Chapter 2

Self-adjointness and spectrum

2.1. Some quantum mechanics

In quantum mechanics, a single particle living in $\mathbb{R}^3$ is described by a complex-valued function (the **wave function**)

$$\psi(x,t), \qquad (x,t) \in \mathbb{R}^3 \times \mathbb{R}, \tag{2.1}$$

where x corresponds to a point in space and t corresponds to time. The quantity $\rho_t(x) = |\psi(x,t)|^2$ is interpreted as the **probability density** of the particle at the time t. In particular, ψ must be normalized according to

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 d^3x = 1, \qquad t \in \mathbb{R}. \tag{2.2}$$

The location x of the particle is a quantity which can be observed (i.e., measured) and is hence called **observable**. Due to our probabilistic interpretation, it is also a random variable whose **expectation** is given by

$$\mathbb{E}_\psi(x) = \int_{\mathbb{R}^3} x|\psi(x,t)|^2 d^3x. \tag{2.3}$$

In a real life setting, it will not be possible to measure x directly and one will only be able to measure certain functions of x. For example, it is possible to check whether the particle is inside a certain area Ω of space (e.g., inside a detector). The corresponding observable is the characteristic function $\chi_\Omega(x)$ of this set. In particular, the number

$$\mathbb{E}_\psi(\chi_\Omega) = \int_{\mathbb{R}^3} \chi_\Omega(x)|\psi(x,t)|^2 d^3x = \int_\Omega |\psi(x,t)|^2 d^3x \tag{2.4}$$

corresponds to the probability of finding the particle inside $\Omega \subseteq \mathbb{R}^3$. An important point to observe is that, in contradistinction to classical mechanics, the particle is no longer localized at a certain point. In particular, the **mean-square deviation** (or **variance**) $\Delta_\psi(x)^2 = \mathbb{E}_\psi(x^2) - \mathbb{E}_\psi(x)^2$ is always nonzero.

In general, the **configuration space** (or **phase space**) of a quantum system is a (complex) Hilbert space $\mathfrak{H}$ and the possible states of this system are represented by the elements ψ having norm one, $\|\psi\| = 1$.

An observable a corresponds to a linear operator A in this Hilbert space and its expectation, if the system is in the state ψ, is given by the real number

$$\mathbb{E}_\psi(A) = \langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle, \tag{2.5}$$

where $\langle ., .. \rangle$ denotes the scalar product of $\mathfrak{H}$. Similarly, the mean-square deviation is given by

$$\Delta_\psi(A)^2 = \mathbb{E}_\psi(A^2) - \mathbb{E}_\psi(A)^2 = \|(A - \mathbb{E}_\psi(A))\psi\|^2. \tag{2.6}$$

Note that $\Delta_\psi(A)$ vanishes if and only if ψ is an eigenstate corresponding to the eigenvalue $\mathbb{E}_\psi(A)$; that is, $A\psi = \mathbb{E}_\psi(A)\psi$.

From a physical point of view, (2.5) should make sense for any $\psi \in \mathfrak{H}$. However, this is not in the cards as our simple example of one particle already shows. In fact, the reader is invited to find a square integrable function $\psi(x)$ for which $x\psi(x)$ is no longer square integrable. The deeper reason behind this nuisance is that $\mathbb{E}_\psi(x)$ can attain arbitrarily large values if the particle is not confined to a finite domain, which renders the corresponding operator unbounded. But unbounded operators cannot be defined on the entire Hilbert space in a natural way by the closed graph theorem (Theorem 2.8 below).

Hence, A will only be defined on a subset $\mathfrak{D}(A) \subseteq \mathfrak{H}$ called the **domain** of A. Since we want A to be defined for at least *most* states, we require $\mathfrak{D}(A)$ to be dense.

However, it should be noted that there is no general prescription for how to find the operator corresponding to a given observable.

Now let us turn to the time evolution of such a quantum mechanical system. Given an initial state $\psi(0)$ of the system, there should be a unique $\psi(t)$ representing the state of the system at time $t \in \mathbb{R}$. We will write

$$\psi(t) = U(t)\psi(0). \tag{2.7}$$

Moreover, it follows from physical experiments that **superposition of states** holds; that is, $U(t)(\alpha_1\psi_1(0) + \alpha_2\psi_2(0)) = \alpha_1\psi_1(t) + \alpha_2\psi_2(t)$ ($|\alpha_1|^2 + |\alpha_2|^2 = 1$). In other words, $U(t)$ should be a linear operator. Moreover, since $\psi(t)$

is a state (i.e., $\|\psi(t)\| = 1$), we have

$$\|U(t)\psi\| = \|\psi\|. \tag{2.8}$$

Such operators are called **unitary**. Next, since we have assumed uniqueness of solutions to the initial value problem, we must have

$$U(0) = \mathbb{I}, \qquad U(t+s) = U(t)U(s). \tag{2.9}$$

A family of unitary operators $U(t)$ having this property is called a **one-parameter unitary group**. In addition, it is natural to assume that this group is **strongly continuous**; that is,

$$\lim_{t\to t_0} U(t)\psi = U(t_0)\psi, \qquad \psi \in \mathfrak{H}. \tag{2.10}$$

Each such group has an **infinitesimal generator** defined by

$$H\psi = \lim_{t\to 0} \frac{\mathrm{i}}{t}(U(t)\psi - \psi), \quad \mathfrak{D}(H) = \{\psi \in \mathfrak{H} | \lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\}. \tag{2.11}$$

This operator is called the **Hamiltonian** and corresponds to the energy of the system. If $\psi(0) \in \mathfrak{D}(H)$, then $\psi(t)$ is a solution of the **Schrödinger equation** (in suitable units)

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\psi(t). \tag{2.12}$$

This equation will be the main subject of our course.

In summary, we have the following **axioms of quantum mechanics**.

Axiom 1. The configuration space of a quantum system is a complex separable Hilbert space $\mathfrak{H}$ and the possible states of this system are represented by the elements of $\mathfrak{H}$ which have norm one.

Axiom 2. Each observable a corresponds to a linear operator A defined maximally on a dense subset $\mathfrak{D}(A)$. Moreover, the operator corresponding to a polynomial $P_n(a) = \sum_{j=0}^{n} \alpha_j a^j$, $\alpha_j \in \mathbb{R}$, is $P_n(A) = \sum_{j=0}^{n} \alpha_j A^j$, $\mathfrak{D}(P_n(A)) = \mathfrak{D}(A^n) = \{\psi \in \mathfrak{D}(A) | A\psi \in \mathfrak{D}(A^{n-1})\}$ ($A^0 = \mathbb{I}$).

Axiom 3. The expectation value for a measurement of a, when the system is in the state $\psi \in \mathfrak{D}(A)$, is given by (2.5), which must be real for all $\psi \in \mathfrak{D}(A)$.

Axiom 4. The time evolution is given by a strongly continuous one-parameter unitary group $U(t)$. The generator of this group corresponds to the energy of the system.

In the following sections we will try to draw some mathematical consequences from these assumptions:

First we will see that Axioms 2 and 3 imply that observables correspond to self-adjoint operators. Hence these operators play a central role in quantum mechanics and we will derive some of their basic properties. Another crucial role is played by the set of all possible expectation values for the measurement of a, which is connected with the spectrum $\sigma(A)$ of the corresponding operator A.

The problem of defining functions of an observable will lead us to the spectral theorem (in the next chapter), which generalizes the diagonalization of symmetric matrices.

Axiom 4 will be the topic of Chapter 5.

2.2. Self-adjoint operators

Let $\mathfrak{H}$ be a (complex separable) Hilbert space. A **linear operator** is a linear mapping

$$A : \mathfrak{D}(A) \to \mathfrak{H}, \tag{2.13}$$

where $\mathfrak{D}(A)$ is a linear subspace of $\mathfrak{H}$, called the **domain** of A. It is called **bounded** if the operator norm

$$\|A\| = \sup_{\|\psi\|=1} \|A\psi\| = \sup_{\|\varphi\|=\|\psi\|=1} |\langle\psi, A\varphi\rangle| \tag{2.14}$$

is finite. The second equality follows since equality in $|\langle\psi, A\varphi\rangle| \le \|\psi\|\,\|A\varphi\|$ is attained when $A\varphi = z\psi$ for some $z \in \mathbb{C}$. If A is bounded, it is no restriction to assume $\mathfrak{D}(A) = \mathfrak{H}$ and we will always do so. The Banach space of all bounded linear operators is denoted by $\mathfrak{L}(\mathfrak{H})$. Products of (unbounded) operators are defined naturally; that is, $AB\psi = A(B\psi)$ for $\psi \in \mathfrak{D}(AB) = \{\psi \in \mathfrak{D}(B) | B\psi \in \mathfrak{D}(A)\}$.

The expression $\langle\psi, A\psi\rangle$ encountered in the previous section is called the **quadratic form**,

$$q_A(\psi) = \langle\psi, A\psi\rangle, \qquad \psi \in \mathfrak{D}(A), \tag{2.15}$$

associated to A. An operator can be reconstructed from its quadratic form via the **polarization identity**

$$\langle\varphi, A\psi\rangle = \frac{1}{4}\left(q_A(\varphi+\psi) - q_A(\varphi-\psi) + \mathrm{i}q_A(\varphi-\mathrm{i}\psi) - \mathrm{i}q_A(\varphi+\mathrm{i}\psi)\right). \tag{2.16}$$

A densely defined linear operator A is called **symmetric** (or **hermitian**) if

$$\langle\varphi, A\psi\rangle = \langle A\varphi, \psi\rangle, \qquad \psi, \varphi \in \mathfrak{D}(A). \tag{2.17}$$

The justification for this definition is provided by the following

Lemma 2.1. *A densely defined operator A is symmetric if and only if the corresponding quadratic form is real-valued.*

Proof. Clearly (2.17) implies that $\mathrm{Im}(q_A(\psi)) = 0$. Conversely, taking the imaginary part of the identity

$$q_A(\psi + \mathrm{i}\varphi) = q_A(\psi) + q_A(\varphi) + \mathrm{i}(\langle\psi, A\varphi\rangle - \langle\varphi, A\psi\rangle)$$

shows $\mathrm{Re}\langle A\varphi, \psi\rangle = \mathrm{Re}\langle\varphi, A\psi\rangle$. Replacing φ by $\mathrm{i}\varphi$ in this last equation shows $\mathrm{Im}\langle A\varphi, \psi\rangle = \mathrm{Im}\langle\varphi, A\psi\rangle$ and finishes the proof. □

In other words, a densely defined operator A is symmetric if and only if

$$\langle\psi, A\psi\rangle = \langle A\psi, \psi\rangle, \qquad \psi \in \mathfrak{D}(A). \tag{2.18}$$

This already narrows the class of admissible operators to the class of symmetric operators by Axiom 3. Next, let us tackle the issue of the correct domain.

By Axiom 2, A should be defined maximally; that is, if $\tilde{A}$ is another symmetric operator such that $A \subseteq \tilde{A}$, then $A = \tilde{A}$. Here we write $A \subseteq \tilde{A}$ if $\mathfrak{D}(A) \subseteq \mathfrak{D}(\tilde{A})$ and $A\psi = \tilde{A}\psi$ for all $\psi \in \mathfrak{D}(A)$. The operator $\tilde{A}$ is called an **extension** of A in this case. In addition, we write $A = \tilde{A}$ if both $\tilde{A} \subseteq A$ and $A \subseteq \tilde{A}$ hold.

The **adjoint operator** A^* of a densely defined linear operator A is defined by

$$\begin{aligned} \mathfrak{D}(A^*) &= \{\psi \in \mathfrak{H} | \exists \tilde{\psi} \in \mathfrak{H} : \langle\psi, A\varphi\rangle = \langle\tilde{\psi}, \varphi\rangle, \forall \varphi \in \mathfrak{D}(A)\}, \\ A^*\psi &= \tilde{\psi}. \end{aligned} \tag{2.19}$$

The requirement that $\mathfrak{D}(A)$ be dense implies that A^* is well-defined. However, note that $\mathfrak{D}(A^*)$ might not be dense in general. In fact, it might contain no vectors other than 0.

Clearly we have $(\alpha A)^* = \alpha^* A^*$ for $\alpha \in \mathbb{C}$ and $(A + B)^* \supseteq A^* + B^*$ provided $\mathfrak{D}(A + B) = \mathfrak{D}(A) \cap \mathfrak{D}(B)$ is dense. However, equality will not hold in general unless one operator is bounded (Problem 2.2).

For later use, note that (Problem 2.4)

$$\mathrm{Ker}(A^*) = \mathrm{Ran}(A)^{\perp}. \tag{2.20}$$

For symmetric operators we clearly have $A \subseteq A^*$. If, in addition, $A = A^*$ holds, then A is called **self-adjoint**. Our goal is to show that observables correspond to self-adjoint operators. This is for example true in the case of the position operator x, which is a special case of a multiplication operator.

Example. (Multiplication operator) Consider the multiplication operator

$$(Af)(x) = A(x)f(x), \quad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}^n, d\mu) \,|\, Af \in L^2(\mathbb{R}^n, d\mu)\} \tag{2.21}$$

given by multiplication with the measurable function $A : \mathbb{R}^n \to \mathbb{C}$. First of all note that $\mathfrak{D}(A)$ is dense. In fact, consider $\Omega_n = \{x \in \mathbb{R}^n \,|\, |A(x)| \leq$

$n\} \nearrow \mathbb{R}^n$. Then, for every $f \in L^2(\mathbb{R}^n, d\mu)$ the function $f_n = \chi_{\Omega_n} f \in \mathfrak{D}(A)$ converges to f as $n \to \infty$ by dominated convergence.

Next, let us compute the adjoint of A. Performing a formal computation, we have for $h, f \in \mathfrak{D}(A)$ that

$$\langle h, Af \rangle = \int h(x)^* A(x) f(x) d\mu(x) = \int (A(x)^* h(x))^* f(x) d\mu(x) = \langle \tilde{A} h, f \rangle, \tag{2.22}$$

where $\tilde{A}$ is multiplication by $A(x)^*$,

$$(\tilde{A} f)(x) = A(x)^* f(x), \quad \mathfrak{D}(\tilde{A}) = \{f \in L^2(\mathbb{R}^n, d\mu) \,|\, \tilde{A} f \in L^2(\mathbb{R}^n, d\mu)\}. \tag{2.23}$$

Note $\mathfrak{D}(\tilde{A}) = \mathfrak{D}(A)$. At first sight this seems to show that the adjoint of A is $\tilde{A}$. But for our calculation we had to assume $h \in \mathfrak{D}(A)$ and there might be some functions in $\mathfrak{D}(A^*)$ which do not satisfy this requirement! In particular, our calculation only shows $\tilde{A} \subseteq A^*$. To show that equality holds, we need to work a little harder:

If $h \in \mathfrak{D}(A^*)$, there is some $g \in L^2(\mathbb{R}^n, d\mu)$ such that

$$\int h(x)^* A(x) f(x) d\mu(x) = \int g(x)^* f(x) d\mu(x), \qquad f \in \mathfrak{D}(A), \tag{2.24}$$

and thus

$$\int (h(x) A(x)^* - g(x))^* f(x) d\mu(x) = 0, \qquad f \in \mathfrak{D}(A). \tag{2.25}$$

In particular,

$$\int \chi_{\Omega_n}(x) (h(x) A(x)^* - g(x))^* f(x) d\mu(x) = 0, \qquad f \in L^2(\mathbb{R}^n, d\mu), \tag{2.26}$$

which shows that $\chi_{\Omega_n}(h(x) A(x)^* - g(x))^* \in L^2(\mathbb{R}^n, d\mu)$ vanishes. Since n is arbitrary, we even have $h(x) A(x)^* = g(x) \in L^2(\mathbb{R}^n, d\mu)$ and thus A^* is multiplication by $A(x)^*$ and $\mathfrak{D}(A^*) = \mathfrak{D}(A)$.

In particular, A is self-adjoint if A is real-valued. In the general case we have at least $\|Af\| = \|A^* f\|$ for all $f \in \mathfrak{D}(A) = \mathfrak{D}(A^*)$. Such operators are called **normal**. ⋄

Now note that

$$A \subseteq B \quad \Rightarrow \quad B^* \subseteq A^*; \tag{2.27}$$

that is, increasing the domain of A implies decreasing the domain of A^*. Thus there is no point in trying to extend the domain of a self-adjoint operator further. In fact, if A is self-adjoint and B is a symmetric extension, we infer $A \subseteq B \subseteq B^* \subseteq A^* = A$ implying $A = B$.

Corollary 2.2. *Self-adjoint operators are maximal; that is, they do not have any symmetric extensions.*

Furthermore, if A^* is densely defined (which is the case if A is symmetric), we can consider A^{**}. From the definition (2.19) it is clear that $A \subseteq A^{**}$ and thus A^{**} is an extension of A. This extension is closely related to extending a linear subspace M via $M^{\perp\perp} = \overline{M}$ (as we will see a bit later) and thus is called the **closure** $\overline{A} = A^{**}$ of A.

If A is symmetric, we have $A \subseteq A^*$ and hence $\overline{A} = A^{**} \subseteq A^*$; that is, $\overline{A}$ lies between A and A^*. Moreover, $\langle \psi, A^*\varphi\rangle = \langle \overline{A}\psi, \varphi\rangle$ for all $\psi \in \mathfrak{D}(\overline{A})$, $\varphi \in \mathfrak{D}(A^*)$ implies that $\overline{A}$ is symmetric since $A^*\varphi = \overline{A}\varphi$ for $\varphi \in \mathfrak{D}(\overline{A})$.

Example. (Differential operator) Take $\mathfrak{H} = L^2(0, 2\pi)$.

(i) Consider the operator

$$A_0 f = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(A_0) = \{f \in C^1[0, 2\pi] \,|\, f(0) = f(2\pi) = 0\}. \tag{2.28}$$

That A_0 is symmetric can be shown by a simple integration by parts (do this). Note that the *boundary conditions* $f(0) = f(2\pi) = 0$ are chosen such that the boundary terms occurring from integration by parts vanish. However, this will also follow once we have computed A_0^*. If $g \in \mathfrak{D}(A_0^*)$, we must have

$$\int_0^{2\pi} g(x)^*(-\mathrm{i}f'(x))dx = \int_0^{2\pi} \tilde{g}(x)^* f(x)dx \tag{2.29}$$

for some $\tilde{g} \in L^2(0, 2\pi)$. Integration by parts (cf. (2.116)) shows

$$\int_0^{2\pi} f'(x) \left(g(x) - \mathrm{i}\int_0^x \tilde{g}(t)dt \right)^* dx = 0. \tag{2.30}$$

In fact, this formula holds for $\tilde{g} \in C[0, 2\pi]$. Since the set of continuous functions is dense, the general case $\tilde{g} \in L^2(0, 2\pi)$ follows by approximating $\tilde{g}$ with continuous functions and taking limits on both sides using dominated convergence.

Hence $g(x) - \mathrm{i}\int_0^x \tilde{g}(t)dt \in \{f' | f \in \mathfrak{D}(A_0)\}^\perp$. But $\{f' | f \in \mathfrak{D}(A_0)\} = \{h \in C[0, 2\pi] | \int_0^{2\pi} h(t)dt = 0\}$ (show this) implying $g(x) = g(0) + \mathrm{i}\int_0^x \tilde{g}(t)dt$ since $\overline{\{f' | f \in \mathfrak{D}(A_0)\}} = \{h \in \mathfrak{H} | \langle 1, h\rangle = 0\} = \{1\}^\perp$ and $\{1\}^{\perp\perp} = \operatorname{span}\{1\}$. Thus $g \in AC[0, 2\pi]$, where

$$AC[a, b] = \{f \in C[a, b] | f(x) = f(a) + \int_a^x g(t)dt,\ g \in L^1(a, b)\} \tag{2.31}$$

denotes the set of all absolutely continuous functions (see Section 2.7). In summary, $g \in \mathfrak{D}(A_0^*)$ implies $g \in AC[0, 2\pi]$ and $A_0^* g = \tilde{g} = -\mathrm{i}g'$. Conversely, for every $g \in H^1(0, 2\pi) = \{f \in AC[0, 2\pi] | f' \in L^2(0, 2\pi)\}$, (2.29) holds with $\tilde{g} = -\mathrm{i}g'$ and we conclude

$$A_0^* f = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(A_0^*) = H^1(0, 2\pi). \tag{2.32}$$

In particular, A_0 is symmetric but not self-adjoint. Since $\overline{A_0} = A_0^{**} \subseteq A_0^*$, we can use integration by parts to compute

$$0 = \langle g, \overline{A_0} f\rangle - \langle A_0^* g, f\rangle = \mathrm{i}(f(0)g(0)^* - f(2\pi)g(2\pi)^*) \tag{2.33}$$

and since the boundary values of $g \in \mathfrak{D}(A_0^*)$ can be prescribed arbitrarily, we must have $f(0) = f(2\pi) = 0$. Thus

$$\overline{A_0} f = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(\overline{A_0}) = \{f \in \mathfrak{D}(A_0^*) \,|\, f(0) = f(2\pi) = 0\}. \tag{2.34}$$

(ii) Now let us take

$$Af = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(A) = \{f \in C^1[0, 2\pi] \,|\, f(0) = f(2\pi)\}, \tag{2.35}$$

which is clearly an extension of A_0. Thus $A^* \subseteq A_0^*$ and we compute

$$0 = \langle g, Af\rangle - \langle A^* g, f\rangle = \mathrm{i}f(0)(g(0)^* - g(2\pi)^*). \tag{2.36}$$

Since this must hold for all $f \in \mathfrak{D}(A)$, we conclude $g(0) = g(2\pi)$ and

$$A^* f = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(A^*) = \{f \in H^1(0, 2\pi) \,|\, f(0) = f(2\pi)\}. \tag{2.37}$$

Similarly, as before, $\overline{A} = A^*$ and thus $\overline{A}$ is self-adjoint. ◇

One might suspect that there is no big difference between the two symmetric operators A_0 and A from the previous example, since they coincide on a dense set of vectors. However, the converse is true: For example, the first operator A_0 has no eigenvectors at all (i.e., solutions of the equation $A_0\psi = z\psi$, $z \in \mathbb{C}$) whereas the second one has an orthonormal basis of eigenvectors!

Example. Compute the eigenvectors of A_0 and A from the previous example.

(i) By definition, an eigenvector is a (nonzero) solution of $A_0 u = zu$, $z \in \mathbb{C}$, that is, a solution of the ordinary differential equation

$$-\,\mathrm{i}\,u'(x) = zu(x) \tag{2.38}$$

satisfying the boundary conditions $u(0) = u(2\pi) = 0$ (since we must have $u \in \mathfrak{D}(A_0)$). The general solution of the differential equation is $u(x) = u(0)\mathrm{e}^{\mathrm{i}zx}$ and the boundary conditions imply $u(x) = 0$. Hence there are no eigenvectors.

(ii) Now we look for solutions of $Au = zu$, that is, the same differential equation as before, but now subject to the boundary condition $u(0) = u(2\pi)$. Again the general solution is $u(x) = u(0)\mathrm{e}^{\mathrm{i}zx}$ and the boundary condition requires $u(0) = u(0)\mathrm{e}^{2\pi\mathrm{i}z}$. Thus there are two possibilities. Either $u(0) = 0$

(which is of no use for us) or $z \in \mathbb{Z}$. In particular, we see that all eigenvectors are given by

$$u_n(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}nx}, \qquad n \in \mathbb{Z}, \tag{2.39}$$

which are well known to form an orthonormal basis. ⋄

We will see a bit later that this is a consequence of self-adjointness of $\overline{A}$. Hence it will be important to know whether a given operator is self-adjoint or not. Our example shows that symmetry is easy to check (in case of differential operators it usually boils down to integration by parts), but computing the adjoint of an operator is a nontrivial job even in simple situations. However, we will learn soon that self-adjointness is a much stronger property than symmetry, justifying the additional effort needed to prove it.

On the other hand, if a given symmetric operator A turns out not to be self-adjoint, this raises the question of self-adjoint extensions. Two cases need to be distinguished. If $\overline{A}$ is self-adjoint, then there is only one self-adjoint extension (if B is another one, we have $\overline{A} \subseteq B$ and hence $\overline{A} = B$ by Corollary 2.2). In this case A is called **essentially self-adjoint** and $\mathfrak{D}(A)$ is called a **core** for $\overline{A}$. Otherwise there might be more than one self-adjoint extension or none at all. This situation is more delicate and will be investigated in Section 2.6.

Since we have seen that computing A^* is not always easy, a criterion for self-adjointness not involving A^* will be useful.

Lemma 2.3. *Let A be symmetric such that* $\mathrm{Ran}(A+z) = \mathrm{Ran}(A+z^*) = \mathfrak{H}$ *for one $z \in \mathbb{C}$. Then A is self-adjoint.*

Proof. Let $\psi \in \mathfrak{D}(A^*)$ and $A^*\psi = \tilde{\psi}$. Since $\mathrm{Ran}(A + z^*) = \mathfrak{H}$, there is a $\vartheta \in \mathfrak{D}(A)$ such that $(A + z^*)\vartheta = \tilde{\psi} + z^*\psi$. Now we compute

$$\langle \psi, (A+z)\varphi\rangle = \langle \tilde{\psi} + z^*\psi, \varphi\rangle = \langle (A+z^*)\vartheta, \varphi\rangle = \langle \vartheta, (A+z)\varphi\rangle, \quad \varphi \in \mathfrak{D}(A),$$

and hence $\psi = \vartheta \in \mathfrak{D}(A)$ since $\mathrm{Ran}(A + z) = \mathfrak{H}$. □

To proceed further, we will need more information on the closure of an operator. We will use a different approach which avoids the use of the adjoint operator. We will establish equivalence with our original definition in Lemma 2.4.

The simplest way of extending an operator A is to take the closure of its **graph** $\Gamma(A) = \{(\psi, A\psi) | \psi \in \mathfrak{D}(A)\} \subset \mathfrak{H}^2$. That is, if $(\psi_n, A\psi_n) \to (\psi, \tilde{\psi})$, we might try to define $A\psi = \tilde{\psi}$. For $A\psi$ to be well-defined, we need that $(\psi_n, A\psi_n) \to (0, \tilde{\psi})$ implies $\tilde{\psi} = 0$. In this case A is called **closable** and the unique operator $\overline{A}$ which satisfies $\Gamma(\overline{A}) = \overline{\Gamma(A)}$ is called the **closure** of A. Clearly, A is called **closed** if $\overline{A} = A$, which is the case if and only if the graph of A is closed. Equivalently, A is closed if and only if $\Gamma(A)$ equipped with the **graph norm** $\|(\psi, A\psi)\|^2_{\Gamma(A)} = \|\psi\|^2 + \|A\psi\|^2$ is a Hilbert space (i.e., closed). By construction, $\overline{A}$ is the smallest closed extension of A.

Example. Suppose A is bounded. Then the closure was already computed in Theorem 0.26. In particular, $\mathfrak{D}(\overline{A}) = \overline{\mathfrak{D}(A)}$ and a bounded operator is closed if and only if its domain is closed. ⋄

Example. Consider again the differential operator A_0 from (2.28) and let us compute the closure without the use of the adjoint operator.

Let $f \in \mathfrak{D}(\overline{A_0})$ and let $f_n \in \mathfrak{D}(A_0)$ be a sequence such that $f_n \to f$, $A_0 f_n \to -\mathrm{i}g$. Then $f_n' \to g$ and hence $f(x) = \int_0^x g(t)dt$. Thus $f \in AC[0, 2\pi]$ and $f(0) = 0$. Moreover $f(2\pi) = \lim_{n\to 0} \int_0^{2\pi} f_n'(t)dt = 0$. Conversely, any such f can be approximated by functions in $\mathfrak{D}(A_0)$ (show this). ⋄

Example. Consider again the multiplication operator by $A(x)$ in $L^2(\mathbb{R}^n, d\mu)$ but now defined on functions with compact support, that is,

$$\mathfrak{D}(A_0) = \{f \in \mathfrak{D}(A) \,|\, \mathrm{supp}(f) \text{ is compact}\}. \tag{2.40}$$

Then its closure is given by $\overline{A_0} = A$. In particular, A_0 is essentially self-adjoint and $\mathfrak{D}(A_0)$ is a core for A.

To prove $\overline{A_0} = A$, let some $f \in \mathfrak{D}(A)$ be given and consider $f_n = \chi_{\{x|\,|x|\le n\}} f$. Then $f_n \in \mathfrak{D}(A_0)$ and $f_n(x) \to f(x)$ as well as $A(x)f_n(x) \to A(x)f(x)$ in $L^2(\mathbb{R}^n, d\mu)$ by dominated convergence. Thus $\mathfrak{D}(\overline{A_0}) \subseteq \mathfrak{D}(A)$ and since A is closed, we even get equality. ⋄

Example. Consider the multiplication $A(x) = x$ in $L^2(\mathbb{R})$ defined on

$$\mathfrak{D}(A_0) = \{f \in \mathfrak{D}(A) \,|\, \int_{\mathbb{R}} f(x)dx = 0\}. \tag{2.41}$$

Then A_0 is closed. Hence $\mathfrak{D}(A_0)$ is not a core for A.

To show that A_0 is closed, suppose there is a sequence $f_n(x) \to f(x)$ such that $x f_n(x) \to g(x)$. Since A is closed, we necessarily have $f \in \mathfrak{D}(A)$ and $g(x) = x f(x)$. But then

$$\begin{aligned} 0 = \lim_{n\to\infty} \int_{\mathbb{R}} f_n(x)dx &= \lim_{n\to\infty} \int_{\mathbb{R}} \frac{1}{1+|x|}(f_n(x) + \mathrm{sign}(x) x f_n(x))dx \\ &= \int_{\mathbb{R}} \frac{1}{1+|x|}(f(x) + \mathrm{sign}(x)g(x))dx = \int_{\mathbb{R}} f(x)dx \end{aligned} \tag{2.42}$$

which shows $f \in \mathfrak{D}(A_0)$. ⋄

Next, let us collect a few important results.

Lemma 2.4. *Suppose A is a densely defined operator.*

(i) *A^* is closed.*

(ii) *A is closable if and only if $\mathfrak{D}(A^*)$ is dense and $\overline{A} = A^{**}$, respectively, $(\overline{A})^* = A^*$, in this case.*

(iii) *If A is injective and $\mathrm{Ran}(A)$ is dense, then $(A^*)^{-1} = (A^{-1})^*$. If A is closable and $\overline{A}$ is injective, then $\overline{A}^{-1} = \overline{A^{-1}}$.*

Proof. Let us consider the following two unitary operators from $\mathfrak{H}^2$ to itself

$$U(\varphi, \psi) = (\psi, -\varphi), \qquad V(\varphi, \psi) = (\psi, \varphi).$$

(i) From

$$\begin{aligned}\Gamma(A^*) &= \{(\varphi, \tilde{\varphi}) \in \mathfrak{H}^2 | \langle \varphi, A\psi \rangle = \langle \tilde{\varphi}, \psi \rangle,\ \forall \psi \in \mathfrak{D}(A)\} \\ &= \{(\varphi, \tilde{\varphi}) \in \mathfrak{H}^2 | \langle (\varphi, \tilde{\varphi}), (\tilde{\psi}, -\psi) \rangle_{\mathfrak{H}^2} = 0,\ \forall (\psi, \tilde{\psi}) \in \Gamma(A)\} \\ &= (U\Gamma(A))^\perp \end{aligned} \tag{2.43}$$

we conclude that A^* is closed.

(ii) Similarly, using $U\Gamma^\perp = (U\Gamma)^\perp$ (Problem 1.4), by

$$\begin{aligned}\overline{\Gamma(A)} &= \Gamma(A)^{\perp\perp} = (U\Gamma(A^*))^\perp \\ &= \{(\psi, \tilde{\psi}) |\, \langle \psi, A^*\varphi \rangle - \langle \tilde{\psi}, \varphi \rangle = 0, \forall \varphi \in \mathfrak{D}(A^*)\}\end{aligned}$$

we see that $(0, \tilde{\psi}) \in \overline{\Gamma(A)}$ if and only if $\tilde{\psi} \in \mathfrak{D}(A^*)^\perp$. Hence A is closable if and only if $\mathfrak{D}(A^*)$ is dense. In this case, equation (2.43) also shows $\overline{A}^* = A^*$. Moreover, replacing A by A^* in (2.43) and comparing with the last formula shows $A^{**} = \overline{A}$.

(iii) Next note that (provided A is injective)

$$\Gamma(A^{-1}) = V\Gamma(A).$$

Hence if $\mathrm{Ran}(A)$ is dense, then $\mathrm{Ker}(A^*) = \mathrm{Ran}(A)^\perp = \{0\}$ and

$$\Gamma((A^*)^{-1}) = V\Gamma(A^*) = VU\Gamma(A)^\perp = UV\Gamma(A)^\perp = U(V\Gamma(A))^\perp$$

shows that $(A^*)^{-1} = (A^{-1})^*$. Similarly, if A is closable and $\overline{A}$ is injective, then $\overline{A}^{-1} = \overline{A^{-1}}$ by

$$\Gamma(\overline{A}^{-1}) = V\Gamma(\overline{A}) = \overline{V\Gamma(A)} = \Gamma(\overline{A^{-1}}).$$

□

Corollary 2.5. *If A is self-adjoint and injective, then A^{-1} is also self-adjoint.*

Proof. Equation (2.20) in the case $A = A^*$ implies $\mathrm{Ran}(A)^\perp = \mathrm{Ker}(A) = \{0\}$ and hence (iii) is applicable. □

If A is densely defined and bounded, we clearly have $\mathfrak{D}(A^*) = \mathfrak{H}$ and by Corollary 1.9, $A^* \in \mathfrak{L}(\mathfrak{H})$. In particular, since $\overline{A} = A^{**}$, we obtain

Theorem 2.6. *We have $\overline{A} \in \mathfrak{L}(\mathfrak{H})$ if and only if $A^* \in \mathfrak{L}(\mathfrak{H})$.*

Now we can also generalize Lemma 2.3 to the case of essential self-adjoint operators.

Lemma 2.7. *A symmetric operator A is essentially self-adjoint if and only if one of the following conditions holds for one $z \in \mathbb{C}\backslash\mathbb{R}$:*

- $\overline{\mathrm{Ran}(A+z)} = \overline{\mathrm{Ran}(A+z^*)} = \mathfrak{H}$,
- $\mathrm{Ker}(A^*+z) = \mathrm{Ker}(A^*+z^*) = \{0\}$.

If A is nonnegative, that is, $\langle\psi, A\psi\rangle \geq 0$ for all $\psi \in \mathfrak{D}(A)$, we can also admit $z \in (-\infty, 0)$.

Proof. First of all note that by (2.20) the two conditions are equivalent. By taking the closure of A, it is no restriction to assume that A is closed. Let $z = x + \mathrm{i}y$. From

$$\begin{aligned}\|(A+z)\psi\|^2 &= \|(A+x)\psi + \mathrm{i}y\psi\|^2 \\ &= \|(A+x)\psi\|^2 + y^2\|\psi\|^2 \geq y^2\|\psi\|^2,\end{aligned} \tag{2.44}$$

we infer that $\mathrm{Ker}(A+z) = \{0\}$ and hence $(A+z)^{-1}$ exists. Moreover, setting $\psi = (A+z)^{-1}\varphi$ ($y \neq 0$) shows $\|(A+z)^{-1}\| \leq |y|^{-1}$. Hence $(A+z)^{-1}$ is bounded and closed. Since it is densely defined by assumption, its domain $\mathrm{Ran}(A+z)$ must be equal to $\mathfrak{H}$. Replacing z by z^*, we see $\mathrm{Ran}(A+z^*) = \mathfrak{H}$ and applying Lemma 2.3 shows that A is self-adjoint. Conversely, if $A = A^*$, the above calculation shows $\mathrm{Ker}(A^*+z) = \{0\}$, which finishes the case $z \in \mathbb{C}\backslash\mathbb{R}$.

The argument for the nonnegative case with $z < 0$ is similar using $\varepsilon\|\psi\|^2 \leq \langle\psi, (A+\varepsilon)\psi\rangle \leq \|\psi\|\|(A+\varepsilon)\psi\|$ which shows $(A+\varepsilon)^{-1} \leq \varepsilon^{-1}$, $\varepsilon > 0$. □

In addition, we can also prove the closed graph theorem which shows that an unbounded closed operator cannot be defined on the entire Hilbert space.

Theorem 2.8 (Closed graph). *Let $\mathfrak{H}_1$ and $\mathfrak{H}_2$ be two Hilbert spaces and $A: \mathfrak{H}_1 \to \mathfrak{H}_2$ an operator defined on all of $\mathfrak{H}_1$. Then A is bounded if and only if $\Gamma(A)$ is closed.*

Proof. If A is bounded, then it is easy to see that $\Gamma(A)$ is closed. So let us assume that $\Gamma(A)$ is closed. Then A^* is well-defined and for all unit vectors

$\varphi \in \mathfrak{D}(A^*)$ we have that the linear functional $\ell_\varphi(\psi) = \langle A^*\varphi, \psi\rangle$ is pointwise bounded, that is,

$$\|\ell_\varphi(\psi)\| = |\langle\varphi, A\psi\rangle| \le \|A\psi\|.$$

Hence by the uniform boundedness principle there is a constant C such that $\|\ell_\varphi\| = \|A^*\varphi\| \le C$. That is, A^* is bounded and so is $A = A^{**}$. □

Note that since symmetric operators are closable, they are automatically closed if they are defined on the entire Hilbert space.

Theorem 2.9 (Hellinger-Toeplitz)**.** *A symmetric operator defined on the entire Hilbert space is bounded.*

Problem 2.1 (Jacobi operator)**.** *Let a and b be some real-valued sequences in $\ell^\infty(\mathbb{Z})$. Consider the operator*

$$Jf_n = a_n f_{n+1} + a_{n-1} f_{n-1} + b_n f_n, \qquad f \in \ell^2(\mathbb{Z}).$$

Show that J is a bounded self-adjoint operator.

Problem 2.2. *Show that $(\alpha A)^* = \alpha^* A^*$ and $(A+B)^* \supseteq A^* + B^*$ (where $\mathfrak{D}(A^* + B^*) = \mathfrak{D}(A^*) \cap \mathfrak{D}(B^*)$) with equality if one operator is bounded. Give an example where equality does not hold.*

Problem 2.3. *Suppose AB is densely defined. Show that $(AB)^* \supseteq B^* A^*$. Moreover, if B is bounded, then $(BA)^* = A^* B^*$.*

Problem 2.4. *Show* (2.20).

Problem 2.5. *An operator is called* **normal** *if $\|A\psi\| = \|A^*\psi\|$ for all $\psi \in \mathfrak{D}(A) = \mathfrak{D}(A^*)$.*

Show that if A is normal, so is $A + z$ for any $z \in \mathbb{C}$.

Problem 2.6. *Show that normal operators are closed. (Hint: A^* is closed.)*

Problem 2.7. *Show that a bounded operator A is normal if and only if $AA^* = A^*A$.*

Problem 2.8. *Show that the kernel of a closed operator is closed.*

Problem 2.9. *Show that if A is closed and B bounded, then AB is closed.*

2.3. Quadratic forms and the Friedrichs extension

Finally we want to draw some further consequences of Axiom 2 and show that observables correspond to self-adjoint operators. Since self-adjoint operators are already maximal, the difficult part remaining is to show that an observable has at least one self-adjoint extension. There is a good way of doing this for nonnegative operators and hence we will consider this case first.

An operator is called **nonnegative** (resp. **positive**) if $\langle\psi, A\psi\rangle \ge 0$ (resp. > 0 for $\psi \ne 0$) for all $\psi \in \mathfrak{D}(A)$. If A is positive, the map $(\varphi,\psi) \mapsto \langle\varphi, A\psi\rangle$ is a scalar product. However, there might be sequences which are Cauchy with respect to this scalar product but not with respect to our original one. To avoid this, we introduce the scalar product

$$\langle\varphi,\psi\rangle_A = \langle\varphi,(A+1)\psi\rangle, \qquad A \ge 0, \tag{2.45}$$

defined on $\mathfrak{D}(A)$, which satisfies $\|\psi\| \le \|\psi\|_A$. Let $\mathfrak{H}_A$ be the completion of $\mathfrak{D}(A)$ with respect to the above scalar product. We claim that $\mathfrak{H}_A$ can be regarded as a subspace of $\mathfrak{H}$; that is, $\mathfrak{D}(A) \subseteq \mathfrak{H}_A \subseteq \mathfrak{H}$.

If (ψ_n) is a Cauchy sequence in $\mathfrak{D}(A)$, then it is also Cauchy in $\mathfrak{H}$ (since $\|\psi\| \le \|\psi\|_A$ by assumption) and hence we can identify the limit in $\mathfrak{H}_A$ with the limit of (ψ_n) regarded as a sequence in $\mathfrak{H}$. For this identification to be unique, we need to show that if $(\psi_n) \subset \mathfrak{D}(A)$ is a Cauchy sequence in $\mathfrak{H}_A$ such that $\|\psi_n\| \to 0$, then $\|\psi_n\|_A \to 0$. This follows from

$$\begin{aligned}\|\psi_n\|_A^2 &= \langle\psi_n,\psi_n-\psi_m\rangle_A + \langle\psi_n,\psi_m\rangle_A \\ &\le \|\psi_n\|_A\|\psi_n-\psi_m\|_A + \|\psi_n\|\|(A+1)\psi_m\|\end{aligned} \tag{2.46}$$

since the right-hand side can be made arbitrarily small choosing m, n large.

Clearly the quadratic form q_A can be extended to every $\psi \in \mathfrak{H}_A$ by setting

$$q_A(\psi) = \langle\psi,\psi\rangle_A - \|\psi\|^2, \qquad \psi \in \mathfrak{Q}(A) = \mathfrak{H}_A. \tag{2.47}$$

The set $\mathfrak{Q}(A)$ is also called the **form domain** of A.

Example. (Multiplication operator) Let A be multiplication by $A(x) \ge 0$ in $L^2(\mathbb{R}^n, d\mu)$. Then

$$\mathfrak{Q}(A) = \mathfrak{D}(A^{1/2}) = \{f \in L^2(\mathbb{R}^n, d\mu) \,|\, A^{1/2} f \in L^2(\mathbb{R}^n, d\mu)\} \tag{2.48}$$

and

$$q_A(x) = \int_{\mathbb{R}^n} A(x)|f(x)|^2 d\mu(x) \tag{2.49}$$

(show this). ⋄

Now we come to our extension result. Note that $A+1$ is injective and the best we can hope for is that for a nonnegative extension $\tilde{A}$, the operator $\tilde{A}+1$ is a bijection from $\mathfrak{D}(\tilde{A})$ onto $\mathfrak{H}$.

Lemma 2.10. *Suppose A is a nonnegative operator. Then there is a nonnegative extension $\tilde{A}$ such that* $\mathrm{Ran}(\tilde{A}+1) = \mathfrak{H}$.

Proof. Let us define an operator $\tilde{A}$ by

$$\begin{aligned}\mathfrak{D}(\tilde{A}) &= \{\psi \in \mathfrak{H}_A | \exists \tilde{\psi} \in \mathfrak{H} : \langle\varphi,\psi\rangle_A = \langle\varphi,\tilde{\psi}\rangle, \forall\varphi \in \mathfrak{H}_A\}, \\ \tilde{A}\psi &= \tilde{\psi} - \psi.\end{aligned}$$

Since $\mathfrak{H}_A$ is dense, $\tilde{\psi}$ is well-defined. Moreover, it is straightforward to see that $\tilde{A}$ is a nonnegative extension of A.

It is also not hard to see that $\mathrm{Ran}(\tilde{A}+1) = \mathfrak{H}$. Indeed, for any $\tilde{\psi} \in \mathfrak{H}$, $\varphi \mapsto \langle \tilde{\psi}, \varphi \rangle$ is a bounded linear functional on $\mathfrak{H}_A$. Hence there is an element $\psi \in \mathfrak{H}_A$ such that $\langle \tilde{\psi}, \varphi \rangle = \langle \psi, \varphi \rangle_A$ for all $\varphi \in \mathfrak{H}_A$. By the definition of $\tilde{A}$, $(\tilde{A}+1)\psi = \tilde{\psi}$ and hence $\tilde{A}+1$ is onto. □

Example. Let us take $\mathfrak{H} = L^2(0,\pi)$ and consider the operator

$$Af = -\frac{d^2}{dx^2} f, \quad \mathfrak{D}(A) = \{f \in C^2[0,\pi] \,|\, f(0) = f(\pi) = 0\}, \tag{2.50}$$

which corresponds to the one-dimensional model of a particle confined to a box.

(i) First of all, using integration by parts twice, it is straightforward to check that A is symmetric:

$$\int_0^\pi g(x)^*(-f'')(x)dx = \int_0^\pi g'(x)^* f'(x)dx = \int_0^\pi (-g'')(x)^* f(x)dx. \tag{2.51}$$

Note that the *boundary conditions* $f(0) = f(\pi) = 0$ are chosen such that the boundary terms occurring from integration by parts vanish. Moreover, the same calculation also shows that A is positive:

$$\int_0^\pi f(x)^*(-f'')(x)dx = \int_0^\pi |f'(x)|^2 dx > 0, \quad f \neq 0. \tag{2.52}$$

(ii) Next let us show $\mathfrak{H}_A = \{f \in H^1(0,\pi) \,|\, f(0) = f(\pi) = 0\}$. In fact, since

$$\langle g, f \rangle_A = \int_0^\pi \big(g'(x)^* f'(x) + g(x)^* f(x)\big)\, dx, \tag{2.53}$$

we see that f_n is Cauchy in $\mathfrak{H}_A$ if and only if both f_n and f_n' are Cauchy in $L^2(0,\pi)$. Thus $f_n \to f$ and $f_n' \to g$ in $L^2(0,\pi)$ and $f_n(x) = \int_0^x f_n'(t)dt$ implies $f(x) = \int_0^x g(t)dt$. Thus $f \in AC[0,\pi]$. Moreover, $f(0) = 0$ is obvious and from $0 = f_n(\pi) = \int_0^\pi f_n'(t)dt$ we have $f(\pi) = \lim_{n\to\infty} \int_0^\pi f_n'(t)dt = 0$. So we have $\mathfrak{H}_A \subseteq \{f \in H^1(0,\pi) \,|\, f(0) = f(\pi) = 0\}$. To see the converse, approximate f' by smooth functions g_n. Using $g_n - \frac{1}{\pi}\int_0^\pi g_n(t)dt$ instead of g_n, it is no restriction to assume $\int_0^\pi g_n(t)dt = 0$. Now define $f_n(x) = \int_0^x g_n(t)dt$ and note $f_n \in \mathfrak{D}(A) \to f$.

(iii) Finally, let us compute the extension $\tilde{A}$. We have $f \in \mathfrak{D}(\tilde{A})$ if for all $g \in \mathfrak{H}_A$ there is an $\tilde{f}$ such that $\langle g, f \rangle_A = \langle g, \tilde{f} \rangle$. That is,

$$\int_0^\pi g'(x)^* f'(x)dx = \int_0^\pi g(x)^*(\tilde{f}(x) - f(x))dx. \tag{2.54}$$

Integration by parts on the right-hand side shows

$$\int_0^\pi g'(x)^* f'(x)dx = -\int_0^\pi g'(x)^* \int_0^x (\tilde{f}(t) - f(t))dt\,dx \tag{2.55}$$

or equivalently

$$\int_0^\pi g'(x)^* \left(f'(x) + \int_0^x (\tilde{f}(t) - f(t))dt \right) dx = 0. \tag{2.56}$$

Now observe $\{g' \in \mathfrak{H} | g \in \mathfrak{H}_A\} = \{h \in \mathfrak{H} | \int_0^\pi h(t)dt = 0\} = \{1\}^\perp$ and thus $f'(x) + \int_0^x (\tilde{f}(t) - f(t))dt \in \{1\}^{\perp\perp} = \mathrm{span}\{1\}$. So we see $f \in H^2(0,\pi) = \{f \in AC[0,\pi] | f' \in H^1(0,\pi)\}$ and $\tilde{A}f = -f''$. The converse is easy and hence

$$\tilde{A}f = -\frac{d^2}{dx^2}f, \quad \mathfrak{D}(\tilde{A}) = \{f \in H^2[0,\pi] \,|\, f(0) = f(\pi) = 0\}. \tag{2.57}$$

⋄

Now let us apply this result to operators A corresponding to observables. Since A will, in general, not satisfy the assumptions of our lemma, we will consider A^2 instead, which has a symmetric extension $\tilde{A^2}$ with $\mathrm{Ran}(\tilde{A^2}+1) = \mathfrak{H}$. By our requirement for observables, A^2 is maximally defined and hence is equal to this extension. In other words, $\mathrm{Ran}(A^2+1) = \mathfrak{H}$. Moreover, for any $\varphi \in \mathfrak{H}$ there is a $\psi \in \mathfrak{D}(A^2)$ such that

$$(A - \mathrm{i})(A + \mathrm{i})\psi = (A + \mathrm{i})(A - \mathrm{i})\psi = \varphi \tag{2.58}$$

and since $(A \pm \mathrm{i})\psi \in \mathfrak{D}(A)$, we infer $\mathrm{Ran}(A \pm \mathrm{i}) = \mathfrak{H}$. As an immediate consequence we obtain

Corollary 2.11. *Observables correspond to self-adjoint operators.*

2.4. Resolvents and spectra

Let A be a (densely defined) closed operator. The **resolvent set** of A is defined by

$$\rho(A) = \{z \in \mathbb{C} | (A - z)^{-1} \in \mathfrak{L}(\mathfrak{H})\}. \tag{2.66}$$

More precisely, $z \in \rho(A)$ if and only if $(A - z) : \mathfrak{D}(A) \to \mathfrak{H}$ is bijective and its inverse is bounded. By the closed graph theorem (Theorem 2.8), it suffices to check that $A - z$ is bijective. The complement of the resolvent set is called the **spectrum**

$$\sigma(A) = \mathbb{C} \backslash \rho(A) \tag{2.67}$$

of A. In particular, $z \in \sigma(A)$ if $A - z$ has a nontrivial kernel. A vector $\psi \in \operatorname{Ker}(A - z)$ is called an **eigenvector** and z is called an **eigenvalue** in this case.

The function

$$\begin{array}{rccc} R_A : & \rho(A) & \to & \mathfrak{L}(\mathfrak{H}) \\ & z & \mapsto & (A-z)^{-1} \end{array} \tag{2.68}$$

is called the **resolvent** of A. Note the convenient formula

$$R_A(z)^* = ((A-z)^{-1})^* = ((A-z)^*)^{-1} = (A^* - z^*)^{-1} = R_{A^*}(z^*). \tag{2.69}$$

In particular,

$$\rho(A^*) = \rho(A)^*. \tag{2.70}$$

Example. (Multiplication operator) Consider again the multiplication operator

$$(Af)(x) = A(x)f(x), \quad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}^n, d\mu) \,|\, Af \in L^2(\mathbb{R}^n, d\mu)\}, \tag{2.71}$$

given by multiplication with the measurable function $A : \mathbb{R}^n \to \mathbb{C}$. Clearly $(A - z)^{-1}$ is given by the multiplication operator

$$\begin{aligned} (A-z)^{-1}f(x) &= \frac{1}{A(x)-z} f(x), \\ \mathfrak{D}((A-z)^{-1}) &= \{f \in L^2(\mathbb{R}^n, d\mu) \,|\, \frac{1}{A-z} f \in L^2(\mathbb{R}^n, d\mu)\} \end{aligned} \tag{2.72}$$

whenever this operator is bounded. But $\|(A - z)^{-1}\| = \|\frac{1}{A-z}\|_\infty \le \frac{1}{\varepsilon}$ is equivalent to $\mu(\{x| \,|A(x) - z| < \varepsilon\}) = 0$ and hence

$$\rho(A) = \{z \in \mathbb{C} | \exists \varepsilon > 0 : \, \mu(\{x| \,|A(x) - z| < \varepsilon\}) = 0\}. \tag{2.73}$$

The spectrum

$$\sigma(A) = \{z \in \mathbb{C} | \forall \varepsilon > 0 : \, \mu(\{x| \,|A(x) - z| < \varepsilon\}) > 0\} \tag{2.74}$$

is also known as the **essential range** of $A(x)$. Moreover, z is an eigenvalue of A if $\mu(A^{-1}(\{z\})) > 0$ and $\chi_{A^{-1}(\{z\})}$ is a corresponding eigenfunction in this case. ◇

Example. (Differential operator) Consider again the differential operator

$$Af = -\mathrm{i}\frac{d}{dx} f, \quad \mathfrak{D}(A) = \{f \in AC[0, 2\pi] \,|\, f' \in L^2, \; f(0) = f(2\pi)\} \tag{2.75}$$

in $L^2(0, 2\pi)$. We already know that the eigenvalues of A are the integers and that the corresponding normalized eigenfunctions

$$u_n(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}nx} \tag{2.76}$$

form an orthonormal basis.

To compute the resolvent, we must find the solution of the corresponding inhomogeneous equation $-\mathrm{i}f'(x) - z\,f(x) = g(x)$. By the variation of constants formula the solution is given by (this can also be easily verified directly)

$$f(x) = f(0)\mathrm{e}^{\mathrm{i}zx} + \mathrm{i}\int_0^x \mathrm{e}^{\mathrm{i}z(x-t)} g(t)dt. \tag{2.77}$$

Since f must lie in the domain of A, we must have $f(0) = f(2\pi)$ which gives

$$f(0) = \frac{\mathrm{i}}{\mathrm{e}^{-2\pi\mathrm{i}z} - 1}\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}zt} g(t)dt, \qquad z \in \mathbb{C}\backslash\mathbb{Z}. \tag{2.78}$$

(Since $z \in \mathbb{Z}$ are the eigenvalues, the inverse cannot exist in this case.) Hence

$$(A - z)^{-1} g(x) = \int_0^{2\pi} G(z, x, t) g(t) dt, \tag{2.79}$$

where

$$G(z, x, t) = \mathrm{e}^{\mathrm{i}z(x-t)} \begin{cases} \frac{-\mathrm{i}}{1-\mathrm{e}^{-2\pi\mathrm{i}z}}, & t > x, \\ \frac{\mathrm{i}}{1-\mathrm{e}^{2\pi\mathrm{i}z}}, & t < x, \end{cases} \qquad z \in \mathbb{C}\backslash\mathbb{Z}. \tag{2.80}$$

In particular $\sigma(A) = \mathbb{Z}$. ◇

If $z, z' \in \rho(A)$, we have the **first resolvent formula**

$$R_A(z) - R_A(z') = (z - z')R_A(z)R_A(z') = (z - z')R_A(z')R_A(z). \tag{2.81}$$

In fact,

$$\begin{aligned}(A - z)^{-1} &- (z - z')(A - z)^{-1}(A - z')^{-1} \\ &= (A - z)^{-1}(1 - (z - A + A - z')(A - z')^{-1}) = (A - z')^{-1},\end{aligned} \tag{2.82}$$

which proves the first equality. The second follows after interchanging z and z'. Now fix $z' = z_0$ and use (2.81) recursively to obtain

$$R_A(z) = \sum_{j=0}^{n} (z - z_0)^j R_A(z_0)^{j+1} + (z - z_0)^{n+1} R_A(z_0)^{n+1} R_A(z). \tag{2.83}$$

The sequence of bounded operators

$$R_n = \sum_{j=0}^{n} (z - z_0)^j R_A(z_0)^{j+1} \tag{2.84}$$

converges to a bounded operator if $|z - z_0| < \|R_A(z_0)\|^{-1}$ and clearly we expect $z \in \rho(A)$ and $R_n \to R_A(z)$ in this case. Let $R_\infty = \lim_{n\to\infty} R_n$ and set $\varphi_n = R_n\psi$, $\varphi = R_\infty\psi$ for some $\psi \in \mathfrak{H}$. Then a quick calculation shows

$$AR_n\psi = (A - z_0)R_n\psi + z_0\varphi_n = \psi + (z - z_0)\varphi_{n-1} + z_0\varphi_n. \tag{2.85}$$

Hence $(\varphi_n, A\varphi_n) \to (\varphi, \psi + z\varphi)$ shows $\varphi \in \mathfrak{D}(A)$ (since A is closed) and $(A - z)R_\infty\psi = \psi$. Similarly, for $\psi \in \mathfrak{D}(A)$,

$$R_n A\psi = \psi + (z - z_0)\varphi_{n-1} + z_0\varphi_n \tag{2.86}$$

and hence $R_\infty(A-z)\psi = \psi$ after taking the limit. Thus $R_\infty = R_A(z)$ as anticipated.

If A is bounded, a similar argument verifies the **Neumann series** for the resolvent

$$R_A(z) = -\sum_{j=0}^{n-1} \frac{A^j}{z^{j+1}} + \frac{1}{z^n} A^n R_A(z) \\ = -\sum_{j=0}^{\infty} \frac{A^j}{z^{j+1}}, \quad |z| > \|A\|. \tag{2.87}$$

In summary we have proved the following:

Theorem 2.15. *The resolvent set $\rho(A)$ is open and $R_A : \rho(A) \to \mathfrak{L}(\mathfrak{H})$ is holomorphic; that is, it has an absolutely convergent power series expansion around every point $z_0 \in \rho(A)$. In addition,*

$$\|R_A(z)\| \geq \mathrm{dist}(z, \sigma(A))^{-1} \tag{2.88}$$

and if A is bounded, we have $\{z \in \mathbb{C} | \, |z| > \|A\|\} \subseteq \rho(A)$.

As a consequence we obtain the useful

Lemma 2.16. *We have $z \in \sigma(A)$ if there is a sequence $\psi_n \in \mathfrak{D}(A)$ such that $\|\psi_n\| = 1$ and $\|(A-z)\psi_n\| \to 0$. If z is a boundary point of $\rho(A)$, then the converse is also true. Such a sequence is called a* **Weyl sequence**.

Proof. Let ψ_n be a Weyl sequence. Then $z \in \rho(A)$ is impossible by $1 = \|\psi_n\| = \|R_A(z)(A-z)\psi_n\| \leq \|R_A(z)\|\|(A-z)\psi_n\| \to 0$. Conversely, by (2.88) there is a sequence $z_n \to z$ and corresponding vectors $\varphi_n \in \mathfrak{H}$ such that $\|R_A(z)\varphi_n\|\|\varphi_n\|^{-1} \to \infty$. Let $\psi_n = R_A(z_n)\varphi_n$ and rescale φ_n such that $\|\psi_n\| = 1$. Then $\|\varphi_n\| \to 0$ and hence

$$\|(A-z)\psi_n\| = \|\varphi_n + (z_n - z)\psi_n\| \leq \|\varphi_n\| + |z - z_n| \to 0$$

shows that ψ_n is a Weyl sequence. □

Let us also note the following spectral mapping result.

Lemma 2.17. *Suppose A is injective. Then*

$$\sigma(A^{-1})\backslash\{0\} = (\sigma(A)\backslash\{0\})^{-1}. \tag{2.89}$$

In addition, we have $A\psi = z\psi$ if and only if $A^{-1}\psi = z^{-1}\psi$.

Proof. Suppose $z \in \rho(A)\backslash\{0\}$. Then we claim

$$R_{A^{-1}}(z^{-1}) = -zAR_A(z) = -z - z^2 R_A(z).$$

In fact, the right-hand side is a bounded operator from $\mathfrak{H} \to \mathrm{Ran}(A) = \mathfrak{D}(A^{-1})$ and

$$(A^{-1} - z^{-1})(-zAR_A(z))\varphi = (-z + A)R_A(z)\varphi = \varphi, \quad \varphi \in \mathfrak{H}.$$

Conversely, if $\psi \in \mathfrak{D}(A^{-1}) = \mathrm{Ran}(A)$, we have $\psi = A\varphi$ and hence

$$(-zAR_A(z))(A^{-1} - z^{-1})\psi = AR_A(z)((A - z)\varphi) = A\varphi = \psi.$$

Thus $z^{-1} \in \rho(A^{-1})$. The rest follows after interchanging the roles of A and A^{-1}. □

Next, let us characterize the spectra of self-adjoint operators.

Theorem 2.18. *Let A be symmetric. Then A is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$ and $(A-E) \geq 0$, $E \in \mathbb{R}$, if and only if $\sigma(A) \subseteq [E, \infty)$. Moreover, $\|R_A(z)\| \leq |\,\mathrm{Im}(z)|^{-1}$ and, if $(A - E) \geq 0$, $\|R_A(\lambda)\| \leq |\lambda - E|^{-1}$, $\lambda < E$.*

Proof. If $\sigma(A) \subseteq \mathbb{R}$, then $\mathrm{Ran}(A + z) = \mathfrak{H}$, $z \in \mathbb{C}\backslash\mathbb{R}$, and hence A is self-adjoint by Lemma 2.7. Conversely, if A is self-adjoint (resp. $A \geq E$), then $R_A(z)$ exists for $z \in \mathbb{C}\backslash\mathbb{R}$ (resp. $z \in \mathbb{C}\backslash[E, \infty)$) and satisfies the given estimates as has been shown in the proof of Lemma 2.7. □

In particular, we obtain (show this!)

Theorem 2.19. *Let A be self-adjoint. Then*

$$\inf \sigma(A) = \inf_{\psi \in \mathfrak{D}(A),\, \|\psi\|=1} \langle \psi, A\psi \rangle \tag{2.90}$$

and

$$\sup \sigma(A) = \sup_{\psi \in \mathfrak{D}(A),\, \|\psi\|=1} \langle \psi, A\psi \rangle. \tag{2.91}$$

For the eigenvalues and corresponding eigenfunctions we have

Lemma 2.20. *Let A be symmetric. Then all eigenvalues are real and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. If $A\psi_j = \lambda_j \psi_j$, $j = 1, 2$, we have

$$\lambda_1 \|\psi_1\|^2 = \langle \psi_1, \lambda_1 \psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle = \langle \lambda_1 \psi_1, \psi_1 \rangle = \lambda_1^* \|\psi_1\|^2$$

and

$$(\lambda_1 - \lambda_2)\langle \psi_1, \psi_2 \rangle = \langle A\psi_1, \psi_2 \rangle - \langle A\psi_1, \psi_2 \rangle = 0,$$

finishing the proof. □

The result does not imply that two linearly independent eigenfunctions to the same eigenvalue are orthogonal. However, it is no restriction to assume that they are since we can use Gram–Schmidt to find an orthonormal basis for $\mathrm{Ker}(A - \lambda)$. If $\mathfrak{H}$ is finite dimensional, we can always find an orthonormal basis of eigenvectors. In the infinite dimensional case this is no longer true in general. However, if there is an orthonormal basis of eigenvectors, then A is essentially self-adjoint.

Theorem 2.21. *Suppose A is a symmetric operator which has an orthonormal basis of eigenfunctions $\{\varphi_j\}$. Then A is essentially self-adjoint. In particular, it is essentially self-adjoint on* $\operatorname{span}\{\varphi_j\}$.

Proof. Consider the set of all finite linear combinations $\psi = \sum_{j=0}^n c_j\varphi_j$ which is dense in $\mathfrak{H}$. Then $\phi = \sum_{j=0}^n \frac{c_j}{\lambda_j \pm \mathrm{i}}\varphi_j \in \mathfrak{D}(A)$ and $(A \pm \mathrm{i})\phi = \psi$ shows that $\operatorname{Ran}(A \pm \mathrm{i})$ is dense. □

Similarly, we can characterize the spectra of unitary operators. Recall that a bijection U is called unitary if $\langle U\psi, U\psi\rangle = \langle\psi, U^*U\psi\rangle = \langle\psi,\psi\rangle$. Thus U is unitary if and only if

$$U^* = U^{-1}. \tag{2.92}$$

Theorem 2.22. *Let U be unitary. Then $\sigma(U) \subseteq \{z \in \mathbb{C} | |z| = 1\}$. All eigenvalues have modulus one and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. Since $\|U\| \le 1$, we have $\sigma(U) \subseteq \{z \in \mathbb{C} | |z| \le 1\}$. Moreover, U^{-1} is also unitary and hence $\sigma(U) \subseteq \{z \in \mathbb{C} | |z| \ge 1\}$ by Lemma 2.17. If $U\psi_j = z_j\psi_j$, $j = 1, 2$, we have

$$(z_1 - z_2)\langle\psi_1, \psi_2\rangle = \langle U^*\psi_1, \psi_2\rangle - \langle\psi_1, U\psi_2\rangle = 0$$

since $U\psi = z\psi$ implies $U^*\psi = U^{-1}\psi = z^{-1}\psi = z^*\psi$. □

Problem 2.17. *Suppose A is closed and B bounded:*

- *Show that $\mathbb{I} + B$ has a bounded inverse if $\|B\| < 1$.*
- *Suppose A has a bounded inverse. Then so does $A + B$ if $\|B\| \le \|A^{-1}\|^{-1}$.*

Problem 2.18. *What is the spectrum of an orthogonal projection?*

Problem 2.19. *Compute the resolvent of*

$$Af = f', \qquad \mathfrak{D}(A) = \{f \in H^1[0,1] \,|\, f(0) = 0\}$$

and show that unbounded operators can have empty spectrum.

Problem 2.20. *Compute the eigenvalues and eigenvectors of $A = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A) = \{f \in H^2(0,\pi) | f(0) = f(\pi) = 0\}$. Compute the resolvent of A.*

Problem 2.21. *Find a Weyl sequence for the self-adjoint operator $A = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A) = H^2(\mathbb{R})$ for $z \in (0,\infty)$. What is $\sigma(A)$? (Hint: Cut off the solutions of $-u''(x) = z\,u(x)$ outside a finite ball.)*

Example 2.4.10. Let P, dom $P = \mathcal{H}^1(\mathbb{R})$, be the momentum operator on $\mathbb{R}$ discussed in Example 2.3.11. This operator has no eigenvalues; indeed, if $\lambda \in \mathbb{R}$ (recall that its spectrum is real) satisfies

$$(P\psi)(x) = -i\frac{d\psi}{dx}(x) = \lambda\psi(x), \qquad \psi \in \mathcal{H}^1(\mathbb{R}),$$

then $\psi(x) = ce^{i\lambda x}$, which belongs to $\mathrm{L}^2(\mathbb{R})$ iff $c = 0$; however, by "cutting off" such ψ, it will be possible to determine the spectrum of P. It should be noted that the "cutting off" that follows is a usual procedure.

Now fix $\lambda \in \mathbb{R}$ and let $\phi(x) = (2/\pi)^{1/4}e^{-x^2}$; then $1 = \|\phi\|^2 = \int_{\mathbb{R}} |\phi(x)|^2\,dx$. For each n set

$$\xi_n(x) = \frac{1}{\sqrt{n}}\phi\left(\frac{x}{n}\right)e^{i\lambda x},$$

which belongs to dom P and $\|\xi_n\| = 1$. Since

$$\|P\xi_n - \lambda\xi_n\|^2 = \frac{1}{n^2}\int_{\mathbb{R}} |\phi'(t)|^2\,dt$$

which vanishes as $n \to \infty$. Then (ξ_n) is a Weyl sequence for P at λ, and $\lambda \in \sigma(P)$. Therefore, $\sigma(P) = \mathbb{R}$ and it has no eigenvalues.

Example 2.4.11. Let $q : \mathbb{R} \to \mathbb{R}$, $q(x) = x$ be the position operator on $\mathbb{R}$ (see Exercise 2.3.31; here an alternative solution to that exercise is discussed). If $\lambda \in \mathbb{R}$, for each n set

$$\xi_n(x) = \frac{\sqrt{n}}{\pi^{1/4}}e^{-n^2(x-\lambda)^2},$$

which belongs to dom $\mathcal{M}_q$, $\|\xi_n\|^2 = 1$ and

$$\|q\xi_n - \lambda\xi_n\|^2 = \frac{1}{\sqrt{\pi}\,n^2}\int_{\mathbb{R}} x^2\,e^{-x^2}\,dx,$$

vanishes as $n \to \infty$, then (ξ_n) is a Weyl sequence for q at λ. Therefore, $\sigma(\mathcal{M}_q) = \mathbb{R}$ and it is easy to check that it has no eigenvalues.