional $\langle\psi, A\cdot\rangle$ is zero on $\mathrm{Dom}(A)$, which means that ψ is orthogonal to the image of A. ■

Proposition 9.13 *Suppose A is an unbounded operator on $\mathbf{H}$ and that B is a bounded operator defined on all of $\mathbf{H}$. Let $A + B$ denote the operator with $\mathrm{Dom}(A + B) = \mathrm{Dom}(A)$ and given by $(A + B)\psi = A\psi + B\psi$ for all $\psi \in \mathrm{Dom}(A)$. Then $(A+B)^*$ has the same domain as A^* and $(A+B)^*\psi = A^*\psi + B^*\psi$ for all $\psi \in \mathrm{Dom}(A^*)$.*

In particular, the sum of an unbounded self-adjoint operator and a bounded self-adjoint operator (defined on all of $\mathbf{H}$) is self-adjoint on the domain of the unbounded operator.

Proof. See Exercise 3. ■

The sum of two unbounded self-adjoint operators is not, in general, self-adjoint. See Sect. 9.9 for more information about this issue.

Proposition 9.14 *Let A be a closed operator and λ an element of $\mathbb{C}$. Suppose that there exists $\varepsilon > 0$ such that*

$$\|(A - \lambda I)\psi\| \geq \varepsilon \|\psi\| \tag{9.2}$$

for all A in $\mathrm{Dom}(A)$*. Then the range of $A - \lambda I$ is a closed subspace of* $\mathbf{H}$.

Here, we take the domain of the operator $A - \lambda I$ to coincide with the domain of A, as in Proposition 9.13.

Proof. Assume that ϕ_n is a sequence in the range of $A - \lambda I$ converging to some ϕ. Then $\phi_n = (A - \lambda I)\psi_n$, for some sequence ψ_n in $\mathrm{Dom}(A)$. Applying (9.2) with $\psi = \psi_n - \psi_m$ shows that $\|\psi_n - \psi_m\| \leq (1/\varepsilon) \|\phi_n - \phi_m\|$. This means that ψ_n is Cauchy and thus convergent to some vector ψ. Since $\psi_n \to \psi$ and $(A - \lambda I)\psi_n = \phi_n \to \phi$, we have that

$$A\psi_n = \lambda\psi_n + \phi_n \to \lambda\psi + \phi.$$

Thus, by the definition of a closed operator, $\psi \in \mathrm{Dom}(A)$ and $A\psi = \lambda\psi + \phi$. This means that $(A - \lambda I)\psi = \phi$ and so the range of $A - \lambda I$ is closed. ■

We conclude this section with a simple example for which we can compute the adjoint and closure explicitly.

Example 9.15 *Let $\langle e_j \rangle$ be an orthonormal basis for* $\mathbf{H}$ *and let $\langle \lambda_j \rangle$ be an arbitrary sequence of real numbers. Define an operator A on* $\mathbf{H}$ *with* $\mathrm{Dom}(A)$ *equal to the space of finite linear combinations of the e_j's, with A itself defined by*

$$Ae_j = \lambda_j e_j.$$

Then A is symmetric and closable and $\mathrm{Dom}(A^*) = \mathrm{Dom}(A^{cl}) = V$*, where*

$$V = \left\{ \psi = \sum_j a_j e_j \,\middle|\, \sum_j (1 + \lambda_j^2)\,|a_j|^2 < \infty \right\}. \tag{9.3}$$

For any $\psi = \sum_j a_j e_j$ in V, we have

$$A^*\psi = A^{cl}\psi = \sum_j a_j \lambda_j e_j. \tag{9.4}$$

Thus, $(A^{cl})^* = A^* = A^{cl}$, showing that A is essentially self-adjoint.

Proof. Note that for any sequence $\langle a_j \rangle$ of coefficients satisfying the condition on the right-hand side of (9.3), we have $\sum_j |a_j|^2 < \infty$ and, thus, the sum $\sum_j a_j e_j$ converges in $\mathbf{H}$. Suppose first that $\phi = \sum_j a_j e_j$ belongs V. Then for any $\psi = \sum_j b_j e_j$ (finite sum) in the domain of A we have

$$\langle \phi, A\psi \rangle = \sum_j \overline{a_j} \lambda_j b_j$$

and so by the Cauchy–Schwarz inequality,

$$|\langle \phi, A\psi \rangle| \leq \left(\sum_j \lambda_j^2 \left| a_j \right|^2 \right)^{1/2} \|\psi\| .$$

Thus, $\langle \phi, A\cdot \rangle$ is a bounded linear functional, showing that $\phi \in \mathrm{Dom}(A^*)$. Furthermore, it is apparent that $\langle \phi, A\psi \rangle = \langle \chi, \psi \rangle$ for all $\psi \in \mathrm{Dom}(A)$, where $\chi = \sum_j a_j \lambda_j e_j$.

Meanwhile, suppose $\phi = \sum_j a_j e_j$ belongs to the domain of A^*, and consider $\psi_N := \sum_{j=1}^N \lambda_j a_j e_j$ in $\mathrm{Dom}(A)$. Then

$$|\langle \phi, A\psi_N \rangle| = \sum_{j=1}^N \lambda_j^2 \left| a_j \right|^2 = \left(\sum_{j=1}^N \lambda_j^2 \left| a_j \right|^2 \right)^{1/2} \|\psi_N\| .$$

Since $\phi \in \mathrm{Dom}(A^*)$, the functional $\langle \phi, A\cdot \rangle$ is bounded, and so $\sum_{j=1}^N \lambda_j^2 \left| a_j \right|^2$ must be bounded, independent of N, and so $\sum_j \lambda_j^2 \left| a_j \right|^2 < \infty$. Since ϕ belongs to $\mathbf{H}$, we have also that $\sum_j \left| a_j \right|^2 < \infty$, showing that ϕ is in V.

Turning now to the closure of A, it is apparent that A is symmetric and thus closable, by Proposition 9.8. Suppose $\psi = \sum_j a_j e_j$ belongs to V and consider $\psi_N := \sum_{j=1}^N a_j e_j$. Clearly, ψ_N converges to ψ. Furthermore, since $\psi \in V$, we see that $A\psi_N$ converges to the vector $\sum_j a_j \lambda_j e_j$. This shows that $\psi \in \mathrm{Dom}(A^{cl})$ and that $A^{cl}\psi = \sum_j a_j \lambda_j e_j$. Thus, each element of V belongs to $\mathrm{Dom}(A^{cl})$ and A^{cl} is given on V by (9.4).

Now, the space V forms a Hilbert space with respect to the norm given by

$$\|\psi\|_V^2 = \sum_j (1 + \lambda_j^2) \left| a_j \right|^2 ,$$

where $\psi = \sum_j a_j e_j$. [To establish completeness of V with respect to this norm, note that V can be identified isometrically with $L^2(\mathbb{N})$ with respect to the measure μ for which $\mu(\{j\}) = 1 + \lambda_j^2$.] Suppose, now, that we have a sequence $\langle \psi^m \rangle$ in $\mathrm{Dom}(A)$ for which both $\langle \psi_m \rangle$ and $\langle A\psi_m \rangle$ are convergent. Then $\langle \psi^m \rangle$ forms a Cauchy sequence in V which converges to some element ψ of V. Since $\|\psi\|_{\mathbf{H}} \leq \|\psi\|_V$ for all $\psi \in \mathrm{Dom}(A)$, we see that ψ^m also converges in $\mathbf{H}$ to $\psi \in V$. This shows that each element of $\mathrm{Dom}(A^{cl})$ belongs to V. ∎

9.4 The Spectrum of an Unbounded Operator

Recall that if A is a bounded operator, then a number $\lambda \in \mathbb{C}$ belongs to the *resolvent set* of A if the operator $A - \lambda I$ has a bounded inverse, and λ belongs to the *spectrum* of A if $A - \lambda I$ does not have a bounded inverse. For an unbounded operator A, we will say that a number $\lambda \in \mathbb{C}$ is in the resolvent set of A if $A - \lambda I$ has a bounded inverse. That is, even though A is unbounded, for λ to be in the resolvent set of A, there must be a *bounded* inverse to $A - \lambda I$; otherwise, λ is in the spectrum of A. We make this characterization more precise in the following definition.

Definition 9.16 *Suppose A is an unbounded operator on $\mathbf{H}$. A number $\lambda \in \mathbb{C}$ belongs to the* ***resolvent set*** *of A if there exists a bounded operator B with the following properties: (1) For all $\psi \in \mathbf{H}$, $B\psi$ belongs to* $\mathrm{Dom}(A)$ *and $(A-\lambda I)B\psi = \psi$, and (2) for all $\psi \in \mathrm{Dom}(A)$ we have $B(A-\lambda I)\psi = \psi$.*
If no such bounded operator B exists, then λ belongs to the ***spectrum*** *of A.*

Note that we are implicitly taking $\mathrm{Dom}(A - \lambda I)$ to equal $\mathrm{Dom}(A)$, as in Proposition 9.13. As in the bounded case, even if A is self-adjoint, points λ in the spectrum of A are not necessarily eigenvalues; that is, there does not necessarily exist a nonzero $\psi \in \mathrm{Dom}(A)$ with $A\psi = \lambda\psi$. On the other hand, if $A\psi = \lambda\psi$ for some $\psi \in \mathrm{Dom}(A)$, then $A - \lambda I$ is not injective and thus λ certainly does belong to the spectrum of A.

Theorem 9.17 *If A is an unbounded self-adjoint operator on $\mathbf{H}$, the spectrum of A is contained in the real line.*

If A is symmetric but not self-adjoint, then the spectrum of A must contain points not in the real line. Indeed, Theorem 9.21 will show that at least one of $(A - iI)$ and $(A + iI)$ must fail to be surjective, and thus at least one of the numbers i and $-i$ is in the spectrum of A. Nevertheless, a symmetric operator cannot have nonreal eigenvalues, as we showed already in Proposition 3.4.

Proof. Consider a complex number $\lambda = a + ib$ with $b \neq 0$. Since A is symmetric, the proof of Lemma 7.8 applies, giving

$$\langle (A - \lambda I)\psi, (A - \lambda I)\psi \rangle \geq b^2 \langle \psi, \psi \rangle \tag{9.5}$$

for all $\psi \in \mathrm{Dom}(A)$. This shows that $(A - \lambda I)$ is injective.

Meanwhile, applying Propositions 9.12 and 9.13 with $B = -\lambda I$ we see that

$$(\mathrm{Range}(A - \lambda I))^{\perp} = \ker((A - \lambda I)^*) = \ker(A^* - \bar{\lambda} I) = \ker(A - \bar{\lambda} I).$$

Since $\bar{\lambda}$ again has nonzero imaginary part, $A - \bar{\lambda} I$ is also injective, showing that $\mathrm{Range}(A - \lambda I)$ is dense in $\mathbf{H}$. Since $A = A^*$ is closed, (9.5) allows us to apply Proposition 9.14 to show that $\mathrm{Range}(A - \lambda I)$ is closed, hence all of $\mathbf{H}$.

We have shown, then, that $(A-\lambda I)$ maps $\mathrm{Dom}(A)$ injectively onto $\mathbf{H}$. It follows from (9.5) (or the closed graph theorem) that the inverse operator is bounded, so that λ is in the resolvent set of A. ∎

Our next result shows that the spectrum of an unbounded self-adjoint operator has properties similar to that of a bounded self-adjoint operator.

Proposition 9.18 *If A is an unbounded self-adjoint operator on $\mathbf{H}$, then the following hold.*

1. *A number $\lambda \in \mathbb{R}$ belongs to the spectrum of A if and only if there exists a sequence ψ_n of nonzero vectors in $\mathrm{Dom}(A)$ such that*

$$\lim_{n\to\infty} \frac{\|(A-\lambda I)\psi_n\|}{\|\psi_n\|} = 0. \tag{9.6}$$

2. *The spectrum $\sigma(A)$ of A is a closed subset of $\mathbb{R}$.*

Although the spectrum of a bounded self-adjoint operator is a bounded subset of $\mathbb{R}$, the spectrum of an unbounded self-adjoint operator will be unbounded. Indeed, it can be shown (using the spectral theorem) that if a self-adjoint operator has bounded spectrum, then the operator must be bounded.

Proof. For Point 1, if a sequence as in (9.6) existed, then as in the proof of Proposition 7.7, $A-\lambda I$ could not have a *bounded* inverse, so λ must be in the spectrum of A. Conversely, suppose no such sequence exists. Then there is some $\varepsilon > 0$ such that

$$\|(A-\lambda I)\psi\| \geq \varepsilon \|\psi\| \tag{9.7}$$

for all $\psi \in \mathrm{Dom}(A)$. This means that $A-\lambda I$ is injective and that, by Proposition 9.14, the range of $A-\lambda I$ is closed. But

$$(A-\lambda I)^* = A^* - \lambda I = A - \lambda I$$

and $A-\lambda I$ is injective, so by Proposition 9.12, the range of $A-\lambda I$ is all of $\mathbf{H}$. This means $A-\lambda I$ has an inverse, which is bounded by (9.7). Thus λ is not in the spectrum of A.

Point 2 is left as an exercise (Exercise 4). ∎

Definition 9.19 *Let A be an unbounded operator on $\mathbf{H}$. Then A is **non-negative** if $\langle \psi, A\psi\rangle \geq 0$ for all $\psi \in \mathrm{Dom}(A)$ and A is **bounded below** by $c \in \mathbb{R}$ if $\langle \psi, A\psi\rangle \geq c\|\psi\|^2$ for all $\psi \in \mathrm{Dom}(A)$.*

Proposition 9.20 *Let A be an unbounded self-adjoint operator on $\mathbf{H}$. If A is non-negative, then the spectrum of A is contained in $[0,\infty)$. More generally, if A is bounded below by c, then the spectrum of A is contained in $[c,\infty)$.*

We will eventually see, using the spectral theorem for unbounded self-adjoint operators, that the converse to Proposition 9.20 also holds: If the spectrum of a self-adjoint operator A is contained in $[0,\infty)$, then A is non-negative, and if the spectrum of A is contained in $[c,\infty)$, then A is bounded below by c. These results follow easily, for example, from the form of the spectral theorem in Theorem 10.9.

Proof. Suppose A is bounded below by c and λ is a point in the spectrum of A. If ψ_n be a sequence as in Point 1 of Proposition 9.18, with the ψ_n's normalized to be unit vectors, then

$$\lim_{n\to\infty} |\langle \psi_n, (A-\lambda I)\psi_n\rangle| \leq \lim_{n\to\infty} \|(A-\lambda I)\psi_n\| = 0.$$

On the other hand, $A = \lambda I + (A-\lambda I)$, and so

$$\langle \psi_n, A\psi_n\rangle = \lambda + \langle \psi_n, (A-\lambda I)\psi_n\rangle .$$

Thus, $\langle \psi_n, A\psi_n\rangle$ converges to λ $(= \lambda \langle \psi_n, \psi_n\rangle)$ as n tends to infinity. Since A is bounded below by c, we must have $\lambda \geq c$. This establishes the result for operators bounded below by c. Specializing to $c = 0$ gives the result for non-negative operators. ∎

9.5 Conditions for Self-Adjointness and Essential Self-Adjointness

In this section, we give criteria for determining whether a symmetric operator is self-adjoint or essentially self-adjoint. See also Sect. 10.2 for the connection between self-adjoint operators and one-parameter unitary groups.

Theorem 9.21 *If A is a symmetric operator on $\mathbf{H}$, then A is essentially self-adjoint if and only if* $\mathrm{Range}(A-iI)$ *and* $\mathrm{Range}(A+iI)$ *are dense subspaces of* $\mathbf{H}$.

Using Proposition 9.12, we can reformulate this result as follows.

Corollary 9.22 *If A is a symmetric operator on $\mathbf{H}$, then A is essentially self-adjoint if and only if the operators A^*+iI and A^*-iI are injective on* $\mathrm{Dom}(A^*)$.

As Exercise 11 shows, it is possible to have one of the operators A^*+iI and A^*-iI be injective and the other fail to be injective.

Proof of Theorem 9.21. Assume first that A is essentially self-adjoint, so that A^{cl} is self-adjoint. Then $A^* = (A^{cl})^* = A^{cl}$, and so

$$[\mathrm{Range}(A-iI)]^{\perp} = \ker(A^*+iI) = \ker(A^{cl}+iI) = \{0\},$$

by Theorem 9.17, and similarly for the range of $A+iI$.

Conversely, assume A is symmetric and that $A - iI$ and $A + iI$ both have dense range. Since $(A^{cl})^* = A^*$ is a closed extension of A, it is also an extension of A^{cl}, showing that A^{cl} is symmetric. We may then apply Lemma 7.8—the proof of which requires only symmetry—to the operator A^{cl} with $\lambda = i$, giving

$$\left\|(A^{cl} - iI)\psi\right\|^2 \geq \|\psi\|^2 \tag{9.8}$$

and showing that $A^{cl} - iI$ is injective. Since the range of $A - iI$ is dense, the range of $A^{cl} - iI$ is certainly also dense. But since A^{cl} is closed, (9.8) and Proposition 9.14 tell us that the range of $A^{cl} - iI$ is closed, hence all of $\mathbf{H}$. Similar reasoning shows that the range of $A^{cl} + iI$ is also all of $\mathbf{H}$.

Now, by Proposition 9.13, $(A^{cl} - iI)^* = (A^{cl})^* + iI$, which is an extension of $A^{cl} + iI$. Suppose $(A^{cl})^* + iI$ is a *proper* extension of $A^{cl} + iI$, that is, that the domain of $(A^{cl})^* + iI$ is strictly bigger than the domain of $A^{cl} + iI$. Then since $A^{cl} + iI$ already maps *onto* $\mathbf{H}$, $(A^{cl})^* + iI$ cannot be injective. Thus, the operator

$$(A^{cl})^* + iI = A^* + iI = (A - iI)^*$$

must have a nontrivial kernel. Then by Proposition 9.12, Range$(A - iI)$ is not dense, contradicting our assumptions.

We conclude, therefore, that $(A^{cl})^* + iI$ is *not* a proper extension of $A^{cl} + iI$, i.e., that $(A^{cl})^* + iI = A^{cl} + iI$ (with equality of domains). This, by Proposition 9.13, means that $(A^{cl})^* = A^*$ (with equality of domains), which is what we are trying to prove. ■

Proposition 9.23 *If A is a symmetric operator on* $\mathbf{H}$*, then A is self-adjoint if and only if*

$$\text{Range}(A - iI) = \text{Range}(A + iI) = \mathbf{H}.$$

Proof. Suppose first that A is self-adjoint. Then by Theorem 9.21, the ranges of $A - iI$ and $A + iI$ are dense in $\mathbf{H}$. On the other hand,

$$\|(A - iI)\psi\|^2 \geq \|\psi\|^2, \tag{9.9}$$

by (the proof of) Lemma 7.8, with $\lambda = i$. Since, also, $A = A^*$ is closed, Proposition 9.14 tells us that the range of $A - iI$ is closed, hence all of $\mathbf{H}$. A similar argument shows that the range of $A + iI$ is all of $\mathbf{H}$.

Conversely, suppose that the ranges of $A - iI$ and $A + iI$ are all of $\mathbf{H}$. Then A is essentially self-adjoint by Theorem 9.21, so that A^* is self-adjoint. Since $A - iI$ already maps *onto* $\mathbf{H}$, if A^* were a nontrivial extension of A, then $A^* - iI$ could not be injective. But (9.9), with A replaced by A^*, shows that $A^* - iI$ is injective. Thus, $A = A^*$ and so A is self-adjoint. ■

In the case that A is positive-semidefinite (i.e., $\langle \psi, A\psi \rangle \geq 0$ for all $\psi \in \text{Dom}(A)$), there is another self-adjointness condition, the proof of which is very similar to that of Theorem 9.22.

Theorem 9.24 *Suppose that A is a symmetric operator on $\mathbf{H}$ and that $\langle\psi, A\psi\rangle \geq 0$ for all $\psi \in \mathrm{Dom}(A)$. Then A is essentially self-adjoint if and only if $A + I$ has dense range. Equivalently, A is essentially self-adjoint if and only if $A^* + I$ is injective.*

Proof. Assume first that A is essentially self-adjoint. Then $(A + I)^* = A^* + I = A^{cl} + I$. It is easily seen that A^{cl} is also positive definite, and so

$$\left\langle\psi, (A^{cl} + I)\psi\right\rangle = \langle\psi, \psi\rangle + \left\langle\psi, A^{cl}\psi\right\rangle \geq \langle\psi, \psi\rangle \tag{9.10}$$

Thus, $A^{cl} + I = (A + I)^*$ is injective. Thus, the range of $A + I$ is dense, by Proposition 9.12.

Now assume that $A + I$ has dense range. By (9.10), $A^{cl} + I$ is injective and by (9.10) and Proposition 9.14, the range of $A^{cl} + I$ is closed, hence all of $\mathbf{H}$. Assume $\mathrm{Dom}(A^*)$ is strictly larger than $\mathrm{Dom}(A^{cl})$. Then because $A^{cl} + I$ is already surjective, $A^* + I$ (which has a domain equal to the domain of A^*) cannot be injective. Thus, $A^* + I = (A + I)^*$ has a nontrivial kernel, which means that the range of $A + I$ is not dense. This is a contradiction, and so the domain of A^* must actually be equal to the domain of A^{cl}. Since A and so also A^{cl} are symmetric, this means that A^{cl} is self-adjoint. ■

Example 9.25 *Suppose that A is a symmetric operator on $\mathbf{H}$ that has an orthonormal basis of eigenvectors. That is to say, suppose there is an orthonormal basis $\{e_j\}$ for $\mathbf{H}$ such that for each j, we have $e_j \in \mathrm{Dom}(A)$ and $Ae_j = \lambda_j e_j$ for some real number λ_j. Then A is essentially self-adjoint.*

This result is a strengthening of Example 9.15, in that we do not assume that the domain of A is equal to the space of finite linear combinations of the e_j's.

Proof. For any j, $(A - iI)e_j = (\lambda_j - i)e_j$. Since λ_j is real, we have a nonzero multiple of e_j belonging to $\mathrm{Range}(A - iI)$, for each j. This shows that $\mathrm{Range}(A - iI)$ is dense, and similarly for $\mathrm{Range}(A + iI)$. ■

Example 9.26 *Suppose $\mathbf{H}$ is a Hilbert space direct sum of a sequence of separable Hilbert spaces $\mathbf{H}_j$:*

$$\mathbf{H} = \bigoplus_{j=1}^{\infty} \mathbf{H}_j.$$

Suppose also that A_j is a bounded self-adjoint operator on $\mathbf{H}_j$, for each j. Define a subspace V of $\mathbf{H}$ by

$$V = \left\{ \psi = (\psi_1, \psi_2, \ldots) \left| \sum_{j=1}^{\infty} \left(\|\psi_j\|_j^2 + \|A_j\psi_j\|_j^2 \right) < \infty \right. \right\}.$$

Suppose now that A is a symmetric operator on $\mathbf{H}$ whose domain contains the finite direct sum of the $\mathbf{H}_j$'s and such that $A|_{\mathbf{H}_j} = A_j$. Then A is *essentially self-adjoint,* $\mathrm{Dom}(A^{cl}) = \mathrm{Dom}(A^*) = V$*, and*

$$A^{cl}\psi = A^*\psi = (A_1\psi_1, A_2\psi_2, \ldots) \tag{9.11}$$

for all $\psi = (\psi_1, \psi_2, \ldots)$ *in* V*.*

See Definition A.45 for the definition of the Hilbert direct sum and the finite direct sum of a sequence of Hilbert spaces. Example 9.25 is the special case of Example 9.26 in which each $\mathbf{H}_j$ has dimension 1. This result will be useful to us in Chap. 10.

Proof. Since A_j is self-adjoint, the ranges of $A_j - iI$ and $A_j + iI$ are dense in $\mathbf{H}_j$. Thus, the closure of the range of $A - iI$ contains each $\mathbf{H}_j$ and is therefore dense in $\mathbf{H}$, and similarly for $A + iI$. This shows that A is essentially self-adjoint.

It remains to show that the domain of $A^* = A^{cl}$ is V. Let W denote the finite direct sum of the $\mathbf{H}_j$'s. By the argument in the previous paragraph, $A|_W$ is essentially self-adjoint. Then A^* is a symmetric extension of $(A|_W)^*$, which must coincide with $(A|_W)^*$. Thus, it suffices to consider the case $\mathrm{Dom}(A) = W$.

If we assume that $\mathrm{Dom}(A) = W$, we can compute the adjoint of A by the argument in Example 9.15. If $\phi \in V$, then the Cauchy–Schwarz inequality shows that the linear functional $\langle \phi, A\cdot \rangle$ is bounded and that $A^*\phi$ is as (9.11). On the other hand, if $\langle \phi, A\cdot \rangle$ is bounded, where $\phi = (\phi_1, \phi_2, \ldots)$, take

$$\psi_N = (\phi_1, \phi_2, \ldots, \phi_N, 0, 0, \ldots).$$

Then, as in the proof of Example 9.15, the only way we can have $|\langle \phi, A\psi_N \rangle| \leq C\,\|\psi_N\|$ is if ϕ belongs to V. ■

9.6 A Counterexample

In this section, we will examine an elementary example of an operator that is symmetric but not essentially self-adjoint. Our example will be essentially the momentum operator on a finite interval, with "wrong" boundary conditions. (A more sophisticated example is given in Sect. 9.10.) We take our Hilbert space to be $L^2([0,1])$.

Proposition 9.27 *Let* $\mathrm{Dom}(A) \subset L^2([0,1])$ *be the space of continuously differentiable functions* f *on* $[0,1]$ *satisfying*

$$\psi(0) = \psi(1) = 0.$$

For $\psi \in \mathrm{Dom}(A)$*, define*

$$A\psi = -i\hbar \frac{d\psi}{dx}.$$

Then A *is symmetric but not essentially self-adjoint.*

We can understand the failure of essential self-adjointness of A in practical terms as a failure of the spectral theorem. The eigenvector equation $A\psi = \lambda\psi$ for $\lambda \in \mathbb{R}$ is a first-order ordinary differential equation, whose general solution is $\psi(x) = ce^{i\lambda x}$, where c is a constant. The only way such a function can satisfy the boundary conditions $\psi(0) = \psi(1) = 0$ is if $c = 0$, in which case ψ is the zero vector. Thus, A has no eigenvectors. Furthermore, taking the closure of A does not help, because, as the proof will show, the boundary conditions survive taking the closure.

Proof of symmetry. Using integration by parts we see that for all ϕ and ψ in $\mathrm{Dom}(A)$ we have

$$\int_0^1 \overline{\phi(x)} \frac{d\psi}{dx}\ dx = \overline{\phi(1)}\psi(1) - \overline{\phi(0)}\psi(0) - \int_0^1 \overline{\frac{d\phi}{dx}} \psi(x)\ dx. \tag{9.12}$$

Since we assume ϕ and ψ are in $\mathrm{Dom}(A)$, the boundary terms are zero and we get

$$\left\langle \phi, \frac{d\psi}{dx} \right\rangle_{L^2([0,1])} = -\left\langle \frac{d\phi}{dx}, \psi \right\rangle_{L^2([0,1])}.$$

Because there is a conjugate in one side of the inner product but not the other, it follows that

$$\left\langle \phi, -i\hbar \frac{d\psi}{dx} \right\rangle_{L^2([0,1])} = \left\langle -i\hbar \frac{d\phi}{dx}, \psi \right\rangle_{L^2([0,1])},$$

as claimed. ■

We now consider A^{cl} and $A^* = (A^{cl})^*$. We will see that there are elements of the domain of the adjoint that are not in the domain of the closure.

Lemma 9.28 *If ϕ is a continuously differentiable function on $[0,1]$, then $\phi \in \mathrm{Dom}(A^*)$ and $A^*\phi = -i\hbar\ d\phi/dx$.*

Proof. If ϕ is continuously differentiable, then for any ψ in $\mathrm{Dom}(A)$, we may integrate by parts as in (9.12). Since ψ is zero at both ends of the interval, the boundary terms vanish and we obtain

$$\begin{aligned} \langle \phi, A\psi \rangle &= i\hbar \int_0^1 \overline{\frac{d\phi}{dx}} \psi(x)\ dx \\ &= \int_0^1 \overline{\left(-i\hbar \frac{d\phi}{dx}\right)} \psi(x)\ dx \end{aligned} \tag{9.13}$$

Since $d\phi/dx$ is continuous and hence in $L^2([0,1])$, we see that (9.13) is a continuous linear functional, as a function of ψ with fixed ϕ. Thus, ψ is in the domain of A^*, and $A^*\phi = -i\ d\phi/dx$. ■

Proof of Proposition 9.27. Suppose ψ is in the domain of A^{cl}. Then there exist ψ_n in $\mathrm{Dom}(A)$ such that ψ_n converges to ψ and $A\psi_n$ converges to some $\chi \in L^2([0,1])$. Since the derivatives of the ψ_n's are converging in L^2, the ψ_n's themselves must be converging uniformly, as can be shown by writing each ψ_n as the integral of its derivative. (See Exercise 10.) It follows that every element of $\mathrm{Dom}(A^{cl})$ is continuous and vanishes at both ends of the interval. On the other hand, $\mathrm{Dom}(A^*)$ contains all smooth functions, including many that do not vanish at the ends of the interval. Thus, A^{cl} and $(A^{cl})^* = A^*$ do not have the same domains. ∎

It follows from Lemma 9.28 that *every* complex number λ belongs to the spectrum of A^{cl}. See Exercise 9.

The reason that A fails to be essentially self-adjoint is that we impose *too many* boundary conditions on functions in the domain of A, which results in there being *too few* boundary conditions (in this case, no boundary conditions at all) on functions in the domain of A^*. In this example, A^* is given by the same *formula* as A ($-id/dx$ in both cases), but the domain of A^* is bigger than the domain of A^{cl}.

Suppose we define another operator B, still given by the formula $-i\, d/dx$, but with the domain of B to be the space of continuously differentiable functions ψ with $\psi(0) = \psi(1)$. If we integrate by parts as in (9.12), the boundary terms will cancel, showing that B is symmetric. Meanwhile, the functions $\psi_n(x) := e^{2\pi i n x}$, $n \in \mathbb{Z}$, form an orthonormal basis for $L^2([0,1])$ consisting of eigenvectors for B, with real eigenvalues $\lambda_n = 2\pi n$. Thus, by Example 9.25, B is essentially self-adjoint.

9.7 An Example

We now give an example of an operator that *is* essentially self-adjoint. Let $C_c^\infty(\mathbb{R})$ denote the space of smooth, compactly supported functions on $\mathbb{R}$.

Proposition 9.29 *Let P be the densely defined operator with* $\mathrm{Dom}(P) = C_c^\infty(\mathbb{R}) \subset L^2(\mathbb{R})$ *and given by $P\psi = -i\hbar\, d\psi/dx$. Then P is essentially self-adjoint.*

Proof. Our strategy is to apply Corollary 9.22. Since P is symmetric, we expect that P^* will be given by the formula $-i\hbar\, d/dx$, on some suitable domain inside $L^2(\mathbb{R})$. Thus, if $\psi \in \ker(P^* + iI)$, this should mean that $-i\hbar\, d\psi/dx = -i\psi$, or $d\psi/dx = (1/\hbar)\psi(x)$, which ought to imply that $\psi(x) = ce^{x/\hbar}$, for some constant c. Since $ce^{x/\hbar}$ belongs to $L^2(\mathbb{R})$ only if $c = 0$, we hope to conclude that $\psi = 0$.

To say that $\psi \in L^2(\mathbb{R})$ belongs to the kernel of $P^* + iI$ means that ψ belongs to $\mathrm{Dom}(P^*)$ and that $P^*\psi = -i\psi$. This holds if and only if

$$-i\hbar \int_{\mathbb{R}} \overline{\frac{d\chi}{dx}} \psi(x)\, dx = i \int_{\mathbb{R}} \overline{\chi(x)} \psi(x)\, dx$$

for all $\chi \in C_c^\infty(\mathbb{R})$. For any $\xi \in C_c^\infty(\mathbb{R})$, if we take $\chi(x) = \xi(x)e^{-x/\hbar}$ and combine the integrals into one, we get

$$\begin{aligned} 0 &= -i \int_{\mathbb{R}} \left[\hbar e^{-x/\hbar} \overline{\frac{d\xi}{dx}} - e^{-x/\hbar}\overline{\xi(x)} + e^{-x/\hbar}\overline{\xi(x)} \right] \psi(x)\ dx \\ &= -i\hbar \int_{\mathbb{R}} \overline{\frac{d\xi}{dx}} e^{-x/\hbar}\psi(x)\ dx. \end{aligned} \tag{9.14}$$

Now, (9.14) says that the derivative of $e^{-x/\hbar}\psi(x)$ in the weak or distributional sense is zero. (See Proposition A.29 in Appendix A.3.3.) Thus, by the remarks immediately following Proposition A.5, we must have $e^{-x/\hbar}\psi(x) = c$ for some c, meaning that $\psi(x) = ce^{x/\hbar}$. Since we also assume that ψ belongs to $\mathrm{Dom}(P^*) \subset L^2(\mathbb{R})$, we must have $c = 0$, so that ψ is the zero element of $L^2(\mathbb{R})$.

We have shown, then, that only 0 belongs to the kernel of $P^* + iI$. A similar argument with i replaced by $-i$ and $e^{x/\hbar}$ by $e^{-x/\hbar}$ shows that only 0 belongs to the kernel of $P^* - iI$. Thus, by Corollary 9.22, P is essentially self-adjoint. ■

9.8 The Basic Operators of Quantum Mechanics

In this section, we consider several of the unbounded self-adjoint operators that arise in quantum mechanics. We find natural domains of self- adjointness for the position, momentum, kinetic energy, and potential energy operators. Since Schrödinger operators are more complicated to analyze, we postpone a discussion of them until the next section. We begin with the potential energy operator.

Proposition 9.30 *Suppose $V : \mathbb{R}^n \to \mathbb{R}$ is a measurable function. Let $V(\mathbf{X})$ be the unbounded operator with domain*

$$\mathrm{Dom}(V(\mathbf{X})) = \left\{ \psi \in L^2(\mathbb{R}^n) \,\middle|\, V(\mathbf{x})\psi(\mathbf{x}) \in L^2(\mathbb{R}^n) \right\}$$

and given by

$$[V(\mathbf{X})\psi](\mathbf{x}) = V(\mathbf{x})\psi(\mathbf{x}).$$

Then $\mathrm{Dom}(V(\mathbf{X}))$ *is dense in* $L^2(\mathbb{R}^n)$ *and* $V(\mathbf{X})$ *is self-adjoint on this domain.*

Proof. Define a subset E_m of $\mathbb{R}^n$ by

$$E_m = \{ \mathbf{x} \in \mathbb{R}^n \,| |V(\mathbf{x})| < m \},$$

so that $\cup_m E_m = \mathbb{R}^n$. Then for any $\psi \in L^2(\mathbb{R}^n)$, the function $\psi 1_{E_m}$ belongs to $\mathrm{Dom}(V(\mathbf{X}))$. On the other hand, using dominated convergence, we have $\psi 1_{E_m} \to \psi$ as $m \to \infty$, establishing that $\mathrm{Dom}(V(\mathbf{X}))$ is dense.

Since V is real-valued, it is easy to see that $V(\mathbf{X})$ is symmetric on $\mathrm{Dom}(V(\mathbf{X}))$. Thus, $V(\mathbf{X})^*$ is an extension of $V(\mathbf{X})$.

Meanwhile, suppose $\phi \in \mathrm{Dom}(V(\mathbf{X})^*)$, meaning that

$$\psi \mapsto \int_X \overline{\phi(x)} V(x)\psi(x)\, dx, \quad \psi \in \mathrm{Dom}(V(\mathbf{X})) \tag{9.15}$$

is a bounded linear functional. This linear functional has a unique bounded extension to L^2 and, thus, Thus, there exists a unique $\chi \in L^2(\mathbb{R}^n)$ such that

$$\int_X \overline{\psi(x)} V(x)\phi(x)\, dx = \int_X \overline{\chi(x)}\phi(x)\, dx, \tag{9.16}$$

or

$$\int_X \left[\overline{\psi(x)} V(x) - \overline{\chi(x)}\right] \phi(x)\, dx = 0$$

for all $\phi \in \mathrm{Dom}(V(\mathbf{X}))$.

Taking $\phi = (\psi V - \chi) 1_{E_m}$, we see that $\psi V - \chi$ is zero almost everywhere on E_m, for all m, hence zero almost everywhere on $\mathbb{R}^n$. Thus, ψV is equal to χ as an element of $L^2(\mathbb{R}^n)$. This shows that $\psi \in \mathrm{Dom}(V(\mathbf{X}))$. Thus, actually, $\mathrm{Dom}(V(\mathbf{X})^*) = \mathrm{Dom}(V(\mathbf{X}))$. Since we have already shown that $V(\mathbf{X})^*$ is an extension of $V(\mathbf{X})$, we conclude that $V(\mathbf{X})$ is self-adjoint on $\mathrm{Dom}(V(\mathbf{X}))$. ■

If we specialize the preceding proposition to the case $V(\mathbf{x}) = x_j$, we obtain the following result about the position operator.

Corollary 9.31 *The position operator X_j is self-adjoint on the domain*

$$\mathrm{Dom}(X_j) = \left\{\psi \in L^2(\mathbb{R}^n) \,\middle|\, x_j\psi(\mathbf{x}) \in L^2(\mathbb{R}^n)\right\}.$$

We now turn to consideration of the momentum operator. Since the Fourier transform converts $\partial/\partial x_j$ into multiplication by ik_j (Proposition A.17) we can use the preceding results on multiplication operators to obtain a natural domain on which the momentum operator is self-adjoint.

Proposition 9.32 *For each $j = 1, 2, \ldots, n$, define a domain* $\mathrm{Dom}(P_j) \subset L^2(\mathbb{R}^n)$ *as follows:*

$$\mathrm{Dom}(P_j) = \left\{\psi \in L^2(\mathbb{R}^n) \,\middle|\, k_j\hat{\psi}(\mathbf{k}) \in L^2(\mathbb{R}^n)\right\},$$

where $\hat{\psi}$ is the Fourier transform of ψ. Define P_j on this domain by

$$P_j\psi = \mathcal{F}^{-1}(\hbar k_j \hat{\psi}(\mathbf{k})).$$

Then P_j is self-adjoint on $\mathrm{Dom}(P_j)$.

The domain $\mathrm{Dom}(P_j)$ *of P_j can also be described as the set of all $\psi \in L^2(\mathbb{R}^n)$ such that $\partial\psi/\partial x_j$, computed in the distribution sense, belongs to $L^2(\mathbb{R}^n)$. For any $\psi \in \mathrm{Dom}(P_j)$, we have $P_j\psi = -i\hbar\partial\psi/\partial x_j$, where $\partial\psi/\partial x_j$ is computed in the distribution sense.*

Saying that the distributional derivative of ψ belongs to $L^2(\mathbb{R}^n)$ means (Proposition A.29) that there exists a (unique) ϕ in $L^2(\mathbb{R}^n)$ such that

$$-\left\langle \frac{\partial\chi}{\partial x_j},\psi\right\rangle = \langle\chi,\phi\rangle$$

for all $\chi\in C_c^\infty(\mathbb{R}^n)$. If ψ is continuously differentiable, then the distributional derivative of ψ coincides with the ordinary derivative of ψ. Thus, if $\psi\in L^2(\mathbb{R}^n)$ is continuously differentiable, then ψ belongs to $\mathrm{Dom}(P_j)$ if and only if $\partial\psi/\partial x_j$, computed in the pointwise sense, belongs to $L^2(\mathbb{R}^n)$, in which case $P_j\psi=-i\hbar\partial\psi/\partial x_j$. On the other hand, if $\psi\in\mathrm{Dom}(P_j)$, it is not necessarily the case that ψ is *continuously* differentiable.

In the case $n=1$, the domain of P_1 certainly contains $C_c^\infty(\mathbb{R})$, since each element ψ of $C_c^\infty(\mathbb{R})$ is a Schwartz function (Definition A.15), so that $\hat\psi$ is also a Schwartz function, in which case $k\hat\psi(k)$ belongs to $L^2(\mathbb{R})$. Now, as shown in Sect. 9.7, the operator $-i\hbar d/dx$ is essentially self-adjoint on $C_c^\infty(\mathbb{R})$, which means that this operator has a unique self-adjoint extension. This self-adjoint extension must, therefore, agree with the operator P_1 in the $n=1$ case of Proposition 9.32.

Lemma 9.33 *Suppose $\psi\in L^2(\mathbb{R}^n)$ has the property that $\partial\psi/\partial x_j$, computed in the distribution sense, is equal to an L^2 function ϕ. Then $\hat\phi(\mathbf{k})=ik_j\hat\psi(\mathbf{k})$, showing that $k_j\hat\psi(\mathbf{k})$ belongs to $L^2(\mathbb{R}^n)$.*

Conversely, suppose $\psi\in L^2(\mathbb{R}^n)$ has the property that $k_j\hat\psi(\mathbf{k})$ belongs to $L^2(\mathbb{R}^n)$. Then $\partial\psi/\partial x_j$, computed in the distribution sense, is equal to the L^2 function $\mathcal{F}^{-1}(ik_j\mathcal{F}(\psi))$.

Proof. Suppose $\partial\psi/\partial x_j$, computed in the distribution sense, is equal to the L^2 function ϕ (see Definition A.28). Then by the unitarity of the Fourier transform (Theorem A.19) and its behavior with respect to differentiation (Proposition A.17), we have

$$\begin{aligned}\langle\chi,\phi\rangle &= -\left\langle\frac{\partial\chi}{\partial x_j},\psi\right\rangle\\ &= -\left\langle ik_j\mathcal{F}(\chi),\mathcal{F}(\psi)\right\rangle,\end{aligned}$$

for all $\chi\in C_c^\infty(\mathbb{R})$. Thus,

$$\langle\mathcal{F}(\chi),\mathcal{F}(\phi)\rangle = -\left\langle ik_j\mathcal{F}(\chi),\mathcal{F}(\psi)\right\rangle,\quad \chi\in C_c^\infty(\mathbb{R}).$$

Writing this equality out as an integral, we have

$$\begin{aligned}\int_{\mathbb{R}^n}\overline{\hat\chi(\mathbf{k})}\hat\phi(\mathbf{k})\;d\mathbf{k} &= -\int_{\mathbb{R}^n}\overline{ik_j\hat\chi(\mathbf{k})}\hat\psi(\mathbf{k})\;d\mathbf{k}\\ &= \int_{\mathbb{R}^n}\overline{\hat\chi(\mathbf{k})}ik_j\hat\psi(\mathbf{k})\;d\mathbf{k}\end{aligned}\qquad(9.17)$$

for all $\chi\in C_c^\infty(\mathbb{R}^n)$.

We now claim that because (9.17) holds for *all* $\chi \in C_c^\infty(\mathbb{R}^n)$, we must have $\hat{\phi}(\mathbf{k}) = ik_j\hat{\psi}(\mathbf{k})$ for almost every $\mathbf{k}$. Using the Stone–Weierstrass theorem and Theorem A.10, it is not hard to show that the space of smooth functions with support in $[a,b]$ is dense in $L^2([a,b])$, for all $a < b \in \mathbb{R}$. Since both $\hat{\phi}$ and $k_j\hat{\psi}(\mathbf{k})$ are locally square-integrable, we see that these two functions are equal almost everywhere on $[a,b]$, for all $a < b \in \mathbb{R}$, and hence equal almost everywhere on $\mathbb{R}$.

Since $\hat{\phi}$ is globally square-integrable, so is $k_j\hat{\psi}(\mathbf{k})$. Furthermore, by the injectivity of the L^2 Fourier transform, we have

$$\frac{\partial\psi}{\partial x_j} = \phi = \mathcal{F}^{-1}(ik_j\mathcal{F}(\psi))$$

as claimed.

The argument for the second part of the lemma is similar and left as an exercise (Exercise 12). ∎

Proof of Proposition 9.32. By Proposition 9.30, the operator of multiplication by k_j is an unbounded self-adjoint operator on $L^2(\mathbb{R}^n)$, with domain equal to the set of ϕ for which $k_j\phi(\mathbf{k})$ belongs to $L^2(\mathbb{R}^n)$. It then follows from the unitarity of the Fourier transform that $P_j = \hbar\mathcal{F}^{-1}M_{k_j}\mathcal{F}$ is self-adjoint on $\mathcal{F}^{-1}(\mathrm{Dom}(M_{k_j}))$, where M_{k_j} denotes multiplication by k_j.

The second characterization of $\mathrm{Dom}(P_j)$ follows from Lemma 9.33. ∎

Proposition 9.34 *Define a domain* $\mathrm{Dom}(\Delta)$ *as follows:*

$$\mathrm{Dom}(\Delta) = \left\{\psi \in L^2(\mathbb{R}^n) \,\middle|\, |\mathbf{k}|^2\,\hat{\psi}(\mathbf{k}) \in L^2(\mathbb{R}^n)\right\}.$$

Define Δ *on this domain by the expression*

$$\Delta\psi = -\mathcal{F}^{-1}(|\mathbf{k}|^2\,\hat{\psi}(\mathbf{k})), \tag{9.18}$$

where $\hat{\psi}$ *is the Fourier transform of* ψ *and* $\mathcal{F}^{-1}$ *is the inverse Fourier. Then* Δ *is self-adjoint on* $\mathrm{Dom}(\Delta)$*.*

The domain $\mathrm{Dom}(\Delta)$ *may also be described as the set of all* $\psi \in L^2(\mathbb{R}^n)$ *such that* $\Delta\psi$*, computed in the distribution sense, belongs to* $L^2(\mathbb{R}^n)$*. If* $\psi \in \mathrm{Dom}(\Delta)$*, then* $\Delta\psi$ *as defined by (9.18) agrees with* $\Delta\psi$ *computed in the distribution sense.*

The proof of Proposition 9.34 is extremely similar to that of Proposition 9.32 and is omitted. Of course, the kinetic energy operator $-\hbar^2\Delta/(2m)$ is also self-adjoint on the same domain as Δ. It is easy to see from (9.18) and the unitarity of the Fourier transform that $-\hbar^2\Delta/(2m)$ is non-negative, that is, that

$$\left\langle\psi, -\frac{\hbar^2}{2m}\Delta\psi\right\rangle \geq 0$$

for all $\psi \in \mathrm{Dom}(\Delta)$.

Using the same reasoning as in Sects. 9.6 and 9.7, it is not hard to show that the operators P_j and Δ are essentially self-adjoint on $C_c^\infty(\mathbb{R}^n)$. See Exercise 16.

Care must be exercised in applying Proposition 9.34. Although the function

$$\psi(\mathbf{x}) := \frac{1}{|\mathbf{x}|}$$

is harmonic on $\mathbb{R}^3\backslash\{0\}$, the Laplacian over $\mathbb{R}^3$ of ψ in the distribution sense is *not* zero (Exercise 13). (It can be shown, by carefully analyzing the calculation in the proof of Proposition 9.35, that $\Delta\psi$ is a nonzero multiple of a δ-function.) This example shows that if a function ψ has a singularity, calculating the Laplacian of ψ away from the singularity may not give the correct distributional Laplacian of ψ. For example, the function ϕ in $L^2(\mathbb{R}^3)$ given by

$$\phi(\mathbf{x}) := \frac{e^{-|\mathbf{x}|^2}}{|\mathbf{x}|} \tag{9.19}$$

is not in $\mathrm{Dom}(\Delta)$, even though both ϕ and $\Delta\phi$ are (by direct computation) square-integrable over $\mathbb{R}^3\backslash\{0\}$. Indeed, when $n \leq 3$, every element of $\mathrm{Dom}(\Delta)$ is continuous (Exercise 14).

Proposition 9.35 *Suppose $\psi(\mathbf{x}) = g(\mathbf{x})f(|\mathbf{x}|)$, where g is a smooth function on $\mathbb{R}^n$ and f is a smooth function on $(0,\infty)$. Suppose also that f satisfies*

$$\lim_{r\to 0^+} r^{n-1}f(r) = 0$$
$$\lim_{r\to 0^+} r^{n-1}f'(r) = 0.$$

If both ψ and $\Delta\psi$ are square-integrable over $\mathbb{R}^n\backslash\{0\}$, then ψ belongs to $\mathrm{Dom}(\Delta)$.

Note that the second condition in the proposition fails if $n = 3$ and $f(r) = 1/r$. We will make use of this result in Chap. 18.

Proof. To apply Proposition 9.34, we need to compute $\langle\psi, \Delta\chi\rangle$, for each $\chi \in C_c^\infty(\mathbb{R}^n)$. We choose a large cube C, centered at the origin and such that the support of χ is contained in the interior of C. Then we consider the integral of $\bar{\psi}(\partial^2\chi/\partial x_j^2)$ over $C\backslash C_\varepsilon$, where C_ε is a cube centered at the origin and having side-length ε. We evaluate the x_j-integral first and we integrate by parts twice. For "good" values of the remaining variables, x_j ranges over all of C, in which case there are no boundary terms to worry about. For "bad" values of the remaining variables, we get two kinds of boundary terms, one involving $\bar{\psi}(\partial\chi/\partial x_j)$ and one involving $(\partial\bar{\psi}/\partial x_j)\chi$, in both cases integrated over two opposite faces of C_ε.

Now,

$$\frac{\partial\psi}{\partial x_j} = \frac{\partial g}{\partial x_j}f(|\mathbf{x}|) + g(\mathbf{x})\frac{df}{dr}\frac{x_j}{r}.$$

Since the area of the faces of the cube is ε^{n-1}, the assumption on f will cause the boundary terms to disappear in the limit as ε tends to zero. Furthermore, both ψ and $\Delta\psi$ are in $L^2(\mathbb{R}^n)$ and thus in $L^1(C)$, where in the case of $\Delta\psi$, we simply leave the value at the origin (which is a set of measure zero) undefined. Thus, integrals of $\bar{\psi}\Delta\chi$ and $(\Delta\bar{\psi})\chi$ over $C\backslash C_\varepsilon$ will converge to integrals over C. Since the boundary terms vanish in the limit, we are left with

$$\langle \psi, \Delta\chi \rangle = \langle \Delta\psi, \chi \rangle .$$

Thus, the distributional Laplacian of ψ is simply integration against the "pointwise" Laplacian, ignoring the origin. Proposition 9.34 then tells us that $\psi \in \mathrm{Dom}(\Delta)$. ∎

9.9 Sums of Self-Adjoint Operators

In the previous section, we have succeeded in defining the Laplacian Δ, and hence also the kinetic energy operator $-\hbar^2\Delta/(2m)$, as a self-adjoint operator on a natural dense domain in $L^2(\mathbb{R}^n)$. We have also defined the potential energy operator $V(\mathbf{X})$ as a self-adjoint operator on a different dense domain, for any measurable function $V : \mathbb{R}^n \to \mathbb{R}$. To obtain the Schrödinger operator $-\hbar^2\Delta/(2m)+V(\mathbf{X})$, we "merely" have to make sense of the sum of two unbounded self-adjoint operators. This task, however, turns out to be more difficult than might be expected. In particular, if V is a highly singular function, then $-\hbar^2\Delta/(2m) + V(\mathbf{X})$ may fail to be self-adjoint or essentially self-adjoint on any natural domain.

Definition 9.36 *If A and B are unbounded operators on $\mathbf{H}$, then $A + B$ is the operator with domain*

$$\mathrm{Dom}(A + B) := \mathrm{Dom}(A) \cap \mathrm{Dom}(B)$$

and given by $(A + B)\psi = A\psi + B\psi$.

The sum of two unbounded self-adjoint operators A and B may fail to be self-adjoint or even essentially self-adjoint. [If, however, B is bounded with $\mathrm{Dom}(B) = \mathbf{H}$, then Proposition 9.13 shows that $A + B$ is self-adjoint on $\mathrm{Dom}(A) \cap \mathrm{Dom}(B) = \mathrm{Dom}(A)$.] For one thing, if A and B are unbounded, then $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$ may fail to be dense in $\mathbf{H}$. But even if $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$ is dense in $\mathbf{H}$, it can easily happen that $A + B$ is not essentially self-adjoint on this domain. (See, for example, Sect. 9.10.) Many things that are simple for bounded self-adjoint operators becomes complicated when dealing with unbounded self-adjoint operators!

In this section, we examine criteria on a function V under which the Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V$$

is self-adjoint or essentially self-adjoint on some natural domain inside $L^2(\mathbb{R}^n)$.

Theorem 9.37 (Kato–Rellich Theorem) *Suppose that A and B are unbounded self-adjoint operators on $\mathbf{H}$. Suppose that* $\mathrm{Dom}(A) \subset \mathrm{Dom}(B)$ *and that there exist positive constants a and b with $a < 1$ such that*

$$\|B\psi\| \leq a\,\|A\psi\| + b\,\|\psi\| \tag{9.20}$$

for all $\psi \in \mathrm{Dom}(A)$. Then $A+B$ is self-adjoint on $\mathrm{Dom}(A)$ and essentially self-adjoint on any subspace of $\mathrm{Dom}(A)$ on which A is essentially self-adjoint. Furthermore, if A is non-negative, then the spectrum of $A+B$ is bounded below by $-b/(1-a)$.

Note that since we assume $\mathrm{Dom}(B) \supset \mathrm{Dom}(A)$, the natural domain for $A+B$ is $\mathrm{Dom}(A) \cap \mathrm{Dom}(B) = \mathrm{Dom}(A)$. An operator B satisfying (9.20) is said to be *relatively bounded* with respect to A, with relative bound a.

Proof. We use the trivial variant of Theorem 9.21 given in Exercise 8. Choose a positive real number μ large enough that $a + b/\mu < 1$, which is possible because we assume $a < 1$. Then for any $\psi \in \mathrm{Dom}(A)$, we have

$$(A+B+i\mu I)\psi = \left(B(A+i\mu I)^{-1} + I\right)(A+i\mu I)\psi. \tag{9.21}$$

For any $\psi \in \mathbf{H}$, we compute that

$$\begin{aligned}\left\|B(A+i\mu I)^{-1}\psi\right\| &\leq a\left\|A(A+i\mu I)^{-1}\psi\right\| + b\left\|(A+i\mu I)^{-1}\psi\right\| \\ &\leq \left(a + \frac{b}{\mu}\right)\|\psi\|. \end{aligned} \tag{9.22}$$

Here we have made use of the estimates

$$\left\|A(A+i\mu I)^{-1}\right\| < 1, \quad \left\|(A+i\mu I)^{-1}\right\| < \frac{1}{\mu},$$

both of which are elementary (Exercise 17).

If C denotes the operator $B(A+i\mu I)^{-1}$, (9.22) tells us that $\|C\| < (a+b/\mu) < 1$. Thus, by Lemma 7.6, $C+I$ is invertible. Furthermore, since A is self-adjoint, $A+i\mu I$ maps $\mathrm{Dom}(A)$ *onto* $\mathbf{H}$. Thus, (9.21) tells us that $A+B+i\mu I$ also maps $\mathrm{Dom}(A)$ onto $\mathbf{H}$. The same argument shows that $A+B-i\mu I$ maps $\mathrm{Dom}(A)$ onto $\mathbf{H}$ and we conclude, by Exercise 8, that $A+B$ is self-adjoint on $\mathrm{Dom}(A)$.

Suppose, in addition, that A is non-negative. Let us replace $i\mu$ by $\lambda > 0$, in (9.21). Calculating as in (9.22), using the estimates in Exercise 18, we obtain that

$$\left\|B(A+\lambda I)^{-1}\psi\right\| \leq \left(a + \frac{b}{\lambda}\right)\|\psi\|$$

for all $\psi \in \mathbf{H}$. If $\lambda > b/(1-a)$, then $a + b/\lambda < 1$, and by the above argument, $\mathrm{Range}(A+B+\lambda I) = \mathbf{H}$. Furthermore, since $A+B+\lambda I$ is self-adjoint, Proposition 9.12 tells us that $\ker(A+B+\lambda I) = \{0\}$. This shows that $A+B+\lambda I$ is invertible and $-\lambda$ is in the resolvent set of $A+B$. We conclude, then, that the spectrum of $A+B$ is contained in $[-b/(1-a),+\infty)$.

The last part of the theorem, concerning essential self-adjointness, is left as an exercise (Exercise 19). ■

Theorem 9.38 *Suppose n is at most 3 and $V:\mathbb{R}^n\to\mathbb{R}$ is a measurable function that can be decomposed as a sum of two real-valued, measurable functions V_1 and V_2, with V_1 belonging to $L^2(\mathbb{R}^n)$ and V_2 being bounded. Then the Schrödinger operator $-\hbar^2\Delta/(2m)+V(\mathbf{X})$ is self-adjoint on* $\mathrm{Dom}(\Delta)$*. Furthermore, $-\hbar^2\Delta/(2m)+V(\mathbf{X})$ is bounded below.*

Implicit in the statement of the theorem is that $\mathrm{Dom}(V(\mathbf{X}))$, as given in Proposition 9.30, contains $\mathrm{Dom}(\Delta)$. A result similar to Theorem 9.38 in $\mathbb{R}^n$, $n\geq 4$, but the condition that V_1 belongs to $L^2(\mathbb{R}^n)$ is replaced by the condition that V_1 belongs to $L^p(\mathbb{R}^n)$ for some $p>n/2$. See Theorem X.20 in Volume II of [34].

Proof. We apply the Kato–Rellich theorem with $A=-\hbar^2\Delta/2m$ and $B=V(\mathbf{X})$. Assume $\psi\in\mathrm{Dom}(\Delta)$ and fix some $\varepsilon>0$. By Exercise 14, there exists a constant c_ε such that

$$|\psi(\mathbf{x})|\leq\varepsilon\left\|\Delta\psi\right\|+c_\varepsilon\left\|\psi\right\|$$

for all $\mathbf{x}\in\mathbb{R}^n$. Thus, if V is as in the theorem and $\psi\in\mathrm{Dom}(\Delta)$,

$$\begin{aligned}\|V\psi\|&\leq\sup|\psi(\mathbf{x})|\,\|V_1\|+\sup|V_2(\mathbf{x})|\,\|\psi\|\\&\leq\varepsilon\,\|V_1\|\,\|\Delta\psi\|+(c_\varepsilon\,\|V_1\|+\sup|V_2(\mathbf{x})|)\,\|\psi\|\,.\end{aligned}$$

This shows that $\mathrm{Dom}(V(\mathbf{X}))\supset\mathrm{Dom}(\Delta)$. Since ε is arbitrary, we can arrange for the constant in front of $\|\Delta\psi\|$ to be less than one and the Kato–Rellich theorem applies. ■

Theorem 9.39 *Suppose n is at most 3 and $V:\mathbb{R}^n\to\mathbb{R}$ is a measurable function that can be decomposed as a sum of three real-valued, measurable functions V_1, V_2, and V_3, with V_1 belonging to $L^2(\mathbb{R}^n)$, V_2 being bounded, and V_3 being non-negative and locally square-integrable. Then the Schrödinger operator $-\hbar^2\Delta/(2m)+V(\mathbf{X})$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^n)$.*

The proof of this result would take us too far afield and is omitted. See Theorem X.29 in Volume II of [34]. Note that we assume only that V_3 is non-negative and *locally* square-integrable; V_3 can tend to $+\infty$ arbitrarily fast at infinity. Again, the same result applies in $\mathbb{R}^n$, $n\geq 4$, if the condition on V_1 is replaced by the assumption that $V_1\in L^p(\mathbb{R}^n)$ for some $p>n/2$.

Proposition 9.40 *Fix* $\mathbf{a}$ *and* $\mathbf{b}$ *in $\mathbb{R}^n$ and let $\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}$ denote the operator given by*

$$(\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P})\psi(\mathbf{x})=(\mathbf{a}\cdot\mathbf{x})\psi(\mathbf{x})-i\hbar\sum_{j=1}^n b_j\frac{\partial\psi}{\partial x_j}.$$

Then $\mathbf{a}\cdot\mathbf{X}+\mathbf{b}\cdot\mathbf{P}$ *is essentially self-adjoint on* $C_c^\infty(\mathbb{R}^n)$*.*

Proof. We use the same strategy as in Sect. 9.7, namely we explicitly solve the equation $A^*\psi=\pm i\psi$ and find that there are no nonzero, square-integrable solutions.

The case $\mathbf{b}=0$ is not hard to analyze and is left as an exercise (Exercise 20). Assume, then, that $\mathbf{b}\neq 0$. By making a rotational change of variables, we can assume that $\mathbf{b}=\alpha\mathbf{e}_1$ and $\mathbf{a}=\beta\mathbf{e}_1+\gamma\mathbf{e}_2$, so that

$$(A\psi)(\mathbf{x})=(\beta x_1+\gamma x_2)\psi(\mathbf{x})-i\hbar\alpha\frac{\partial\psi}{\partial x_1}. \tag{9.23}$$

(If $n=1$, the γx_2 term is not present.) As in the proof of Proposition 9.29, the adjoint A^* of A will be given by the same formula as A, with $\mathrm{Dom}(A^*)$ consisting of those elements ψ of $L^2(\mathbb{R}^n)$ for which the right-hand side of (9.23), computed in the distributional sense, belongs to $L^2(\mathbb{R}^n)$.

We now apply the criterion for essential self-adjointness in Corollary 9.22. We need to show that the equations $A^*\psi=i\psi$ and $A^*\psi=-i\psi$ have no nonzero solutions in $\mathrm{Dom}(A^*)$. After rewriting the equation $A^*\psi=i\psi$ as

$$\frac{\partial\psi}{\partial x_1}=-\frac{i}{\hbar\alpha}(\beta x_1+\gamma x_2)\psi(\mathbf{x})-\frac{1}{\hbar\alpha}\psi(\mathbf{x}), \tag{9.24}$$

we can easily find the general distributional solution as

$$\psi(\mathbf{x})=c(x_2,\ldots,x_n)\exp\left\{-\frac{i\beta}{2\alpha\hbar}x_1^2-\frac{i\gamma}{\alpha\hbar}x_1x_2-\frac{1}{\alpha\hbar}x_1\right\}. \tag{9.25}$$

[It is easily verified that if we let ϕ equal ψ divided by the exponential on the right-hand side of (9.25), then ϕ satisfies $\partial\phi/\partial x_1=0$ in the distributional sense. Exercise 21 then tells us that ϕ must be a function of $x_2,\ldots,x_n$.] Since the exponential factor is never square integrable as a function of x_1 with x_2 fixed, the only way that ψ can be square integrable is if c is zero for almost every value of $(x_2,\ldots,x_n)$, in which case ψ is the zero element of $L^2(\mathbb{R}^n)$. A similar argument shows that the equation $A^*\psi=-i\psi$ has no nonzero solutions. ∎

9.10 Another Counterexample

In this section, we will show that the Schrödinger operator $\hat{H}=P^2/(2m)-X^4$ is *not* essentially self-adjoint on $C_c^\infty(\mathbb{R})$, even though $\hat{H}$ is certainly symmetric. By contrast, $P^2/(2m)+X^4$ is essentially self-adjoint, by Theorem 9.39. The operator $P^2/(2m)-X^4$ is a more serious counterexample than the one in Sect. 12.2, in that it does not involve any obviously incorrect choice of boundary conditions. On the other hand, it should not be surprising that something goes "wrong" in a quantum system with a potential equal to $-x^4$. After all, a classical system with this potential has trajectories that go to infinity in finite time (see Exercise 4 in Chap. 2).

To show that $\hat{H}$ is not essentially self-adjoint, we will show that the adjoint $\hat{H}^*$ is not symmetric. Suppose ψ is a C^∞ function such that both ψ and the function

$$-\frac{\hbar^2}{2m}\psi''(x) - x^4\psi(x) \tag{9.26}$$

belong to $L^2(\mathbb{R})$. Using integration by parts, as in the proof of Lemma 9.28, we can see that ψ is in the domain of $\hat{H}^*$ and $\hat{H}^*\psi$ is the function in (9.26). We will construct an approximate eigenvector $\psi \in \mathrm{Dom}(\hat{H}^*)$ for $\hat{H}^*$ with an imaginary eigenvalue $i\alpha$, which will show that $\hat{H}^*$ is not symmetric and thus $\hat{H}$ is not essentially self-adjoint.

Theorem 9.41 *Define an operator $\hat{H}$ with* $\mathrm{Dom}(\hat{H}) = C_c^\infty(\mathbb{R})$ *by the formula*

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - x^4.$$

Then $\hat{H}$ is not essentially self-adjoint.

In preparation for the proof, let us define a function $p(x)$ on $\mathbb{R}$ such that

$$\frac{p(x)^2}{2m} - x^4 = i\alpha,$$

that is,

$$p(x) = \sqrt{2m}\sqrt{x^4 + i\alpha}. \tag{9.27}$$

Here we take the square root that is in the first quadrant. The function $p(x)$ represents "the momentum of a classical particle with energy $i\alpha$."

Lemma 9.42 *If ψ_α is given by*

$$\psi_\alpha(x) = \frac{1}{\sqrt{p(x)}}\exp\left\{\frac{i}{\hbar}\int_0^x p(y)\ dy\right\}, \tag{9.28}$$

then ψ_α belongs to $L^2(\mathbb{R})$ and the function

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_\alpha}{dx^2} - x^4\psi_\alpha \tag{9.29}$$

also belongs to $L^2(\mathbb{R})$. Furthermore, we have

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - x^4 - i\alpha\right]\psi_\alpha(x) = -\frac{\hbar^2}{2m}\psi_\alpha(x)m_\alpha(x),$$

where

$$m_\alpha(x) = \frac{5}{4}\frac{x^6}{(x^4+i\alpha)^2} - 3\frac{x^2}{(x^4+i\alpha)}.$$

It will be apparent from the proof that the two terms in (9.29) are *not* separately in $L^2(\mathbb{R})$. The motivation for the definition of ψ_α comes from the WKB approximation (Chap. 15) with a complex value for the energy.
Proof. Let us consider the integral of p,

$$\int_0^x p(y)\ dy = \sqrt{2m}\int_0^x \sqrt{y^4+i\alpha}\ dy.$$

Using the power series for $(1+x)^a$ we see that for large y,

$$\sqrt{y^4+i\alpha} = y^2\sqrt{1+i\alpha/y^4} = y^2\left(1+\frac{i\alpha}{2y^4}+O\left(\frac{1}{y^8}\right)\right).$$

From this estimate, it is easy to see that the imaginary part of $\int_0^x p(y)\ dy$ remains bounded as x tends to $\pm\infty$. It follows that the exponential in the definition of ψ is bounded, from which it is easy to see that ψ is square integrable.

Now, using the formula for the second derivative of a product, we obtain

$$\begin{aligned} -\hbar^2\frac{d^2}{dx^2}\psi_\alpha = \Bigg[&\frac{p(x)^2}{\sqrt{p(x)}} - i\hbar\frac{p'(x)}{\sqrt{p(x)}} - 2\hbar^2\left(-\frac{1}{2}\frac{p'(x)}{p(x)^{3/2}}\right)\frac{ip(x)}{\hbar} \\ &-\hbar^2\frac{d^2}{dx^2}\frac{1}{\sqrt{p(x)}}\Bigg]\exp\left\{\frac{i}{\hbar}\int_0^x p(y)\ dy\right\}. \end{aligned} \tag{9.30}$$

The factor of $1/\sqrt{p(x)}$ in the definition of ψ_α was chosen precisely so that the second and third terms in square brackets will cancel. If we replace $p^2(x)$ in the numerator of the first term by $2m(x^4+i\alpha)$, we obtain

$$-\frac{\hbar^2}{2m}\psi_\alpha''(x) - x^4\psi_\alpha - i\alpha\psi_\alpha = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}p(x)^{-1/2}\right)\exp\left\{\frac{i}{\hbar}\int_0^x p(y)\ dy\right\}.$$

It is then an elementary calculation to show that

$$\frac{d^2}{dx^2}p(x)^{-1/2} = p(x)^{-1/2}\left[\frac{5}{4}(x^4+i\alpha)^{-2}x^6 - 3(x^4+i\alpha)^{-1}x^2\right],$$

from which the lemma follows. ■

Proof of Theorem 9.41. If $\hat{H}$ were essentially self-adjoint, $\hat{H}^*$ (which would coincide with $\hat{H}^{cl}$) would be self-adjoint and, in particular, symmetric. If this were the case, we would have, by the proof of Lemma 7.8,

$$\left\langle(\hat{H}^* - i\alpha I)\psi, (\hat{H}^* - i\alpha I)\psi\right\rangle \geq \alpha^2\left\langle\psi,\psi\right\rangle \tag{9.31}$$

for all $\psi \in \mathrm{Dom}(\hat{H}^*)$ and $\alpha \in \mathbb{R}$. But if ψ_α is the function in Lemma 9.42, the discussion preceding Theorem 9.41 shows that ψ_α belongs to $\mathrm{Dom}(\hat{H}^*)$.

Furthermore, it is easily verified that there is a constant C such that $|m_\alpha(x)| \leq C$ for all $\alpha \geq 1$ and $x \in \mathbb{R}$. Thus, for all sufficiently large α, we have

$$\left\|(\hat{H}^* - i\alpha I)\psi_\alpha\right\|^2 \leq \frac{\hbar^4}{4m^2}C^2 \left\|\psi_\alpha\right\|^2 < \alpha^2 \left\|\psi_\alpha\right\|^2,$$

contradicting (9.31). ■

See Exercise 22 for a more explicit approach to showing that $\hat{H}^*$ is not symmetric.

9.11 Exercises

1. Show that an unbounded operator A fails to be closable if and only if the closure of the graph of A contains an element of the form $(0, \psi)$ with $\psi \neq 0$.

2. Define an unbounded operator A on $L^2([0,1])$ with domain $\mathrm{Dom}(A) = C([0,1])$ by
$$Af = f(0)\mathbf{1},$$
where $\mathbf{1}$ is the constant function. Show that A is not closable.

3. Prove Proposition 9.13.

4. Suppose that A is an unbounded self-adjoint operator on $\mathbf{H}$ and that numbers λ_n in $\sigma(A)$ converge to some $\lambda \in \mathbb{R}$. Using Point 1 of Proposition 9.18, show that $\lambda \in \sigma(A)$.

5. Suppose A is a closed operator on $\mathbf{H}$. Show that the kernel of A is a closed subspace of $\mathbf{H}$.

6. Suppose A is a closed operator on $\mathbf{H}$. Define a norm $\|\cdot\|_1$ on $\mathrm{Dom}(A)$ by
$$\|\psi\|_1 = \|\psi\| + \|A\psi\|.$$
Show that $\mathrm{Dom}(A)$ is a Banach space with respect to $\|\cdot\|_1$.

7. Let A be an unbounded operator on $\mathbf{H}$.
   (a) Show that if A is symmetric, then A^{cl} is also symmetric.
   (b) Show that if B is an extension of A, then A^* is an extension of B^*.
   (c) Suppose A is self-adjoint and B is an extension of A. Show that if B is symmetric, then $\mathrm{Dom}(A) = \mathrm{Dom}(B)$. (That is to say, a self-adjoint operator has no proper symmetric extensions.)

8. Fix a positive real number μ.

   (a) Show that a symmetric operator A is self-adjoint if and only if $\operatorname{Range}(A + i\mu I)$ and $\operatorname{Range}(A - i\mu I)$ are equal to $\mathbf{H}$.

   (b) Show that a symmetric operator A is essentially self-adjoint if and only if $\operatorname{Range}(A+i\mu I)$ and $\operatorname{Range}(A-i\mu I)$ are dense in $\mathbf{H}$.

9. Let A be the operator considered in Sect. 9.6. Using Lemma 9.28, show that for each $\lambda \in \mathbb{C}$, there exists $\psi \in \operatorname{Dom}(A^*)$ with $A^*\psi = \lambda\psi$. Conclude that each $\lambda \in \mathbb{C}$ belongs to the spectrum of A^{cl}.

   Hint: Recall that $(A^{cl})^* = A^*$.

10. Let A be the operator considered in Sect. 9.6 and suppose ψ is in the domain of A^{cl}. Then there exists a sequence ψ_n in $\operatorname{Dom}(A)$ such that ψ_n converges to ψ in $L^2([0,1])$ and such that $A\psi_n$ converges to some χ in $L^2([0,1])$.

    (a) Show that

    $$\psi_n(x) = \left\langle 1_{[0,x]}, \frac{d\psi_n}{dx} \right\rangle = i \left\langle 1_{[0,x]}, A\psi_n \right\rangle$$

    for all $x \in [0,1]$.

    (b) Show that ψ_n converges *uniformly* to the function

    $$\psi(x) = i \left\langle 1_{[0,x]}, \chi \right\rangle .$$

    (c) Conclude that ψ is continuous and satisfies $\psi(0) = \psi(1) = 0$.

11. Take $\mathbf{H} = L^2((0,\infty))$ and let A be the operator $-i\ d/dx$, with $\operatorname{Dom}(A)$ consisting of those smooth functions that are supported on a compact subset of $(0,\infty)$. (Such a function is, in particular, zero on $(0,\varepsilon)$ for some $\varepsilon > 0$.) Show that A is symmetric and that $A^* + iI$ is injective but that $A^* - iI$ is not injective.

    Hint: Imitate the arguments in the proof of Propositions 9.27 and 9.29.

12. Prove the second part of Lemma 9.33.

13. Let χ be a smooth, radial function on $\mathbb{R}^3$ such that for $|\mathbf{x}| < 1$ we have $\chi(\mathbf{x}) = 1$, for $|\mathbf{x}| > 2$ we have $\chi(\mathbf{x}) = 0$, and for $1 < |\mathbf{x}| < 2$, we have $\partial\chi/\partial r < 0$. Show that

    $$\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}|} \Delta\chi(\mathbf{x})\ d\mathbf{x} < 0,$$

    which shows that the Laplacian of $1/|\mathbf{x}|$, in the distribution sense, is not zero.

Hint: Let $E = C_1 \backslash C_2$, where C_1 is a cube centered at the origin with side length 3 and where C_2 is a cube centered at the origin with side length 1/2. Then E contains the support of $\Delta\chi$. Using integration by parts on E, show that

$$\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}|} \Delta\chi(\mathbf{x})\ d\mathbf{x} = -\int_{\mathbb{R}^3} \nabla\left(\frac{1}{|\mathbf{x}|}\right) \cdot \nabla\chi(\mathbf{x})\ d\mathbf{x}.$$

14. Let $\mathrm{Dom}(\Delta) \subset L^2(\mathbb{R}^n)$ denote the domain of the Laplacian, as given in Proposition 9.34, and assume $n \leq 3$.

    (a) Show that each $\psi \in \mathrm{Dom}(\Delta)$ is continuous and that there exists constants c_1 and c_2 such that

    $$|\psi(\mathbf{x})| \leq c_1 \|\psi\| + c_2 \left\| |\mathbf{k}|^{9/5} \left|\hat{\psi}(\mathbf{k})\right| \right\|,$$

    for all $\psi \in \mathrm{Dom}(\Delta)$.

    Hint: Show that $\hat{\psi}$ is in L^1 by expressing $\hat{\psi}$ as the product of two L^2 functions.

    (b) Show that for any $\varepsilon > 0$, there exists a constant c_ε such that

    $$|\psi(\mathbf{x})| \leq c_\varepsilon \|\psi\| + \varepsilon \|\Delta\psi\|$$

    for all $\psi \in \mathrm{Dom}(\Delta)$.

15. Recall the definitions of $\mathrm{Dom}(P_j)$ and $\mathrm{Dom}(\Delta)$ in Sect. 9.8. Let $\mathrm{Dom}(P_j^2)$ be the set of all ψ belonging to $\mathrm{Dom}(P_j)$ such that $P_j\psi$ again belongs to $\mathrm{Dom}(P_j)$. Show that

    $$\bigcap_{j=1}^{n} \mathrm{Dom}(P_j^2) = \mathrm{Dom}(\Delta).$$

16. Let Q_j denote the restriction to $C_c^\infty(\mathbb{R}^n)$ of the momentum operator P_j. Show that $\mathrm{Dom}(Q_j^*) = \mathrm{Dom}(P_j)$. Conclude that Q_j is essentially self-adjoint.

17. Let A be an unbounded self-adjoint operator on $\mathbf{H}$ and let μ be a nonzero real number.

    (a) Show that $\left\|(A + i\mu I)^{-1}\right\| \leq 1/|\mu|$. Note that $(A+i\mu I)^{-1}$ exists, by Theorem 9.17.

    (b) Show that for all $\psi \in \mathbf{H}$,

    $$\|\psi\|^2 = \left\|A(A + i\mu I)^{-1}\psi\right\|^2 + \mu^2 \left\|(A + i\mu I)^{-1}\psi\right\|^2.$$

    Conclude that $\left\|A(A + i\mu I)^{-1}\right\| \leq 1$.

18. Let A be an unbounded self-adjoint operator on $\mathbf{H}$. Suppose A is non-negative (Definition 9.19) and let λ be a positive real number.

    (a) Show that $\left\|(A+\lambda I)^{-1}\right\| \leq 1/\lambda$.

    (b) Show that for all $\psi \in \mathbf{H}$,

    $$\|\psi\|^2 \geq \left\|A(A+\lambda I)^{-1}\psi\right\|^2 + \lambda^2 \left\|(A+\lambda I)^{-1}\psi\right\|^2.$$

    Conclude that $\left\|A(A+\lambda I)^{-1}\right\| < 1$.

19. Prove the last part of Theorem 9.37, concerning domains of essential self-adjointness.

    Hint: If A is self-adjoint on $\mathrm{Dom}(A)$ and $V \subset \mathrm{Dom}(A)$ is a dense subspace of $\mathbf{H}$, then A is essentially self-adjoint on V if and only if the closure of $A|_V$ is equal to A.

20. Let A be the operator $\mathbf{b}\cdot\mathbf{X}$ on the domain $C_c^\infty(\mathbb{R}^n)$, for some $\mathbf{b} \in \mathbb{R}^n$.

    (a) Using the definition of the adjoint of an unbounded operator, show that $\mathrm{Dom}(A^*)$ consists of all those ψ in $L^2(\mathbb{R}^n)$ for which the function $(\mathbf{b}\cdot\mathbf{x})\psi(\mathbf{x})$ again belongs to $L^2(\mathbb{R}^n)$.

    (b) Using Proposition 9.30, show that A is essentially self-adjoint.

21. (a) Show that a function $\phi \in C_c^\infty(\mathbb{R}^n)$ can be expressed as $\phi = \partial\chi/\partial x_1$ for some $\chi \in C_c^\infty(\mathbb{R}^n)$ if and only if ϕ satisfies

    $$\int_{-\infty}^{\infty} \phi(x_1, x_2, \ldots, x_n)\, dx_1 = 0$$

    for all $(x_2, \ldots, x_n)$.

    (b) Fix a function $\gamma \in C_c^\infty(\mathbb{R})$ such that $\int_{-\infty}^{\infty} \gamma(x)\, dx = 1$. Show that any $\phi \in C_c^\infty(\mathbb{R}^n)$ can be expressed as

    $$\phi(\mathbf{x}) = f(x_2, \ldots, x_n)\gamma(x_1) + \frac{\partial\chi}{\partial x_1}$$

    for some $\chi \in C_c^\infty(\mathbb{R}^n)$, where f is the element of $C_c^\infty(\mathbb{R}^{n-1})$ given by

    $$f(x_2, \ldots, x_n) = \int_{-\infty}^{\infty} \phi(x_1, x_2, \ldots, x_n)\, dx_1.$$

    (c) Suppose T is a distribution on $\mathbb{R}^n$ with the property that

    $$\frac{\partial T}{\partial x_1} = 0.$$

Define a distribution c on $\mathbb{R}^{n-1}$ by the formula

$$c(f) = T(f(x_2, \ldots, x_n)\gamma(x_1)).$$

Show that for all $\phi \in C_c^\infty(\mathbb{R}^n)$ we have

$$T(\phi) = c(\tilde{\phi}),$$

where $\tilde{\phi} \in C_c^\infty(\mathbb{R}^{n-1})$ is given by

$$\tilde{\phi}(x_2, \ldots, x_n) = \int_{\mathbb{R}} \phi(x_1, x_2, \ldots, x_n)\ dx_1.$$

22. Let $\hat{H}$ denote the Schrödinger operator in Theorem 9.41 and let ψ_α be the function defined in Lemma 9.42.

(a) Show that

$$\begin{aligned}&\left\langle \psi_\alpha, \hat{H}^*\psi_\alpha \right\rangle - \left\langle \hat{H}^*\psi_\alpha, \psi_\alpha \right\rangle \\ &= -\frac{\hbar^2}{2m} \lim_{A\to\infty} \left[\overline{\psi_\alpha(x)}\psi_\alpha'(x)\Big|_{-A}^{A} - \overline{\psi_\alpha'(x)}\psi_\alpha(x)\Big|_{-A}^{A} \right].\end{aligned}$$

(b) Now show by direct calculation that $\left\langle \psi, \hat{H}^*\psi \right\rangle \neq \left\langle \hat{H}^*\psi, \psi \right\rangle$.