13 Hilbert spaces

13.1 Definitions and examples

Let V be a complex vector space with an inner product $\langle \cdot \,|\, \cdot \rangle : V \times V \to \mathbb{C}$ satisfying (IP1)–(IP3) of Section 5.2. Such a space is sometimes called a **pre-Hilbert space**. As in Eq. (5.11) define a norm on an inner product space by

$$\|u\| = \sqrt{\langle u \,|\, u \rangle}. \tag{13.1}$$

The properties (Norm1)–(Norm3) of Section 10.9 hold for this choice of $\|\cdot\|$. Condition (Norm1) is equivalent to (IP3), and (Norm2) is an immediate consequence of (IP1) and (IP2), for

$$\|\lambda v\| = \sqrt{\langle \lambda v \,|\, \lambda v \rangle} = \sqrt{\lambda \overline{\lambda} \langle v \,|\, v \rangle} = |\lambda| \, \|v\|.$$

The triangle inequality (Norm3) is a consequence of Theorem 5.6. These properties hold equally in finite or infinite dimensional vector spaces. A **Hilbert space** $(\mathcal{H}, \langle \cdot \,|\, \cdot \rangle)$ is an inner product space that is complete in the induced norm; that is, $(\mathcal{H}, \|\cdot\|)$ is a Banach space. An introduction to Hilbert spaces at the level of this chapter may be found in [1–6], while more advanced topics are dealt with in [7–11].

The **parallelogram law**

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2 \tag{13.2}$$

holds for all pairs of vectors x, y in an inner product space $\mathcal{H}$. The proof is straightforward, by substituting $\|x + y\|^2 = \langle x + y \,|\, x + y \rangle = \|x\|^2 + \|y\|^2 + 2\mathrm{Re}(\langle x \,|\, y \rangle)$, etc. It immediately gives rise to the inequality

$$\|x + y\|^2 \leq 2\|x\|^2 + 2\|y\|^2. \tag{13.3}$$

For complex numbers (13.2) and (13.3) hold with norm replaced by modulus.

Example 13.1 The typical inner product defined on $\mathbb{C}^n$ in Example 5.4 by

$$\langle (u_1, \dots, u_n) \,|\, (v_1, \dots, v_n) \rangle = \sum_{i=1}^{n} \overline{u_i} v_i$$

makes it into a Hilbert space. The norm is

$$\|\mathbf{v}\| = \sqrt{|v_1|^2 + |v_2|^2 + \cdots + |v_n|^2},$$

which was shown to be complete in Example 10.27. In any finite dimensional inner product space the Schmidt orthonormalization procedure creates an orthonormal basis for which the inner product takes this form (see Section 5.2). Thus every finite dimensional Hilbert space is isomorphic to $\mathbb{C}^n$ with the above inner product. The only thing that distinguishes finite dimensional Hilbert spaces is their dimension.

Example 13.2 Let ℓ^2 be the set of all complex sequences $u = (u_1, u_2, \dots)$ where $u_i \in \mathbb{C}$ such that

$$\sum_{i=1}^{\infty} |u_i|^2 < \infty.$$

This space is a complex vector, for if u, v are any pair of sequences in ℓ^2, then $u + v \in \ell^2$. For, using the complex number version of the inequality (13.3),

$$\sum_{i=1}^{\infty} |u_i + v_i|^2 \leq 2\sum_{i=1}^{\infty} |u_i|^2 + 2\sum_{i=1}^{\infty} |v_i|^2 < \infty.$$

It is trivial that $u \in \ell^2$ implies $\lambda u \in \ell^2$ for any complex number λ.

Let the inner product be defined by

$$\langle u \mid v \rangle = \sum_{i=1}^{\infty} \overline{u_i} v_i.$$

This is well-defined for any pair of sequences $u, v \in \ell^2$, for

$$\begin{aligned} \Big| \sum_{i=1}^{\infty} \overline{u_i} v_i \Big| &\leq \sum_{i=1}^{\infty} |\overline{u_i} v_i| \\ &\leq \frac{1}{2} \sum_{i=1}^{\infty} \big(|u_i|^2 + |v_i|^2 \big) < \infty. \end{aligned}$$

The last step follows from

$$2\big|\overline{a}b\big|^2 = 2|a|^2|b|^2 = |a|^2 + |b|^2 - (|a| - |b|)^2 \leq |a|^2 + |b|^2.$$

The norm defined by this inner product is

$$\|u\| = \sqrt{\sum_{i=1}^{\infty} |u_i|^2} \leq \infty.$$

For any integer M and $n, m > N$

$$\sum_{i=1}^{M} |u_i^{(m)} - u_i^{(n)}|^2 \leq \sum_{i=1}^{\infty} |u_i^{(m)} - u_i^{(n)}|^2 = \|u^{(m)} - u^{(n)}\|^2 < \epsilon^2,$$

and taking the limit $n \to \infty$ we have

$$\sum_{i=1}^{M} \big|u_i^{(m)} - u_i\big|^2 \leq \epsilon^2.$$

In the limit $M \to \infty$

$$\sum_{i=1}^{\infty} \left| u_i^{(m)} - u_i \right|^2 \leq \epsilon^2$$

so that $u^{(m)} - u \in \ell^2$. Hence $u = u^{(m)} - (u^{(m)} - u)$ belongs to ℓ^2 since it is the difference of two vectors from ℓ^2 and it is the limit of the sequence $u^{(m)}$ since $\|u^{(m)} - u\| < \epsilon$ for all $m > N$. It turns out, as we shall see, that ℓ^2 is isomorphic to most Hilbert spaces of interest – the so-called *separable Hilbert spaces*.

Example 13.3 On $\mathcal{C}[0, 1]$, the continuous complex functions on $[0, 1]$, set

$$\langle f \,|\, g \rangle = \int_0^1 \overline{f} g \, \mathrm{d}x.$$

This is a pre-Hilbert space, but fails to be a Hilbert space since a sequence of continuous functions may have a discontinuous limit.

Exercise: Find a sequence of functions in $\mathcal{C}[0, 1]$ that have a discontinuous step function as their limit.

Example 13.4 Let $(X, \mathcal{M}, \mu)$ be a measure space, and $\mathcal{L}^2(X)$ be the set of all square integrable complex-valued functions $f : X \to \mathbb{C}$, such that

$$\int_X |f|^2 \, \mathrm{d}\mu < \infty.$$

This space is a complex vector space, for if f and g are square integrable then

$$\int_X |f + \lambda g|^2 \, \mathrm{d}\mu \leq 2 \int_X |f|^2 \, \mathrm{d}\mu + 2|\lambda|^2 \int_X |g|^2 \, \mathrm{d}\mu$$

by (13.3) applied to complex numbers.

Write $f \sim f'$ iff $f(x) = f'(x)$ almost everywhere on X; this is clearly an equivalence relation on X. We set $L^2(X)$ to be the factor space $\mathcal{L}^2(X)/\sim$. Its elements are equivalence classes $\tilde{f}$ of functions that differ at most on a set of measure zero. Define the inner product of two classes by

$$\langle \tilde{f} \,|\, \tilde{g} \rangle = \int_X \overline{f} g \, \mathrm{d}\mu,$$

which is well-defined (see Example 5.6) and independent of the choice of representatives. For, if $f' \sim f$ and $g' \sim g$ then let A_f and A_g be the sets on which $f(x) \neq f'(x)$ and $g'(x) \neq g(x)$, respectively. These sets have measure zero, $\mu(A_f) = \mu(A_g) = 0$. The set on which $\overline{f'(x)} g'(x) \neq \overline{f(x)} g(x)$ is a subset of $A_f \cup A_g$ and therefore must also have measure zero, so that $\int_X \overline{f} g \, \mathrm{d}\mu = \int_X \overline{f'} g' \, \mathrm{d}\mu$.

The inner product axioms (IP1) and (IP2) are trivial, and (IP3) follows from

$$\|\tilde{f}\| = 0 \implies \int_X |f|^2 \, \mathrm{d}\mu = 0 \implies f = 0 \text{ a.e.}$$

It is common to replace an equivalence class of functions $\tilde{f} \in \mathcal{L}^2(X)$ simply by a representative function f when there is no danger of confusion.

It turns out that the inner product space $\mathcal{L}^2(X)$ is in fact a Hilbert space. The following theorem is needed in order to show completeness.

Theorem 13.1 (Riesz–Fischer) *If $f_1, f_2, \dots$ is a Cauchy sequence of functions in $\mathcal{L}^2(X)$, there exists a function $f \in \mathcal{L}^2(X)$ such that $\|f - f_n\| \to 0$ as $n \to \infty$.*

Proof: The Cauchy sequence condition $\|f_n - f_m\| \to 0$ implies that for any $\epsilon > 0$ there exists N such that

$$\int_X |f_n - f_m|^2 \, \mathrm{d}\mu < \epsilon \qquad \text{for all } m, n > N.$$

We may, with some relabelling, pick a subsequence such that $f_0 = 0$ and

$$\|f_n - f_{n-1}\| < 2^{-n}.$$

Setting

$$h(x) = \sum_{n=1}^{\infty} |f_n(x) - f_{n-1}(x)|$$

we have from (Norm3),

$$\|h\| \le \sum_{n=1}^{\infty} \|f_n - f_{n-1}\| < \sum_{n=1}^{\infty} 2^{-n} = 1.$$

The function $x \mapsto h^2(x)$ is thus a positive real integrable function on X, and the set of points where its defining sequence diverges, $E = \{x \mid h(x) = \infty\}$, is a set of measure zero, $\mu(E) = 0$. Let g_n be the sequence of functions

$$g_n(x) = \begin{cases} f_n - f_{n-1} & \text{if } x \notin E, \\ 0 & \text{if } x \in E. \end{cases}$$

Since $g_n = f_n - f_{n-1}$ a.e. these functions are measurable and $\|g_n\| = \|f_n - f_{n-1}\| < 2^{-n}$. The function

$$f(x) = \sum_{n=1}^{\infty} g_n(x)$$

is defined almost everywhere, since the series is absolutely convergent to $h(x)$ almost everywhere. Furthermore it belongs to $\mathcal{L}^2(X)$, for

$$|f(x)|^2 = \Big|\sum g_n(x)\Big|^2 \le \Big(\sum |g_n(x)|\Big)^2 \le \big(h(x)\big)^2.$$

Since

$$f_n = \sum_{k=1}^{n} (f_k - f_{k-1}) = \sum_{k=1}^{n} g_k \quad \text{a.e.}$$

it follows that

$$\begin{aligned}\|f - f_n\| &= \Big\| f - \sum_{k=1}^{n} g_k \Big\| \\ &= \Big\| \sum_{k=n+1}^{\infty} g_k \Big\| \\ &\le \sum_{k=n+1}^{\infty} \|g_k\| \\ &< \sum_{k=n+1}^{\infty} 2^{-k} = 2^{-n}.\end{aligned}$$

Hence $\|f - f_n\| \to 0$ as $n \to \infty$ and the result is proved. ■

Problems

Problem 13.1 Let E be a Banach space in which the norm satisfies the parallelogram law (13.2). Show that it is a Hilbert space with inner product given by

$$\langle x \,|\, y\rangle = \tfrac{1}{4}\big(\|x+y\|^2 - \|x-y\|^2 + i\|x - iy\|^2 - i\|x + iy\|^2\big).$$

Problem 13.2 On the vector space $\mathcal{F}^1[a,b]$ of complex continuous differentiable functions on the interval $[a,b]$, set

$$\langle f \,|\, g\rangle = \int_a^b \overline{f'(x)}g'(x)\,\mathrm{d}x \quad \text{where} \quad f' = \frac{\mathrm{d}f}{\mathrm{d}x}, \quad g' = \frac{\mathrm{d}g}{\mathrm{d}x}.$$

Show that this is not an inner product, but becomes one if restricted to the space of functions $f \in \mathcal{F}^1[a,b]$ having $f(c) = 0$ for some fixed $a \le c \le b$. Is it a Hilbert space?

Give a similar analysis for the case $a = -\infty$, $b = \infty$, and restricting functions to those of compact support.

Problem 13.3 In the space $L^2([0,1])$ which of the following sequences of functions (i) is a Cauchy sequence, (ii) converges to 0, (iii) converges everywhere to 0, (iv) converges almost everywhere to 0, and (v) converges almost nowhere to 0?

(a) $f_n(x) = \sin^n(x)$, $n = 1, 2, \dots$

(b) $f_n(x) = \begin{cases} 0 & \text{for } x < 1 - \frac{1}{n}, \\ nx + 1 - n & \text{for } 1 - \frac{1}{n} \le x \le 1. \end{cases}$

(c) $f_n(x) = \sin^n(nx)$.

(d) $f_n(x) = \chi_{U_n}(x)$, the characteristic function of the set

$$U_n = \Big[\frac{k}{2^m}, \frac{k+1}{2^m}\Big] \quad \text{where} \quad n = 2^m + k,\ m = 0, 1, \dots \text{and } k = 0, \dots, 2^m - 1.$$

13.2 Expansion theorems

Subspaces

A **subspace** V of a Hilbert space $\mathcal{H}$ is a vector subspace that is **closed** with respect to the norm topology. For a vector subspace to be closed we require the limit of any sequence of vectors in V to belong to V,

$$u_1, u_2, \ldots \to u \text{ and all } u_n \in V \implies u \in V.$$

If V is any vector subspace of $\mathcal{H}$, its **closure** $\overline{V}$ is the smallest subspace containing V. It is the intersection of all subspaces containing V.

If K is any subset of $\mathcal{H}$ then, as in Chapter 3, the *vector subspace* generated by K is

$$L(K) = \left\{ \sum_{i=1}^{n} \alpha^i u_i \,|\, \alpha^i \in \mathbb{C}, u_i \in K \right\},$$

but the **subspace generated** by K will always refer to the *closed* subspace $\overline{L(K)}$ generated by K. A Hilbert space $\mathcal{H}$ is called **separable** if there is a countable set $K = \{u_1, u_2, \ldots\}$ such that $\mathcal{H}$ is generated by K,

$$\mathcal{H} = \overline{L(K)} = \overline{L(u_1, u_2, \ldots)}.$$

Orthonormal bases

If the Hilbert space $\mathcal{H}$ is separable and is generated by $\{u_1, u_2, \ldots\}$, we may use the **Schmidt orthonormalization** procedure (see Section 5.2) to produce an orthonormal set $\{e_1, e_2, \ldots, e_n\}$,

$$\langle e_i \,|\, e_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

The steps of the procedure are

$$\begin{aligned} f_1 &= u_1 & e_1 &= f_1/\|f_1\| \\ f_2 &= u_2 - \langle e_1 \,|\, u_2 \rangle e_1 & e_2 &= f_2/\|f_2\| \\ f_3 &= u_3 - \langle e_1 \,|\, u_3 \rangle e_1 - \langle e_2 \,|\, u_3 \rangle e_2 & e_3 &= f_3/\|f_3\|, \text{ etc.} \end{aligned}$$

from which it can be seen that each u_n is a linear combination of $\{e_1, e_2, \ldots, e_n\}$. Hence $\mathcal{H} = \overline{L(\{e_1, e_2, \ldots\})}$ and the set $\{e_n \,|\, n = 1, 2, \ldots\}$ is called a **complete orthonormal set** or **orthonormal basis** of $\mathcal{H}$.

Theorem 13.2 *If $\mathcal{H}$ is a separable Hilbert space and $\{e_1, e_2, \ldots\}$ is a complete orthonormal set, then any vector $u \in \mathcal{H}$ has a unique expansion*

$$u = \sum_{n=1}^{\infty} c_n e_n \quad \textit{where} \quad c_n = \langle e_n \,|\, u \rangle. \tag{13.4}$$

The meaning of the sum in this theorem is

$$\left\| u - \sum_{n=1}^{N} c_n e_n \right\| \to 0 \quad \text{as} \quad N \to \infty.$$

A critical part of the proof is **Bessel's inequality**:

$$\sum_{n=1}^{N} \left| \langle e_n \,|\, u \rangle \right|^2 \le \|u\|^2. \tag{13.5}$$

Proof: For any $N > 1$

$$\begin{aligned}
0 &\le \left\| u - \sum_{n=1}^{N} \langle e_n \,|\, u \rangle \, e_n \right\|^2 \\
&= \langle u - \textstyle\sum_n \langle e_n \,|\, u \rangle e_n \,|\, u - \sum_m \langle e_m \,|\, u \rangle e_m \rangle \\
&= \|u\|^2 - 2 \sum_{n=1}^{N} \overline{\langle e_n \,|\, u \rangle} \langle e_n \,|\, u \rangle + \sum_{n=1}^{N} \sum_{m=1}^{N} \overline{\langle e_n \,|\, u \rangle} \delta_{mn} \langle e_m \,|\, u \rangle \\
&= \|u\|^2 - \sum_{n=1}^{N} |\langle e_n \,|\, u \rangle|^2,
\end{aligned}$$

which gives the desired inequality. ■

Taking the limit $N \to \infty$ in Bessel's inequality (13.5) shows that the series

$$\sum_{n=1}^{\infty} \left| \langle e_n \,|\, u \rangle \right|^2$$

is bounded above and therefore convergent since it consists entirely of non-negative terms. To prove the expansion theorem 13.2, we first show two lemmas.

Lemma 13.3 *If $v_n \to v$ in a Hilbert space $\mathcal{H}$, then for all vectors $u \in \mathcal{H}$*

$$\langle u \,|\, v_n \rangle \to \langle u \,|\, v \rangle.$$

Proof: By the Cauchy–Schwarz inequality (5.13)

$$\begin{aligned}
\left| \langle u \,|\, v_n \rangle - \langle u \,|\, v \rangle \right| &= \left| \langle u \,|\, v_n - v \rangle \right| \\
&\le \|u\| \, \|v_n - v\| \\
&\to 0
\end{aligned}$$

■

Lemma 13.4 *If $\{e_1, e_2, \dots\}$ is a complete orthonormal set and $\langle v \,|\, e_n \rangle = 0$ for $n = 1, 2, \dots$ then $v = 0$.*

Proof: Since $\{e_n\}$ is a complete o.n. set, every vector $v \in \mathcal{H}$ is the limit of a sequence of vectors spanned by the vectors $\{e_1, e_2, \dots\}$,

$$v = \lim_{n \to \infty} v_n \quad \text{where} \quad v_n = \sum_{i=1}^{N} v_{ni} e_i.$$

Setting $u = v$ in Lemma 13.3, we have

$$\|v\|^2 = \langle v \,|\, v\rangle = \lim_{n\to\infty} \langle v \,|\, v_n\rangle = 0.$$

Hence $v = 0$ by the condition (Norm1). ■

We now return to the proof of the expansion theorem.

Proof of Theorem 13.2: Set

$$u_N = \sum_{n=1}^{N} \langle e_n \,|\, u\rangle\, e_n.$$

This is a Cauchy sequence,

$$\|u_N - u_M\|^2 = \sum_{n=M}^{N} \big|\langle e_n \,|\, u\rangle\big|^2 \to 0 \quad \text{as} \quad M, N \to \infty$$

since the series $\sum_n \big|\langle e_n \,|\, u\rangle\big|^2$ is absolutely convergent by Bessel's inequality (13.5). By completeness of the Hilbert space $\mathcal{H}$, $u_N \to u'$ for some vector $u' \in \mathcal{H}$. But

$$\langle e_k \,|\, u - u'\rangle = \lim_{N\to\infty} \langle e_k \,|\, u - u_N\rangle = \langle e_k \,|\, u\rangle - e_k u = 0$$

since $\langle e_k \,|\, u_N\rangle = \langle e_k \,|\, u\rangle$ for all $N \geq k$. Hence, by Lemma 13.4,

$$u = u' = \lim_{N\to\infty} u_N,$$

and Theorem 13.2 is proved. ■

Exercise: Show that every separable Hilbert space is either a finite dimensional inner product space, or is isomorphic with ℓ^2.

Example 13.5 For any real numbers $a < b$ the Hilbert space $L^2([a, b])$ is separable. The following is an outline proof; details may be found in [1]. By Theorem 11.2 any positive measurable function $f \geq 0$ on $[a, b]$ may be approximated by an increasing sequence of positive simple functions $0 < s_n(x) \to f(x)$. If $f \in \mathcal{L}^2([a, b])$ then by the dominated convergence, Theorem 11.11, $\|f - s_n\| \to 0$. By a straightforward, but slightly technical, argument these simple functions may be approximated with continuous functions, and prove that for any $\epsilon > 0$ there exists a positive continuous function $h(x)$ such that $\|f - h\| < \epsilon$. Using a famous theorem of Weierstrass that any continuous function on a closed interval can be arbitrarily closely approximated by polynomials, it is possible to find a complex-valued polynomial $p(x)$ such that $\|f - p\| < \epsilon$. Since all polynomials are of the form $p(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_n x^n$ where $c \in \mathbb{C}$, the functions $1, x, x^2, \ldots$ form a countable sequence of functions on $[a, b]$ that generate $L^2([a, b])$. This proves separability of $L^2([a, b])$.

Separability of $L^2(\mathbb{R})$ is proved by showing the restricted polynomial functions $f_{n,N} = x^n \chi_{[-N,N]}$ are a countable set that generates $L^2(\mathbb{R})$.

Example 13.6 On $L^2([-\pi, \pi])$ the functions

$$\phi_n(x) = \frac{e^{inx}}{\sqrt{2\pi}}$$

form an orthonormal basis,

$$\langle \phi_m \,|\, \phi_n \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(n-m)x}\, dx = \delta_{mn}$$

as is easily calculated for the two separate cases $n \neq m$ and $n = m$. These generate the Fourier series of an arbitrary square integrable function f on $[-\pi, \pi]$

$$f = \sum_{n=-\infty}^{\infty} c_n \phi_n \quad \text{a.e.}$$

where c_n are the Fourier coefficients

$$c_n = \langle \phi_n \,|\, f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-inx} f(x)\, dx.$$

Example 13.7 The *hermite polynomials* $H_n(x)$ $(n = 0, 1, 2, \dots)$ are defined by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n}.$$

The first few are

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x, \dots$$

The nth polynomial is clearly of degree n with leading term $(-2x)^n$. The functions $\psi_n(x) = e^{-(1/2)x^2} H_n(x)$ form an orthogonal system in $L^2(\mathbb{R})$:

$$\begin{aligned}
\langle \psi_m \,|\, \psi_n \rangle &= (-1)^{n+m} \int_{-\infty}^{\infty} e^{x^2} \frac{d^m e^{-x^2}}{dx^m} \frac{d^n e^{-x^2}}{dx^n}\, dx \\
&= (-1)^{n+m} \left(\left[e^{x^2} \frac{d^m e^{-x^2}}{dx^m} \frac{d^{n-1} e^{-x^2}}{dx^{n-1}} \right]_{-\infty}^{\infty} \right. \\
&\qquad \left. - \int_{-\infty}^{\infty} \frac{d}{dx} \left(e^{x^2} \frac{d^m e^{-x^2}}{dx^m} \right) \frac{d^{n-1} e^{-x^2}}{dx^{n-1}}\, dx \right)
\end{aligned}$$

on integration by parts. The first expression on the right-hand side of this equation vanishes since it involves terms of order $e^{-x^2} x^k$ that approach 0 as $x \to \pm\infty$. We may repeat the integration by parts on the remaining integral, until we arrive at

$$\langle \psi_m \,|\, \psi_n \rangle = (-1)^m \int_{-\infty}^{\infty} e^{-x^2} \frac{d^n}{dx^n} \left(e^{x^2} \frac{d^m e^{-x^2}}{dx^m} \right) dx,$$

which vanishes if $n > m$ since the expression in the brackets is a polynomial of degree m. A similar argument for $n < m$ yields

$$\langle \psi_m \,|\, \psi_n \rangle = 0 \qquad \text{for } n \neq m.$$

For $n = m$ we have, from the leading term in the hermite polynomials,

$$\begin{aligned}\|\psi_n\|^2 = \langle \psi_n \,|\, \psi_n \rangle &= (-1)^n \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(\mathrm{e}^{x^2} \frac{\mathrm{d}^n \mathrm{e}^{-x^2}}{\mathrm{d}x^n} \right) \mathrm{d}x \\ &= (-1)^n \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \big((-2x)^n \big) \, \mathrm{d}x \\ &= 2^n n! \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \, \mathrm{d}x \\ &= 2^n n! \sqrt{\pi}.\end{aligned}$$

Thus the functions

$$\phi_n(x) = \frac{\mathrm{e}^{-(1/2)x^2}}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) \tag{13.6}$$

form an orthonormal set. From Weierstrass's theorem they form a complete o.n. basis for $L^2(\mathbb{R})$.

The following generalization of Lemma 13.3 is sometimes useful.

Lemma 13.5 *If $u_n \to u$ and $v_n \to v$ then $\langle u_n \,|\, v_n \rangle \to \langle u \,|\, v \rangle$.*

Proof: Using the Cauchy–Schwarz inequality (5.13)

$$\begin{aligned}\big| \langle u_n \,|\, v_n \rangle - \langle u \,|\, v \rangle \big| &= \big| \langle u_n \,|\, v_n \rangle - \langle u_n \,|\, v \rangle + \langle u_n \,|\, v \rangle - \langle u \,|\, v \rangle \big| \\ &\le \big| \langle u_n \,|\, v_n \rangle - \langle u_n \,|\, v \rangle \big| + \big| \langle u_n \,|\, v \rangle - \langle u \,|\, v \rangle \big| \\ &\le \|u_n\| \, \|v_n - v\| + \|u_n - u\| \, \|v\| \\ &\to \|u\|.0 + 0.\|v\| \to 0.\end{aligned}$$

■

Exercise: If $u_n \to u$ show that $\|u_n\| \to \|u\|$, used in the last step of the above proof.

The following identity has widespread application in quantum mechanics.

Theorem 13.6 (Parseval's identity)

$$\langle u \,|\, v \rangle = \sum_{i=1}^{\infty} \langle u \,|\, e_i \rangle \langle e_i \,|\, v \rangle. \tag{13.7}$$

Proof: Set

$$u_n = \sum_{i=1}^{n} \langle e_i \,|\, u \rangle \, e_i \quad \text{and} \quad v_n = \sum_{i=1}^{n} \langle e_i \,|\, v \rangle \, e_i .$$

By Theorem 13.2, $u_n \to u$ and $v_n \to v$ as $n \to \infty$. Now using Lemma 13.5,

$$\begin{aligned}\langle u \mid v\rangle &= \lim_{n\to\infty} \langle u_n \mid v_n\rangle \\ &= \lim_{n\to\infty} \sum_{i=1}^{n}\sum_{j=1}^{n} \overline{\langle e_i \mid u\rangle}\langle e_j \mid v\rangle\langle e_i \mid e_j\rangle \\ &= \lim_{n\to\infty} \sum_{i=1}^{n}\sum_{j=1}^{n} \langle u \mid e_i\rangle\langle e_j \mid v\rangle\delta_{ij} \\ &= \lim_{n\to\infty} \sum_{i=1}^{n} \langle u \mid e_i\rangle\langle e_i \mid v\rangle. \\ &= \sum_{i=1}^{\infty} \langle u \mid e_i\rangle\langle e_i \mid v\rangle.\end{aligned}$$

■

For a function $f(x) = \sum_{n=-\infty}^{\infty} c_n\phi_n$ on $[-\pi, \pi]$, where $\phi_n(x)$ are the standard Fourier functions given in Example 13.6, Parseval's identity becomes the well-known formula

$$\|f\|^2 = \int_{-\pi}^{\pi} |f(x)|^2 \,\mathrm{d}x = \sum_{n=-\infty}^{\infty} |c_n|^2.$$

Problems

Problem 13.4 Show that a vector subspace is a closed subset of $\mathcal{H}$ with respect to the norm topology iff the limit of every sequence of vectors in V belongs to V.

Problem 13.5 Let ℓ_0 be the subset of ℓ^2 consisting of sequences with only finitely many terms different from zero. Show that ℓ_0 is a vector subspace of ℓ^2, but that it is not closed. What is its closure $\overline{\ell_0}$?

Problem 13.6 We say a sequence $\{x_n\}$ *converges weakly* to a point x in a Hilbert space $\mathcal{H}$, written $x_n \rightharpoonup x$ if $\langle x_n \mid y\rangle \to \langle x \mid y\rangle$ for all $y \in \mathcal{H}$. Show that every strongly convergent sequence, $\|x_n - x\| \to 0$ is weakly convergent to x. In finite dimensional Hilbert spaces show that every weakly convergent sequence is strongly convergent.

Give an example where $x_n \rightharpoonup x$ but $\|x_n\| \not\to \|x\|$. Is it true in general that the weak limit of a sequence is unique?

Show that if $x_n \rightharpoonup x$ and $\|x_n\| \not\to \|x\|$ then $x_n \not\to x$.

Problem 13.7 In the Hilbert space $L^2([-1, 1])$ let $\{f_n(x)\}$ be the sequence of functions $1, x, x^2, \dots, f_n(x) = x^n, \dots$

(a) Apply Schmidt orthonormalization to this sequence, writing down the first three polynomials so obtained.

(b) The nth *Legendre polynomial* $P_n(x)$ is defined as

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(x^2 - 1\right)^n.$$

Prove that

$$\int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = \frac{2}{2n+1}\delta_{mn}.$$

(c) Show that the nth member of the o.n. sequence obtained in (a) is $\sqrt{n + \frac{1}{2}}\,P_n(x)$.

Problem 13.8 Show that Schmidt orthonormalization in $L^2(\mathbb{R})$, applied to the sequence of functions

$$f_n(x) = x^n e^{-x^2/2},$$

leads to the normalized hermite functions (13.6) of Example 13.7.

Problem 13.9 Show that applying Schmidt orthonormalization in $L^2([0, \infty])$ to the sequence of functions

$$f_n(x) = x^n e^{-x/2}$$

leads to a normalized sequence of functions involving the *Laguerre polynomials*

$$L_n(x) = e^x \frac{d^n}{dx^n}\big(x^n e^{-x}\big).$$

13.3 Linear functionals

Orthogonal subspaces

Two vectors $u, v \in \mathcal{H}$ are said to be **orthogonal** if $\langle u|v\rangle = 0$, written $u \perp v$. If V is a subspace of $\mathcal{H}$ we denote its **orthogonal complement** by

$$V^\perp = \{u \mid u \perp v \text{ for all } v \in V\}.$$

Theorem 13.7 *If V is a subspace of $\mathcal{H}$ then $V^\perp$ is also a subspace.*

Proof: $V^\perp$ is clearly a vector subspace, for $v, v' \in V^\perp$ since

$$\langle \alpha v + \beta v' \,|\, u\rangle = \overline{\alpha}\langle v \,|\, u\rangle + \overline{\beta}\langle v' \,|\, u\rangle = 0$$

for all $u \in V$. The space $V^\perp$ is closed, for if $v_n \to v$ where $v_n \in V^\perp$, then

$$\langle v \,|\, u\rangle = \lim_{n\to\infty} \langle v_n \,|\, u\rangle = \lim_{n\to\infty} 0 = 0$$

for all $u \in V$. Hence $v \in V$. ■

Theorem 13.8 *If V is a subspace of a Hilbert space $\mathcal{H}$ then every $u \in \mathcal{H}$ has a unique decomposition*

$$u = u' + u'' \quad \textit{where} \quad u' \in V,\ u'' \in V^\perp.$$

Proof: The idea behind the proof of this theorem is to find the element of V that is 'nearest' to u. Just as in Euclidean space, this is the orthogonal projection of the vector u onto the subspace V. Let

$$d = \inf\{\|u - v\| \mid v \in V\}$$

and $v_n \in V$ a sequence of vectors such that $\|u - v_n\| \to d$. The sequence $\{v_n\}$ is Cauchy, for if we set $x = u - \frac{1}{2}(v_n + v_m)$ and $y = \frac{1}{2}(v_n - v_m)$ in the parallelogram law (13.2), then

$$\|v_n - v_m\|^2 = 2\|u - v_n\|^2 + 2\|u - v_m\|^2 - 4\|u - \tfrac{1}{2}(v_n + v_m)\|^2. \tag{13.8}$$

For any $\epsilon > 0$ let $N > 0$ be such that for all $k > N$, $\|u - v_k\|^2 \leq d^2 + \frac{1}{4}\epsilon$. Setting n, m both $> N$ in Eq. (13.8) we find $\|v_n - v_m\|^2 \leq \epsilon$. Hence v_n is a Cauchy sequence.

Since $\mathcal{H}$ is complete and V is a closed subspace, there exists a vector $u' \in V$ such that $v_n \to u'$. Setting $u'' = u - u'$, it follows from the exercise after Lemma 13.5 that

$$\|u''\| = \lim_{n\to\infty} \|u - v_n\| = d.$$

For any $v \in V$ set $v_0 = v/\|v\|$, so that $\|v_0\| = 1$. Then

$$\begin{aligned} d^2 &\leq \|u - (u' + \langle v_0 \,|\, u''\rangle\, v_0)\|^2 \\ &= \|u'' - \langle v_0 \,|\, u''\rangle v_0\|^2 \\ &= \langle u'' - \langle v_0 \,|\, u''\rangle v_0 \,|\, u'' - \langle v_0 \,|\, u''\rangle v_0\rangle \\ &= d^2 - |\langle v_0 \,|\, u''\rangle|^2. \end{aligned}$$

Hence $\langle v_0 \,|\, u''\rangle = 0$, so that $\langle v \,|\, u''\rangle = 0$. Since v is an arbitrary vector in V, we have $u'' \in V^\perp$.

A subspace and its orthogonal complement can only have the zero vector in common, $V \cap V^\perp = \{0\}$, for if $w \in V \cap V^\perp$ then $\langle w \,|\, w\rangle = 0$, which implies that $w = 0$. If $u = u' + u'' = v' + v''$, with $u', v' \in V$ and $u'', v'' \in V^\perp$, then the vector $u' - v' \in V$ is equal to $v'' - u'' \in V^\perp$. Hence $u' = v'$ and $u'' = v''$, the decomposition is unique. ∎

Corollary 13.9 *For any subspace V, $V^{\perp\perp} = V$.*

Proof: $V \subseteq V^{\perp\perp}$ for if $v \in V$ then $\langle v \,|\, u\rangle = 0$ for all $u \in V^\perp$. Conversely, let $v \in V^{\perp\perp}$. By Theorem 13.8 v has a unique decomposition $v = v' + v''$ where $v' \in V \subseteq V^{\perp\perp}$ and $v'' \in V^\perp$. Using Theorem 13.8 again but with V replaced by $V^\perp$, it follows that $v'' = 0$. Hence $v = v' \in V$. ∎

Riesz representation theorem

For every $v \in \mathcal{H}$ the map $\varphi_v : u \mapsto \langle v \,|\, u\rangle$ is a linear functional on $\mathcal{H}$. Linearity is obvious and continuity follows from Lemma 13.3. The following theorem shows that all (continuous) linear functionals on a Hilbert space are of this form, a result of considerable significance in quantum mechanics, as it motivates Dirac's *bra-ket notation*.

Theorem 13.10 (Riesz representation theorem) *If φ is a linear functional on a Hilbert space $\mathcal{H}$, then there is a unique vector $v \in \mathcal{H}$ such that*

$$\varphi(u) = \varphi_v(u) = \langle v \,|\, u\rangle \qquad \textit{for all } u \in \mathcal{H}.$$

Proof: Since a linear functional $\varphi : \mathcal{H} \to \mathbb{C}$ is required to be continuous, we always have

$$|\varphi(x_n) - \varphi(x)| \to 0 \quad \text{whenever} \quad \|x - x_n\| \to 0.$$

Let V be the null space of φ,

$$V = \{x \mid \varphi(x) = 0\}.$$

This is a closed subspace, for if $x_n \to x$ and $\varphi(x_n) = 0$ for all n, then $\varphi(x) = 0$ by continuity. If $V = \mathcal{H}$ then φ vanishes on $\mathcal{H}$ and one can set $v = 0$. Assume therefore that $V \neq \mathcal{H}$, and let

w be a non-zero vector such that $w \notin V$. By Theorem 13.8, there is a unique decomposition

$$w = w' + w'' \quad \text{where} \quad w' \in V, \quad w'' \in V^{\perp}.$$

Then $\varphi(w'') = \varphi(w) - \varphi(w') = \varphi(w) \neq 0$ since $w \notin V$. For any $u \in \mathcal{H}$ we may write

$$u = \left(u - \frac{\varphi(u)}{\varphi(w'')} w''\right) + \frac{\varphi(u)}{\varphi(w'')} w'',$$

where the first term on the right-hand side belongs to V since the linear functional φ gives the value 0 when applied to it, while the second term belongs to $V^{\perp}$ as it is proportional to w''. For any $v \in V^{\perp}$ we have then

$$\langle v \,|\, u \rangle = \frac{\varphi(u)}{\varphi(w'')} \langle v \,|\, w'' \rangle.$$

In particular, setting

$$v = \frac{\overline{\varphi(w'')}}{\|w''\|^2} w'' \ \in V^{\perp}$$

gives

$$\langle v \,|\, u \rangle = \frac{\varphi(u)}{\varphi(w'')} \frac{\varphi(w'')}{\|w''\|^2} \langle w'' \,|\, w'' \rangle = \varphi(u).$$

Hence this v is the vector required for the theorem. It is the unique vector with this property, for if $\langle v - v' \,|\, u \rangle = 0$ for all $u \in \mathcal{H}$ then $v = v'$, on setting $u = v - v'$. ■

Problems

Problem 13.10 If S is any subset of $\mathcal{H}$, and V the closed subspace generated by S, $V = \overline{L(S)}$, show that $S^{\perp} = \{u \in \mathcal{H} \,|\, \langle u \,|\, x \rangle = 0 \text{ for all } x \in S\} = V^{\perp}$.

Problem 13.11 Which of the following is a vector subspace of ℓ^2, and which are closed? In each case find the space of vectors orthogonal to the set.

(a) $V_N = \{(x_1, x_2, \dots) \in \ell^2 \,|\, x_i = 0 \text{ for } i > N\}$.

(b) $V = \bigcup_{N=1}^{\infty} V_N = \{(x_1, x_2, \dots) \in \ell^2 \,|\, x_i = 0 \text{ for } i > \text{some } N\}$.

(c) $U = \{(x_1, x_2, \dots) \in \ell^2 \,|\, x_i = 0 \text{ for } i = 2n\}$.

(d) $W = \{(x_1, x_2, \dots) \in \ell^2 \,|\, x_i = 0 \text{ for some } i\}$.

Problem 13.12 Show that the real Banach space $\mathbb{R}^2$ with the norm $\|(x, y)\| = \max\{|x|, |y|\}$ does not have the closest point property of Theorem 13.8. Namely for a given point $\mathbf{x}$ and one-dimensional subspace L, there does not in general exist a unique point in L that is closest to $\mathbf{x}$.

Problem 13.13 If $A : \mathcal{H} \to \mathcal{H}$ is an operator such that $Au \perp u$ for all $u \in \mathcal{H}$, show that $A = 0$.

13.4 Bounded linear operators

Let V be any normed vector space. A linear operator $A : V \to V$ is said to be **bounded** if

$$\|Au\| \leq K\|u\|$$

for some constant $K \geq 0$ and all $u \in V$.

Theorem 13.11 *A linear operator on a normed vector space is bounded if and only if it is continuous with respect to the norm topology.*

Proof: If A is bounded then it is continuous, for if $\epsilon > 0$ then for any pair of vectors u, v such that $\|u - v\| < \epsilon/K$

$$\|Au - Av\| = \|A(u - v)\| \leq K\|u - v\| < \epsilon.$$

Conversely, let A be a continuous operator on V. If A is *not* bounded, then for each $N > 0$ there exists u_N such that $\|Au_N\| \geq N\|u_N\|$. Set

$$w_N = \frac{u_N}{N\|u_N\|},$$

so that

$$\|w_N\| = \frac{1}{N} \to 0.$$

Hence $w_N \to 0$, but $\|Aw_N\| \geq 1$, so that Aw_n definitely does *not* $\to 0$, contradicting the assumption that A is continuous. ■

The **norm** of a bounded operator A is defined as

$$\|A\| = \sup\{\|Au\| \mid \|u\| \leq 1\}.$$

By Theorem 13.11, A is continuous at $x = 0$. Hence there exists $\epsilon > 0$ such that $\|Ax\| \leq 1$ for all $\|x\| \leq \epsilon$. For any u with $\|u\| \leq 1$ let $v = \epsilon u$ so that $\|v\| \leq \epsilon$ and

$$\|Au\| = \frac{1}{\epsilon}\|Av\| \leq \frac{1}{\epsilon}.$$

This shows $\|A\|$ always exists for a bounded operator.

Example 13.8 On ℓ^2 define the two *shift operators* S and S' by

$$S\big((x_1, x_2, x_3, \dots)\big) = (0, x_1, x_2, \dots)$$

and

$$S'\big((x_1, x_2, x_3, \dots)\big) = (x_2, x_3, \dots).$$

These operators are clearly linear, and satisfy

$$\|Sx\| = \|x\| \quad \text{and} \quad \|S'x\| \leq \|x\|.$$

Hence the norm of the operator S is 1, while $\|S'\|$ is also 1 since equality holds for $x_1 = 0$.

Example 13.9 Let α be any bounded measurable function on the Hilbert space $L^2(X)$ of square integrable functions on a measure space X. The *multiplication operator* $A_\alpha : L^2(X) \to L^2(X)$ defined by $A_\alpha(f) = \alpha f$ is a bounded linear operator, for αf is measurable for every $f \in L^2(X)$, and it is square integrable since

$$|\alpha f|^2 \leq M^2 |f|^2 \quad \text{where} \quad M = \sup_{x \in X} |\alpha(x)|.$$

The multiplication operator is well-defined on $L^2(X)$, for if f and f' are equal almost everywhere, $f \sim f'$, then $\alpha f \sim \alpha f'$; thus there is no ambiguity in writing $A_\alpha f$ for $A_\alpha[f]$. Linearity is trivial, while boundedness follows from

$$\|A_\alpha f\|^2 = \int_X |\alpha f|^2 \, d\mu \leq M^2 \int_X |f|^2 \, d\mu = M^2 \|f\|^2.$$

Exercise: If A and B are bounded linear operators on a normed vector space, show that $A + \lambda B$ and AB are also bounded.

A bounded operator $A : V \to V$ is said to be **invertible** if there exists a bounded operator $A^{-1} : V \to V$ such that $AA^{-1} = A^{-1}A = I \equiv \mathrm{id}_V$. A^{-1} is called the **inverse** of A. It is clearly unique, for if $BA = CA$ then $B = BI = BAA^{-1} = CAA^{-1} = C$. It is important that we specify A^{-1} to be both a right and left inverse. For example, in ℓ^2, the shift operator S defined in Example 13.8 has left inverse S', since $S'S = I$, but it is not a right inverse for $SS'(x_1, x_2, \dots) = (0, x_2, x_3, \dots)$. Thus S is not an invertible operator, despite the fact that it is injective and an isometry, $\|Sx\| = \|x\|$. For a finite dimensional space these conditions would be enough to guarantee invertibility.

Theorem 13.12 *If A is a bounded operator on a Banach space V, with $\|A\| < 1$, then the operator $I - A$ is invertible and*

$$(I - A)^{-1} = \sum_{n=0}^{\infty} A^n.$$

Proof: Let x be any vector in V. Since $\|A^k x\| \leq \|A\|(A^{k-1}x)$ it follows by simple induction that A^k is bounded and has norm $\|A^k\| \leq (\|A\|)^k$. The vectors $u_n = (I + A + A^2 + \dots + A^n)x$ form a Cauchy sequence, since

$$\begin{aligned}
\|u_n - u_m\| &= \|(A^{m+1} + \dots + A^n)x\| \\
&\leq \big(\|A\|^{m+1} + \dots + \|A\|^n\big)\|x\| \\
&\leq \frac{\|A\|^{m+1}}{1 - \|A\|}\|x\| \\
&\to 0 \quad \text{as } m \to \infty.
\end{aligned}$$

Since V is a Banach space, $u_m \to u$ for some $u \in V$, so there is a linear operator $T : V \to V$ such that $u = Tx$. Furthermore, since $T - (I + A + \dots + A^n)$ is a bounded linear operator, it follows that T is bounded. Writing $T = \sum_{k=1}^{\infty} A^k$, in the sense that

$$\lim_{m \to \infty} \Big(T - \sum_{k=1}^{m} A^k\Big)x = 0,$$

it is straightforward to verify that $(I - A)Tx = T(I - A)x = x$, which shows that $T = (I - A)^{-1}$. ■

Adjoint operators

Let $A : \mathcal{H} \to \mathcal{H}$ be a bounded linear operator on a Hilbert space $\mathcal{H}$. We define its **adjoint** to be the operator $A^* : \mathcal{H} \to \mathcal{H}$ that has the property

$$\langle u \,|\, Av \rangle = \langle A^* u \,|\, v \rangle \qquad \text{for all } u, v \in \mathcal{H}. \tag{13.9}$$

This operator is well-defined, linear and bounded.

Proof: For fixed u, the map $\varphi_u : v \mapsto \langle u \,|\, Av \rangle$ is clearly linear and continuous, on using Lemma 13.3. Hence φ_u is a linear functional, and by the Riesz representation theorem there exists a unique element $A * u \in \mathcal{H}$ such that

$$\langle A^* u \,|\, v \rangle = \varphi_u(v) = \langle u \,|\, Av \rangle.$$

The map $u \mapsto A * u$ is linear, since for an arbitrary vector v

$$\begin{aligned} \langle A^*(u + \lambda w) \,|\, v \rangle &= \langle u + \lambda w \,|\, Av \rangle \\ &= \langle u \,|\, Av \rangle + \overline{\lambda} \langle w \,|\, Av \rangle \\ &= \langle A^* u + \lambda A^* w \,|\, v \rangle. \end{aligned}$$

To show that the linear operator A^* is bounded, let u be any vector,

$$\begin{aligned} \|A^* u\|^2 &= |\langle A^* u \,|\, A^* u \rangle| \\ &= |\langle u \,|\, AA^* u \rangle| \\ &\le \|u\| \, \|AA^* u\| \\ &\le \|A\| \, \|u\| \, \|A^* u\|. \end{aligned}$$

Hence, either $A^* u = 0$ or $\|A^* u\| \le \|A\| \, \|u\|$. In either case $\|A^* u\| \le \|A\| \, \|u\|$. ■

Theorem 13.13 *The adjoint satisfies the following properties:*

(i) $(A + B)^* = A^* + B^*$,
(ii) $(\lambda A)^* = \overline{\lambda} A^*$,
(iii) $(AB)^* = B^* A^*$,
(iv) $A^{**} = A$,
(v) *if A is invertible then* $(A^{-1})^* = (A^*)^{-1}$.

Proof: We provide proofs of (i) and (ii), leaving the others as exercises.

(i) For arbitrary $u, v \in \mathcal{H}$

$$\begin{aligned} \langle (A + B)^* u \,|\, v \rangle &= \langle u \,|\, (A + B)v \rangle = \langle u \,|\, Av + Bv \rangle \\ &= \langle u \,|\, Av \rangle + \langle u \,|\, Bv \rangle = \langle A^* u \,|\, v \rangle + \langle B^* u \,|\, v \rangle = \langle A^* u + B^* u \,|\, v \rangle. \end{aligned} \tag{13.10}$$

As $\langle w \,|\, v \rangle = \langle w' \,|\, v \rangle$ for all $v \in \mathcal{H}$ implies $w = w'$, we have

$$(A + B)^* u = A^* u + B^* u.$$

(ii) For any pair of vectors $u, v \in \mathcal{H}$

$$
\begin{aligned}
\langle (\lambda A)^* u \,|\, v\rangle &= \langle u \,|\, \lambda A v\rangle = \lambda \langle u \,|\, A v\rangle \\
&= \lambda \langle A^* u \,|\, v\rangle = \langle \overline{\lambda} A^* u \,|\, v\rangle. \qquad (13.11)
\end{aligned}
$$

The proofs of (iii)–(v) are on similar lines.

Example 13.10 The right shift operator S on ℓ^2 (see Example 13.8) induces the inner product

$$\langle x \,|\, Sy\rangle = \overline{x_1}.0 + \overline{x_2} y_1 + \overline{x_3} y_2 + \cdots = \langle S' x \,|\, y\rangle,$$

where S' is the left shift. Hence $S^* = S'$. Similarly $S'^* = S$, since

$$\langle x \,|\, S' y\rangle = \overline{x_1} y_2 + \overline{x_2} y_3 + \cdots = \langle S' x \,|\, y\rangle.$$

Example 13.11 Let α be a bounded measurable function on the Hilbert space $L^2(X)$ of square integrable functions on a measure space X, and A_α the multiplication operator defined in Example 13.9. For any pair of functions f, g square integrable on X, the equation $\langle A^*_\alpha f \,|\, g\rangle = \langle f \,|\, A_\alpha g\rangle$ reads

$$\int_X \overline{A^*_\alpha f} g \,\mathrm{d}\mu = \int_X \overline{f} A_\alpha g \,\mathrm{d}\mu = \int_X \overline{f} \alpha g \,\mathrm{d}\mu.$$

Since g is an arbitrary function from $\mathcal{L}^2(X)$, we have $\overline{A^*_\alpha f} = \alpha \overline{f}$ a.e., and in terms of the equivalence classes of functions in $L^2(X)$ the adjoint operator reads

$$A^*_\alpha [f] = [\overline{\alpha} f].$$

The adjoint operator of a multiplication operator is the multiplication operator by the complex conjugate function.

We define the **matrix element of the operator** A **between the vectors** u **and** v **in** $\mathcal{H}$ to be $\langle u \,|\, Av\rangle$. If the Hilbert space is separable and e_i is an o.n. basis then, by Theorem 13.2, we may write

$$Ae_j = \sum_i a_{ij} e_i \quad \text{where} \quad a_{ij} = \langle e_i \,|\, Ae_j\rangle.$$

Thus the matrix elements of the operator between the basis vectors are identical with the components of the matrix of the operator with respect to this basis, $\mathsf{A} = [a_{ij}]$. The adjoint operator has decomposition

$$A^* e_j = \sum_i a^*_{ij} e_i \quad \text{where} \quad a^*_{ij} = \langle e_i \,|\, A^* e_j\rangle.$$

The relation between the matrix elements $[a^*_{ij}]$ and $[a_{ij}]$ is determined by

$$a^*_{ij} = \langle e_i \,|\, A^* e_j\rangle = \langle Ae_i \,|\, e_j\rangle = \overline{\langle e_j \,|\, Ae_i\rangle} = \overline{a_{ji}},$$

or, in matrix notation,

$$\mathsf{A}^* \equiv [a^*_{ij}] = [\,\overline{a_{ji}}\,] = \overline{\mathsf{A}^T} = \mathsf{A}^\dagger.$$

In quantum mechanics it is common to use the conjugate transpose notation $A^\dagger$ for the adjoint operator, but the equivalence with the complex adjoint matrix only holds for orthonormal bases.

Exercise: Show that in an o.n. basis $Au = \sum_i u'_i e_i$ where $u = \sum_i u_i e_i$ and $u'_i = \sum_j a_{ij} u_j$.

Hermitian operators

An operator A is called **hermitian** if $A = A^*$, so that

$$\langle u \,|\, Av \rangle = \langle A^* u \,|\, v \rangle = \overline{\langle v \,|\, A^* u \rangle} = \langle Au \,|\, v \rangle.$$

If $\mathcal{H}$ is separable and $e_1, e_2, \dots$ a complete orthonormal set, then the matrix elements in this basis, $a_{ij} = \langle e_i \,|\, Ae_j \rangle$, have the hermitian property

$$a_{ij} = \overline{a_{ji}}.$$

In other words, a bounded operator A is hermitian if and only if its matrix with respect to any o.n. basis is hermitian,

$$\mathsf{A} = [a_{ij}] = \overline{\mathsf{A}^T} = \mathsf{A}^\dagger.$$

These operators are sometimes referred to as *self-adjoint*, but in line with modern usage we will use this term for a more general concept defined in Section 13.6.

Let M be a closed subspace of $\mathcal{H}$ then, by Theorem 13.8, any $u \in \mathcal{H}$ has a unique decomposition

$$u = u' + u'' \quad \text{where} \quad u' \in M, \; u'' \in M^\perp.$$

We define the **projection operator** $P_M : \mathcal{H} \to \mathcal{H}$ by $P_M(u) = u'$, which maps every vector of $\mathcal{H}$ onto its orthogonal projection in the subspace M.

Theorem 13.14 *For every subspace M, the projection operator P_M is a bounded hermitian operator and satisfies $P_M^2 = P_M$ (called an* **idempotent operator***). Conversely any idempotent hermitian operator P is a projection operator into some subspace.*

Proof: 1. P_M is hermitian. For any two vectors from $u, v \in \mathcal{H}$

$$\langle u \,|\, P_M v \rangle = \langle u \,|\, v' \rangle = \langle u' + u'' \,|\, v' \rangle = \langle u' \,|\, v' \rangle$$

since $\langle u'' \,|\, v' \rangle = 0$. Similarly,

$$\langle P_M u \,|\, v \rangle = \langle u' \,|\, v \rangle = \langle u' \,|\, v' + v'' \rangle = \langle u' \,|\, v' \rangle.$$

Thus $P_M = P_M^*$.

2. P_M is bounded, for $\|P_M u\|^2 \le \|u\|^2$ since

$$\|u\|^2 = \langle u \,|\, u \rangle = \langle u' + u'' \,|\, u' + u'' \rangle = \langle u' \,|\, u' \rangle + \langle u'' \,|\, u'' \rangle \ge \|u'\|^2.$$

3. P_M is idempotent, for $P_M^2 u = P_M u' = u'$ since $u' \in M$. Hence $P_M^2 = P_M$.

4. Suppose P is hermitian and idempotent, $P^2 = P$. The operator P is bounded and therefore continuous, for by the Cauchy–Schwarz inequality (5.13),

$$\|Pu\|^2 = |\langle Pu \,|\, Pu\rangle| = |\langle u \,|\, P^2 u\rangle| = |\langle u \,|\, Pu\rangle| \le \|u\|\,\|Pu\|.$$

Hence either $\|Pu\| = 0$ or $\|Pu\| \le \|u\|$.

Let $M = \{u \mid u = Pu\}$. This is obviously a vector subspace of $\mathcal{H}$. It is closed by continuity of P, for if $u_n \to u$ and $Pu_n = u_n$, then $Pu_n \to Pu = \lim_{n\to\infty} u_n = u$. Thus M is a subspace of $\mathcal{H}$. For any vector $v \in \mathcal{H}$, set $v' = Pv$ and $v'' = (I - P)v = v - v'$. Then $v = v' + v''$ and $v' \in M$, $v'' \in M^\perp$, for

$$Pv' = P(Pv) = P^2 v = Pv = v',$$

and for all $w \in M$

$$\langle v'' \,|\, w\rangle = \langle (I-P)v \,|\, w\rangle = \langle v \,|\, w\rangle - \langle Pv \,|\, w\rangle = \langle v \,|\, w\rangle - \langle v \,|\, Pw\rangle = \langle v \,|\, w\rangle - \langle v \,|\, w\rangle = 0.$$

■

Unitary operators

An operator $U : \mathcal{H} \to \mathcal{H}$ is called **unitary** if

$$\langle Uu \,|\, Uv\rangle = \langle u \,|\, v\rangle \qquad \text{for all } u, v \in \mathcal{H}.$$

Since this implies $\langle U^* Uu \,|\, v\rangle = \langle u \,|\, v\rangle$, an operator U is unitary if and only if $U^{-1} = U^*$. Every unitary operator is **isometric**, $\|Uu\| = \|u\|$ for all $u \in \mathcal{H}$ – it preserves the distance $d(u, v) = \|u - v\|$ between any two vectors. Conversely, every isometric operator is unitary, for if U is isometric then

$$\langle U(u+v) \,|\, U(u+v)\rangle - i\langle U(u+iv) \,|\, U(u+iv)\rangle = \langle u+v \,|\, u+v\rangle - i\langle u+iv \,|\, u+iv\rangle.$$

Expanding both sides and using $\langle Uu \,|\, Uu\rangle = \langle u \,|\, u\rangle$ and $\langle Uv \,|\, Uv\rangle = \langle v \,|\, v\rangle$, gives

$$2\langle Uu \,|\, Uv\rangle = 2\langle u \,|\, v\rangle.$$

If $\{e_1, e_2, \dots\}$ is an orthonormal basis then so is

$$e'_1 = Ue_1,\ e'_2 = Ue_2, \dots,$$

for

$$\langle e'_i \,|\, e'_j\rangle = \langle Ue_i \,|\, Ue_j\rangle = \langle U^* Ue_i \,|\, e_j\rangle = \langle e_i \,|\, e_j\rangle = \delta_{ij}.$$

Conversely for any pair of complete orthonormal sets $\{e_1, e_2, \dots\}$ and $\{e'_1, e'_2, \dots\}$ the operator defined by $Ue_i = e'_i$ is unitary, for if u is any vector then, by Theorem 13.2,

$$u = \sum_i u_i e_i \quad \text{where} \quad u_i = \langle e_i \,|\, u\rangle.$$

Hence

$$Uu = \sum_i u_i Ue_i = \sum_i u_i e'_i,$$

which gives

$$u_i = \langle e_i \,|\, u\rangle = \langle e'_i \,|\, Uu\rangle.$$

Parseval's identity (13.7) can be applied in the primed basis,

$$\begin{aligned}\langle Uu \,|\, Uv\rangle &= \sum_i \langle Uu \,|\, e'_i\rangle\langle e'_i \,|\, Uv\rangle \\ &= \sum_i \overline{u_i} v_i \\ &= \sum_i \langle u \,|\, e_i\rangle\langle e_i \,|\, v\rangle \\ &= \langle u \,|\, v\rangle,\end{aligned}$$

which shows that U is a unitary operator.

Exercise: Show that if U is a unitary operator then $\|U\| = 1$.

Exercise: Show that the multiplication operator A_α on $L^2(X)$ is unitary iff $|\alpha(x)| = 1$ for all $x \in X$.

Problems

Problem 13.14 The norm $\|\phi\|$ of a bounded linear operator $\phi : \mathcal{H} \to \mathbb{C}$ is defined as the greatest lower bound of all M such that $|\phi(u)| \le M\|u\|$ for all $u \in \mathcal{H}$. If $\phi(u) = \langle v \,|\, u\rangle$ show that $\|\phi\| = \|v\|$. Hence show that the bounded linear functional norm satisfies the parallelogram law

$$\|\phi + \psi\|^2 + \|\phi - \psi\|^2 = 2\|\phi\|^2 + 2\|\psi\|^2.$$

Problem 13.15 If $\{e_n\}$ is a complete o.n. set in a Hilbert space $\mathcal{H}$, and α_n a bounded sequence of scalars, show that there exists a unique bounded operator A such that $Ae_n = \alpha_n e_n$. Find the norm of A.

Problem 13.16 For bounded linear operators A, B on a normed vector space V show that

$$\|\lambda A\| = |\lambda|\,\|A\|, \qquad \|A + B\| \le \|A\| + \|B\|, \qquad \|AB\| \le \|A\|\,\|B\|.$$

Hence show that $\|A\|$ is a genuine norm on the set of bounded linear operators on V.

Problem 13.17 Prove properties (iii)–(v) of Theorem 13.13. Show that $\|A^*\| = \|A\|$.

Problem 13.18 Let A be a bounded operator on a Hilbert space $\mathcal{H}$ with a one-dimensional range.

(a) Show that there exist vectors u, v such that $Ax = \langle v \,|\, x\rangle u$ for all $x \in \mathcal{H}$.
(b) Show that $A^2 = \lambda A$ for some scalar λ, and that $\|A\| = \|u\|\|v\|$.
(c) Prove that A is hermitian, $A^* = A$, if and only if there exists a real number a such that $v = au$.

Problem 13.19 For every bounded operator A on a Hilbert space $\mathcal{H}$ show that the exponential operator

$$\mathrm{e}^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

is well-defined and bounded on $\mathcal{H}$. Show that

(a) $\mathrm{e}^0 = I$.
(b) For all positive integers n, $(\mathrm{e}^A)^n = \mathrm{e}^{nA}$.
(c) e^A is invertible for all bounded operators A (even if A is not invertible) and $\mathrm{e}^{-A} = (\mathrm{e}^A)^{-1}$.
(d) If A and B are commuting operators then $\mathrm{e}^{A+B} = \mathrm{e}^A \mathrm{e}^B$.
(e) If A is hermitian then e^{iA} is unitary.

Problem 13.20 Show that the sum of two projection operators $P_M + P_N$ is a projection operator iff $P_M P_N = 0$. Show that this condition is equivalent to $M \perp N$.

Problem 13.21 Verify that the operator on three-dimensional Hilbert space, having matrix representation in an o.n. basis

$$\begin{pmatrix} \frac{1}{2} & 0 & \frac{i}{2} \\ 0 & 1 & 0 \\ -\frac{i}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

is a projection operator, and find a basis of the subspace it projects onto.

Problem 13.22 Let $\omega = \mathrm{e}^{2\pi i/3}$. Show that $1 + \omega + \omega^2 = 0$.

(a) In Hilbert space of three dimensions let V be the subspace spanned by the vectors $(1, \omega, \omega^2)$ and $(1, \omega^2, \omega)$. Find the vector u_0 in this subspace that is closest to the vector $u = (1, -1, 1)$.
(b) Verify that $u - u_0$ is orthogonal to V.
(c) Find the matrix representing the projection operator P_V into the subspace V.

Problem 13.23 An operator A is called **normal** if it is bounded and commutes with its adjoint, $A^*A = AA^*$. Show that the operator

$$A\psi(x) = c\psi(x) + i\int_a^b K(x, y)\psi(y)\,\mathrm{d}y$$

on $L^2([a, b])$, where c is a real number and $K(x, y) = \overline{K(y, x)}$, is normal.

(a) Show that an operator A is normal if and only if $\|Au\| = \|A^*u\|$ for all vectors $u \in \mathcal{H}$.

(b) Show that if A and B are commuting normal operators, AB and $A + \lambda B$ are normal for all $\lambda \in \mathbb{C}$.

13.5 Spectral theory

Eigenvectors

As in Chapter 4 a complex number α is an **eigenvalue** of a bounded linear operator $A : \mathcal{H} \to \mathcal{H}$ if there exists a non-zero vector $u \in \mathcal{H}$ such that

$$Au = \alpha u.$$

u is called the **eigenvector** of A corresponding to the eigenvalue α.

Theorem 13.15 *All eigenvalues of a hermitian operator A are real, and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof: If $Au = \alpha u$ then

$$\langle u \,|\, Au\rangle = \langle u \,|\, \alpha u\rangle = \alpha \|u\|^2.$$

Since A is hermitian

$$\langle u \,|\, Au\rangle = \langle Au \,|\, u\rangle = \langle \alpha u \,|\, u\rangle = \overline{\alpha}\|u\|^2.$$

For a non-zero vector $\|u\| \neq 0$, we have $\alpha = \overline{\alpha}$; the eigenvalue α is real.

If $Av = \beta v$ then

$$\langle u \,|\, Av\rangle = \langle u \,|\, \beta v\rangle = \beta\langle u \,|\, v\rangle$$

and

$$\langle u \,|\, Av\rangle = \langle Au \,|\, v\rangle = \langle \alpha u \,|\, v\rangle = \overline{\alpha}\langle u \,|\, v\rangle = \alpha\langle u \,|\, v\rangle.$$

If $\beta \neq \alpha$ then $\langle u \,|\, v\rangle = 0$. ■

A hermitian operator is said to be **complete** if its eigenvectors form a complete o.n. set.

Example 13.12 The eigenvalues of a projection operator P are always 0 or 1, for

$$Pu = \alpha u \implies P^2 u = P(\alpha u) = \alpha P u = \alpha^2 u$$

and since P is idempotent,

$$P^2 u = Pu = \alpha u.$$

Hence $\alpha^2 = \alpha$, so that $\alpha = 0$ or 1. If $P = P_M$ then the eigenvectors corresponding to eigenvalue 1 are the vectors belonging to the subspace M, while those having eigenvalue 0 belong to its orthogonal complement $M^\perp$. Combining Theorems 13.8 and 13.2, we see that every projection operator is complete.

Theorem 13.16 *The eigenvalues of a unitary operator U are of the form $\alpha = \mathrm{e}^{ia}$ where a is a real number, and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof: Since U is an isometry, if $Uu = \alpha u$ where $u \neq 0$, then

$$\|u\|^2 = \langle u \,|\, u\rangle = \langle Uu \,|\, Uu\rangle = \langle \alpha u \,|\, \alpha u\rangle = \overline{\alpha}\alpha\|u\|^2.$$

Hence $\overline{\alpha}\alpha = |\alpha|^2 = 1$, and there exists a real a such that $\alpha = \mathrm{e}^{ia}$.

If $Uu = \alpha u$ and $Uv = \beta v$, then

$$\langle u \,|\, Uv\rangle = \beta uv.$$

But $U^*U = I$ implies $u = U^*Uu = \alpha U^*u$, so that

$$U^*u = \alpha^{-1}u = \overline{\alpha}u \quad \text{since} \quad |\alpha|^2 = 1.$$

Therefore

$$\langle u \,|\, Uv\rangle = \langle U^*u \,|\, v\rangle = \langle \overline{\alpha}u \,|\, v\rangle = \alpha\langle u \,|\, v\rangle.$$

Hence $(\alpha - \beta)\langle u \,|\, v\rangle = 0$. If $\alpha \neq \beta$ then u and v are orthogonal, $\langle u \,|\, v\rangle = 0$. ■

Spectrum of a bounded operator

In the case of a finite dimensional space, the set of eigenvalues of an operator is known as its *spectrum*. The spectrum is non-empty (see Chapter 4), and forms the diagonal elements in the Jordan canonical form. In infinite dimensional spaces, however, operators may have no eigenvalues at all.

Example 13.13 In ℓ^2, the right shift operator S has no eigenvalues, for suppose

$$S(x_1, x_2, \dots) = (0, x_1, x_2, \dots) = \lambda(x_1, x_2, \dots).$$

If $\lambda \neq 0$ then $x_1 = 0, x_2 = 0, \dots$, hence λ is not an eigenvalue. But $\lambda = 0$ also implies $x_1 = x_2 = \cdots = 0$, so this operator has no eigenvalues at all.

Exercise: Show that every λ such that $|\lambda| < 1$ is an eigenvalue of the left shift operator $S' = S^*$. Note that the spectrum of S and its adjoint S^* may be unrelated in the infinite dimensional case.

Example 13.14 Let $\alpha(x)$ be a bounded integrable function on a measure space X, and let $A_\alpha : g \mapsto \alpha g$ be the multiplication operator defined in Example 13.9. There is no normalizable function $g \in L^2(X)$ such that $\alpha(x)g(x) = \lambda g(x)$ unless $\alpha(x)$ has the constant value λ on an interval E of non-zero measure. For example, if $\alpha(x) = x$ on $X = [a, b]$, then $f(x)$ is an eigenvector of A_x iff there exists $\lambda \in \mathbb{C}$ such that

$$xf(x) = \lambda f(x),$$

which is only possible through $[a, b]$ if $f(x) = 0$. In quantum mechanics (see Chapter 14) this problem is sometimes overcome by treating the eigenvalue equation as a distributional equation. Then the Dirac delta function $\delta(x - x_0)$ acts as a distributional eigenfunction, with eigenvalue $a < \lambda = x_0 < b$,

$$x\delta(x - x_0) = x_0\delta(x - x_0).$$

Examples such as 13.14 lead us to consider a new definition for the spectrum of an operator. Every operator A has a degeneracy at an eigenvalue λ, in that $A - \lambda I$ is not an invertible operator. For, if $(A - \lambda I)^{-1}$ exists then $Au \neq \lambda u$, for if $Au = \lambda u$ then

$$u = (A - \lambda I)^{-1}(A - \lambda I)u = (A - \lambda I)^{-1}0 = 0.$$

We say a complex number λ is a **regular value** of a bounded operator A on a Hilbert space $\mathcal{H}$ if $A - \lambda I$ is invertible – that is, $(A - \lambda I)^{-1}$ exists and is bounded. The **spectrum** $\Sigma(A)$ of A is defined to be the set of $\lambda \in \mathbb{C}$ that are not regular values of A. If λ is an eigenvalue of A then, as shown above, it is in the spectrum of A but the converse is not true. The eigenvalues are often called the **point spectrum**. The other points of the spectrum are called the **continuous spectrum**. At such points it is conceivable that the inverse exists but is not bounded. More commonly, the inverse only exists on a dense domain of $\mathcal{H}$ and is unbounded on that domain. We will leave discussion of this to Section 13.6.

Example 13.15 If $\alpha(x) = x$ then the multiplication operator A_α on $L^2([0, 1])$ has spectrum consisting of all real numbers λ such that $0 \leq \lambda \leq 1$. If $\lambda > 1$ or $\lambda < 0$ or has non-zero imaginary part then the function $\beta = x - \lambda$ is clearly invertible and bounded on the interval $[0, 1]$. Hence all these are regular values of the operator A_x. The real values $0 \le \lambda \le 1$ form the spectrum of A_x. From Example 13.14 none of these numbers are eigenvalues, but they do lie in the spectrum of A_x since the function β is not invertible. The operator A_β is then defined, but unbounded, on the dense set $[0, 1] - \{\lambda\}$.

Theorem 13.17 *Let A be a bounded operator on a Hilbert space $\mathcal{H}$.*

(i) Every complex number $\lambda \in \Sigma(A)$ has magnitude $|\lambda| \le \|A\|$.
(ii) The set of regular values of A is an open subset of $\mathbb{C}$.
(iii) The spectrum of A is a compact subset of $\mathbb{C}$.

Proof: (i) Let $|\lambda| > \|A\|$. The operator A/λ then has norm < 1 and by Theorem 13.12 the operator $I - A/\lambda$ is invertible and

$$(A - \lambda I)^{-1} = -\lambda^{-1}\left(I - \frac{A}{\lambda}\right)^{-1} = -\lambda^{-1}\sum_{n=0}^{\infty}\left(\frac{A}{\lambda}\right)^n.$$

Hence λ is a regular value. Spectral values must therefore have $|\lambda| \le \|A\|$.

(ii) If λ_0 is a regular value, then for any other complex number λ

$$\begin{aligned} I - (A - \lambda_0 I)^{-1}(A - \lambda I) &= (A - \lambda_0 I)^{-1}\big((A - \lambda_0 I) - (A - \lambda I)\big) \\ &= (A - \lambda_0 I)^{-1}(\lambda - \lambda_0). \end{aligned}$$

Hence

$$\|I - (A - \lambda_0 I)^{-1}(A - \lambda I)\| = |\lambda - \lambda_0|\,\|(A - \lambda_0 I)^{-1}\| < 1$$

if

$$|\lambda - \lambda_0| < \frac{1}{\|(A - \lambda_0 I)^{-1}\|}.$$

By Theorem 13.12, for λ in a small enough neighbourhood of λ the operator $I - \big(I - (A - \lambda_0 I)^{-1}(A - \lambda)\big) = (A - \lambda_0 I)^{-1}(A - \lambda I)$ is invertible. If B is its inverse, then

$$B(A - \lambda_0 I)^{-1}(A - \lambda) = I$$

and $A - \lambda I$ is invertible with inverse $B(A - \lambda_0 I)^{-1}$. Hence the regular values form an open set.

(iii) The spectrum $\Sigma(A)$ is a closed set since it is the complement of an open set (the regular values). By part (i), it is a subset of a bounded set $|\lambda| \le \|A\|$, and is therefore a compact set. ■

Spectral theory of hermitian operators

Of greatest interest is the spectral theory of hermitian operators. This theory can become quite difficult, and we will only sketch some of the proofs.

Theorem 13.18 *The spectrum $\Sigma(A)$ of a hermitian operator A consists entirely of real numbers.*

Proof: Suppose $\lambda = a + ib$ is a complex number with $b \neq 0$. Then $\|(A - \lambda I)u\|^2 = \|(A - aI)u\|^2 + b^2\|u\|^2$, and

$$\|u\| \leq \frac{1}{|b|}\|(A - \lambda I)u\|. \tag{13.12}$$

The operator $A - \lambda I$ is therefore one-to-one, for if $(A - \lambda I)u = 0$ then $u = 0$.

The set $V = \{(A - \lambda I)u \mid u \in \mathcal{H}\}$ is a subspace of $\mathcal{H}$. To show closure (the vector subspace property is trivial), let $v_n = (A - \lambda I)u_n \to v$ be a convergent sequence of vectors in V. From the fact that it is a Cauchy sequence and the inequality (13.12), it follows that u_n is also a Cauchy sequence, having limit u. By continuity of the operator $A - \lambda I$, it follows that V is closed, for

$$(A - \lambda I)u = \lim_{n\to\infty}(A - \lambda I)u_n = \lim_{n\to\infty} v_n = v.$$

Finally, $V = \mathcal{H}$, for if $w \in V^\perp$, then $\langle (A - \lambda I)u \mid w\rangle = \langle u \mid (A - \overline{\lambda} I)w\rangle = 0$ for all $u \in \mathcal{H}$. Setting $u = (A - \overline{\lambda} I)w$ gives $(A - \overline{\lambda} I)w = 0$. Since $A - \overline{\lambda} I$ is one-to-one, $w = 0$. Hence $V^\perp = \{0\}$, the subspace $V = \mathcal{H}$ and every vector $u \in \mathcal{H}$ can be written in the form $u = (A - \lambda I)v$. Thus $A - \lambda I$ is invertible, and the inequality (13.12) can be used to show it is bounded. ∎

The full spectral theory of a hermitian operator involves reconstructing the operator from its spectrum. In the finite dimensional case, the spectrum consists entirely of eigenvalues, making up the point spectrum. From Theorem 13.15 the eigenvalues may be written as a non-empty ordered set of real numbers $\lambda_1 < \lambda_2 < \cdots < \lambda_k$. For each eigenvalue λ_i there corresponds an eigenspace M_i of eigenvectors, and different spaces are orthogonal to each other. A standard inductive argument can be used to show that every hermitian operator on a finite dimensional Hilbert space is complete, so the eigenspaces span the entire Hilbert space. In terms of projection operators into these eigenspaces $P_i = P_{M_i}$, these statements can be summarized as

$$A = \lambda_1 P_1 + \lambda_2 P_2 + \cdots + \lambda_k P_k$$

where

$$P_1 + P_2 + \cdots + P_k = I, \qquad P_i P_j = P_j P_i = \delta_{ij} P_i.$$

Essentially, this is the familiar statement that a hermitian matrix can be 'diagonalized' with its eigenvalues along the diagonal. If we write, for any two projection operators, $P_M \leq P_N$ iff $M \subseteq N$, we can replace the operators P_i with an increasing family of projection operators $E_i = P_1 + P_2 + \cdots + P_i$. These are projection operators since they are clearly hermitian and idempotent, $(E_i)^2 = E_i$, and project into an increasing family of subspaces, $V_i = L(M_1 \cup M_2 \cup \cdots \cup M_i)$, having the property $V_i \subset V_j$ if $i < j$. Since $P_i = E_i - E_{i-1}$, where $E_0 = 0$, we can write the spectral theorem in the form

$$A = \sum_{i=1}^{n} \lambda_i (E_i - E_{i-1}).$$

For infinite dimensional Hilbert spaces, the situation is considerably more complicated, but the projection operator language can again be used to effect. The full spectral theorem in arbitrary dimensions is as follows:

Theorem 13.19 *Let A be a hermitian operator on a Hilbert space $\mathcal{H}$, with spectrum $\Sigma(A)$. By Theorem 13.17 this is a closed bounded subset of $\mathbb{R}$. There exists an increasing family of projection operators E_λ ($\lambda \in \mathbb{R}$), with $E_\lambda \le P_{\lambda'}$ for $\lambda \le \lambda'$, such that*

$$E_\lambda = 0 \quad \textit{for} \quad \lambda < \inf(\Sigma(A)), \qquad E_\lambda = I \quad \textit{for} \quad \lambda > \sup(\Sigma(A))$$

and

$$A = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}E_\lambda.$$

The integral in this theorem is defined in the **Lebesgue–Stieltjes** sense. Essentially it means that if $f(x)$ is a measurable function, and $g(x)$ is of the form

$$g(x) = c + \int_0^x h(x)\, \mathrm{d}x$$

for some complex constant c and integrable function $h(x)$, then

$$\int_a^b f(x)\, \mathrm{d}(g(x)) = \int_a^b f(x)h(x)\, \mathrm{d}x.$$

A function g of this form is said to be **absolutely continuous**; the function h is uniquely defined almost everywhere by g and we may write it as a kind of derivative of g, $h(x) = g'(x)$. For the finite dimensional case this theorem reduces to the statement above, on setting E_λ to have discrete jumps by P_i at each of the eigenvalues λ_i. The proof of this result is not easy. The interested reader is referred to [3, 6] for details.

Problems

Problem 13.24 Show that a non-zero vector u is an eigenvector of an operator A if and only if $|\langle u \mid Au\rangle| = \|Au\|\|u\|$.

Problem 13.25 For any projection operator P_M show that every value $\lambda \ne 0, 1$ is a regular value, by showing that $(P_M - \lambda I)$ has a bounded inverse.

Problem 13.26 Show that every complex number λ in the spectrum of a unitary operator has $|\lambda| = 1$.

Problem 13.27 Prove that every hermitian operator A on a finite dimensional Hilbert space can be written as

$$A = \sum_{i=1}^{k} \lambda_i P_i \quad \text{where} \quad \sum_{i=1}^{k} P_i = I, \quad P_i P_j = P_j P_i = \delta_{ij} P_i.$$

Problem 13.28 For any pair of hermitian operators A and B on a Hilbert space $\mathcal{H}$, define $A \leq B$ iff $\langle u \mid Au\rangle \leq \langle u \mid Bu\rangle$ for all $u \in \mathcal{H}$. Show that this is a partial order on the set of hermitian operators – pay particular attention to the symmetry property, $A \leq B$ and $B \leq A$ implies $A = B$.

(a) For multiplication operators on $L^2(X)$ show that $A_\alpha \leq A_\beta$ iff $\alpha(x) \leq \beta(x)$ a.e. on X.
(b) For projection operators show that the definition given here reduces to that given in the text, $P_M \leq P_N$ iff $M \subseteq N$.

13.6 Unbounded operators

A linear operator A on a Hilbert space $\mathcal{H}$ is **unbounded** if for any $M > 0$ there exists a vector u such that $\|Au\| \geq M\|u\|$. Very few interesting examples of unbounded operators are defined on all of $\mathcal{H}$ – for self-adjoint operators, there are none at all. It is therefore usual to consider an unbounded operator A as not being necessarily defined over all of $\mathcal{H}$ but only on some vector subspace $D_A \subseteq \mathcal{H}$ called the **domain** of A. Its **range** is defined as the set of vectors that are mapped onto, $R_A = A(D_A)$. In general we will refer to a pair (A, D_A), where D_A is a vector subspace of $\mathcal{H}$ and $A : D_A \to R_A \subseteq \mathcal{H}$ is a linear map, as being an **operator in** $\mathcal{H}$. Often we will simply refer to the operator A when the domain D_A is understood.

We say the domain D_A is a **dense** subspace of $\mathcal{H}$ if for every vector $u \in \mathcal{H}$ and any $\epsilon > 0$ there exists a vector $v \in D_A$ such that $\|u - v\| < \epsilon$. The operator A is then said to be **densely defined**.

We say A is an **extension of** B, written $B \subseteq A$, if $D_B \subseteq D_A$ and $A\big|_{D_B} = B$. Two operators (A, D_A) and (B, D_B) in $\mathcal{H}$ are called **equal** if and only if they are extensions of each other – their domains are equal, $D_A = D_B$ and $Au = Bu$ for all $u \in D_A$.

For any two operators in $\mathcal{H}$ we must be careful about simple operations such as addition $A + B$ and multiplication AB. The former only exists on the domain $D_{A+B} = D_A \cap D_B$, while the latter only exists on the set $B^{-1}(R_B \cap D_A)$. Thus operators in $\mathcal{H}$ do not form a vector space or algebra in any natural sense.

Example 13.16 In $\mathcal{H} = \ell^2$ let $A : \mathcal{H} \to \mathcal{H}$ be the operator defined by

$$(Ax)_n = \frac{1}{n} x_n.$$

This operator is bounded, hermitian and has domain $D_A = \mathcal{H}$ since

$$\sum_{n=1}^{\infty} |x_n|^2 < \infty \Longrightarrow \sum_{n=1}^{\infty} \left|\frac{x_n}{n}\right|^2 < \infty.$$

The range of this operator is

$$R_A = \left\{ y \;\Big|\; \sum_{n=1}^{\infty} n^2 |y_n|^2 < \infty \right\},$$

which is dense in ℓ^2 – since every $x \in \ell^2$ can be approximated arbitrarily closely by, for example, a finite sum $\sum_{n=1}^{N} x_n e_n$ where e_n are the standard basis vectors having components

$(e_n)_m = \delta_{nm}$. The inverse operator A^{-1}, defined on the dense domain $D_{A^{-1}} = R_A$, is unbounded since

$$\|A^{-1}e_n\| = \|ne_n\| = n \to \infty.$$

Example 13.17 In the Hilbert space $L^2(\mathbb{R})$ of equivalence classes of square integrable functions (see Example 13.4), set D to be the vector subspace of elements $\widetilde{\varphi}$ having a representative φ from the C^∞ functions on $\mathbb{R}$ of compact support. This is essentially the space of test functions $\mathcal{D}^\infty(\mathbb{R})$ defined in Chapter 12. An argument similar to that outlined in Example 13.5 shows that D is a dense subspace of $L^2(\mathbb{R})$. We define the *position operator* $Q : D \to D \subset L^2(\mathbb{R})$ by $Q\widetilde{\varphi} = \widetilde{x\varphi}$. We may write this more informally as

$$(Q\varphi)(x) = x\varphi(x).$$

Similarly the *momentum operator* $P : D \to D$ is defined by

$$P\varphi(x) = -i\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x).$$

Both these operators are evidently linear on their domains.

Exercise: Show that the position and momentum operators in $L^2(\mathbb{R})$ are unbounded.

If A is a bounded operator defined on a dense domain D_A, it has a unique extension to all of $\mathcal{H}$ (see Problem 13.30). We may always assume then that a bounded operator is defined on all of $\mathcal{H}$, and when we refer to a densely defined operator whose domain is a proper subspace of $\mathcal{H}$ we implicitly assume it to be an unbounded operator.

Self-adjoint and symmetric operators

Lemma 13.20 *If D_A is a dense domain and u a vector in $\mathcal{H}$ such that $\langle u \,|\, v\rangle = 0$ for all $v \in D_A$, then $u = 0$.*

Proof: Let w be any vector in $\mathcal{H}$ and $\epsilon > 0$. Since D_A is dense there exists a vector $v \in D_A$ such that $\|w - v\| < \epsilon$. By the Cauchy–Schwarz inequality

$$|\langle u \,|\, w\rangle| = |\langle u \,|\, w - v\rangle| \le \|u\|\|w - v\| < \epsilon\|u\|.$$

Since ϵ is an arbitrary positive number, $\langle u \,|\, w\rangle = 0$ for all $w \in \mathcal{H}$; hence $u = 0$. ■

If (A, D_A) is an operator in $\mathcal{H}$ with dense domain D_A, then let D_{A^*} be defined by

$$u \in D_{A^*} \iff \exists u^* \text{such that } \langle u \,|\, Av\rangle = \langle u^* \,|\, v\rangle, \quad \forall v \in D_A.$$

If $u \in D_{A^*}$ we set $A^*u = u^*$. This is uniquely defined, for if $\langle u_1^* - u_2^* \,|\, v\rangle = 0$ for all $v \in D_A$ then $u_1^* = u_2^*$ by Lemma 13.20. The operator (A^*, D_{A^*}) is called the **adjoint of** (A, D_A).

We say a densely defined operator (A, D_A) in $\mathcal{H}$ is **closed** if for every sequence $u_n \in D_A$ such that $u_n \to u$ and $Au_n \to v$ it follows that $u \in D_A$ and $Au = v$. Another way of expressing this is to say that an operator is closed if and only if its graph $G_A = \{(x, Ax) \,|\, x \in D_A\}$ is a closed subset of the product set $\mathcal{H} \times \mathcal{H}$. The notion of closedness is similar to continuity, but differs in that we must *assert* the limit $Au_n \to v$, while for continuity it is *deduced*. Clearly every continuous operator is closed, but the converse does not hold in general.

Theorem 13.21 *If A is a densely defined operator then its adjoint A^* is closed.*

Proof: Let y_n be any sequence of vectors in D_{A^*} such that $y_n \to y$ and $A^* y_n \to z$. Then for all $x \in D_A$

$$\langle y \mid Ax \rangle = \lim_{n\to\infty} \langle y_n \mid Ax \rangle = \lim_{n\to\infty} \langle A^* y_n \mid x \rangle = \langle z \mid x \rangle.$$

Since D_A is a dense domain, it follows from Lemma 13.20 that $y \in D_{A^*}$ and $A^* y = z$. ■

Example 13.18 Let $\mathcal{H}$ be a separable Hilbert space with complete orthonormal basis e_n ($n = 0, 1, 2, \dots$). Let the operators a and a^* be defined by

$$a\, e_n = \sqrt{n} e_{n-1}, \qquad a^*\, e_n = \sqrt{n+1} e_{n+1}.$$

The effect on a typical vector $x = \sum_{n=0}^{\infty} x_n e_n$, where $x_n = \langle x \mid e_n \rangle$, is

$$a\,x = \sum_{n=0}^{\infty} x_{n+1} \sqrt{n+1} e_n, \qquad a^*\,x = \sum_{n=1}^{\infty} x_{n-1} \sqrt{n} e_n.$$

The operator a^* is the adjoint of a since

$$\langle a^* y \mid x \rangle = \langle y \mid ax \rangle = \sum_{n=1}^{\infty} \overline{y_n} \sqrt{n+1} x_{n+1}$$

and both operators have domain of definition

$$D = D_a = D_{a*} = \Big\{ y \;\Big|\; \sum_{n=1} |y_n|^2 n < \infty \Big\},$$

which is dense in $\mathcal{H}$ (see Example 13.16). In physics, $\mathcal{H}$ is the symmetric *Fock space*, in which e_n represents n identical (bosonic) particles in a given state, and a^* and a are interpreted as *creation* and *annihilation operators*, respectively.

Exercise: Show that $N = a^* a$ is the particle number operator, $N e_n = n e_n$, and the commutator is $[a, a^*] = aa^* - a^* a = I$. What are the domains of validity of these equations?

Theorem 13.22 *If (A, D_A) and (B, D_B) are densely defined operators in $\mathcal{H}$ then $A \subseteq B \implies B^* \subseteq A^*$.*

Proof: If $A \subseteq B$ then for any vectors $u \in D_A$ and $v \in D_{B^*}$

$$\langle v \mid Au \rangle = \langle v \mid Bu \rangle = \langle B^* v \mid u \rangle.$$

Hence $v \in D_{A^*}$, so that $D_{B^*} \subseteq D_{A^*}$ and

$$\langle v \mid Au \rangle = \langle A^* v \mid u \rangle = \langle B^* v \mid u \rangle.$$

By Lemma 13.20 $A^* v = B^* v$, hence $B^* \subseteq A^*$. ■

An operator (A, D_A) on a dense domain is said to be **self-adjoint** if $A = A^*$. This means that not only is $Au = A^*u$ wherever both sides are defined, but also that the domains are equal, $D_A = D_{A^*}$. By Theorem 13.21 every self-adjoint operator is closed. This is not the only definition that generalizes the concept of a hermitian operator to unbounded operators. The following related definition is also useful. A densely defined operator (A, D_A) in $\mathcal{H}$ is called a **symmetric operator** if $\langle Au \,|\, v\rangle = \langle u \,|\, Av\rangle$ for all $u, v \in D_A$.

Theorem 13.23 *An operator (A, D_A) on a dense domain in $\mathcal{H}$ is symmetric if and only if A^* is an extension of A, $A \subseteq A^*$.*

Proof: If $A \subseteq A^*$ then for all $u, v \in D_A \subseteq D_{A^*}$

$$\langle u \,|\, Av\rangle = \langle A^*u \,|\, v\rangle.$$

Furthermore, since $A^*u = Au$ for all $u \in D_A$, we have the symmetry condition $\langle u \,|\, Av\rangle = \langle Au \,|\, v\rangle$.

Conversely, if A is symmetric then

$$\langle u \,|\, Av\rangle = \langle Au \,|\, v\rangle \qquad \text{for all } u, v \in D_A.$$

On the other hand, the definition of adjoint gives

$$\langle u \,|\, Av\rangle = \langle A^*u \,|\, v\rangle \qquad \text{for all } u \in D_{A^*},\ v \in D_A.$$

Hence if $u \in D_A$ then $u \in D_{A^*}$ and $Au = A^*u$, which two conditions are equivalent to $A \subseteq A^*$. ■

From this theorem it is immediate that every self-adjoint operator is symmetric, since $A = A^* \Longrightarrow A \subseteq A^*$.

Exercise: Show that the operators A and A^{-1} of Example 13.16 are both self-adjoint.

Example 13.19 In Example 13.17 we defined the position operator (Q, D) having domain D, the space of C^∞ functions of compact support on $\mathbb{R}$. This operator is symmetric in $L^2(\mathbb{R})$, since

$$\langle \varphi \,|\, Q\psi\rangle = \int_{-\infty}^{\infty} \overline{\varphi(x)} x\,\psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \overline{x\varphi(x)}\psi(x)\,\mathrm{d}x = \langle Q\varphi \,|\, \psi\rangle$$

for all functions $\varphi, \psi \in D$. However it is not self-adjoint, since there are many functions $\varphi \notin D$ for which there exists a function φ^* such that $\langle \varphi \,|\, Q\psi\rangle = \langle \varphi^* \,|\, \psi\rangle$ for all $\psi \in D$. For example, the function

$$\varphi(x) = \begin{cases} 1 & \text{for } -1 \le x \le 1 \\ 0 & \text{for } |x| > 1 \end{cases}$$

is not in D since it is not C^∞, yet

$$\langle \varphi \,|\, Q\psi\rangle = \langle \varphi^* \,|\, \psi\rangle, \quad \forall\psi \in D \quad \text{where} \quad \varphi^*(x) = x\varphi(x).$$

Similarly, the function $\varphi = 1/(1 + x^2)$ does not have compact support, yet satisfies the same equation. Thus the domain D_{Q^*} of the adjoint operator Q^* is larger than the domain D, and (Q, D) is not self-adjoint.

To rectify the situation, let D_Q be the subspace of $L^2(\mathbb{R})$ of functions φ such that $x\varphi \in L^2(\mathbb{R})$,

$$\int_{-\infty}^{\infty} |x\varphi(x)|^2 \, dx < \infty.$$

Functions φ and φ' are always to be identified, of course, if they are equal almost everywhere. The operator (Q, D_Q) is symmetric since

$$\langle \varphi \,|\, Q\psi \rangle = \int_{-\infty}^{\infty} \overline{\varphi(x)} x \psi(x) \, dx = \langle Q\varphi \,|\, \psi \rangle$$

for all $\varphi, \psi \in D_Q$. The domain D_Q is dense in $L^2(\mathbb{R})$, for if φ is any square integrable function then the sequence of functions

$$\varphi_n(x) = \begin{cases} \varphi(x) & \text{for } -n \le x \le n \\ 0 & \text{for } |x| > n \end{cases}$$

all belong to D_Q and $\varphi_n \to \varphi$ as $n \to \infty$ since

$$\|\varphi - \varphi_n\|^2 = \int_{-\infty}^{-n} |\varphi(x)|^2 \, dx + \int_{n}^{\infty} |\varphi(x)|^2 \, dx \to 0.$$

By Theorem 13.23, Q^* is an extension of Q since the operator (Q, D_Q) is symmetric. It only remains to show that $D_{Q^*} \subseteq D_Q$. The domain D_{Q^*} is the set of functions $\varphi \in L^2(\mathbb{R})$ such that there exists a function φ^* such that

$$\langle \varphi \,|\, Q\psi \rangle = \langle \varphi^* \,|\, \psi \rangle, \quad \forall \psi \in D_Q.$$

The function φ^* has the property

$$\int_{-\infty}^{\infty} \big(\overline{x\varphi(x)} - \overline{\varphi^*}\big)\psi(x) \, dx = 0, \quad \forall \psi \in D_Q.$$

Since D_Q is a dense domain this is only possible if $\varphi^*(x) = x\varphi(x)$ a.e. Since $\varphi^* \in L^2(\mathbb{R})$ it must be true that $x\varphi(x) \in L^2(\mathbb{R})$, whence $\varphi(x) \in D_Q$. This proves that $D_{Q^*} \subseteq D_Q$. Hence $D_{Q^*} = D_Q$, and since $\varphi^*(x) = x\varphi(x)$ a.e., we have $\varphi^* = Q\varphi$. The position operator is therefore self-adjoint, $Q = Q^*$.

Example 13.20 The momentum operator defined in Example 13.17 on the domain D of differentiable functions of compact support is symmetric, for

$$\begin{aligned} \langle \varphi \,|\, P\psi \rangle &= \int_{-\infty}^{\infty} -i\overline{\varphi(x)} \frac{d\psi}{dx} \, dx \\ &= \big[-i\overline{\varphi(x)}\psi(x)\big]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} i \frac{d\overline{\varphi(x)}}{dx} \psi(x) \, dx \\ &= \int_{-\infty}^{\infty} \overline{i \frac{d\varphi(x)}{dx}} \psi(x) \, dx \\ &= \langle P\varphi \,|\, \psi \rangle \end{aligned}$$

for all $\varphi, \psi \in D$. Again, it is not hard to find functions φ outside D that satisfy this relation for all ψ, so this operator is not self-adjoint. Extending the domain so that the momentum operator becomes self-adjoint is rather trickier than for the position operator. We only give the result; details may be found in [3, 7]. Recall from the discussion following Theorem 13.19 that a function $\varphi : \mathbb{R} \to \mathbb{C}$ is said to be *absolutely continuous* if there exists a measurable function ρ on $\mathbb{R}$ such that

$$\varphi(x) = c + \int_0^x \rho(x)\,\mathrm{d}x.$$

We may then set $D\varphi = \varphi' = \rho$. When ρ is a continuous function, $\varphi(x)$ is differentiable and $D\varphi = \mathrm{d}\varphi(x)/\mathrm{d}x$. Let D_P consist of those absolutely continuous functions such that φ and $D\varphi$ are square integrable. It may be shown that D_P is a dense vector subspace of $L^2(\mathbb{R})$ and that the operator (P, D_P) where $P\varphi = -iD\varphi$ is a self-adjoint extension of the momentum operator P defined in Example 13.17.

Spectral theory of unbounded operators

As for hermitian operators, the eigenvalues of a self-adjoint operator (A, D_A) are real and eigenvectors corresponding to different eigenvalues are orthogonal. If $Au = \lambda u$, then λ is real since

$$\lambda = \frac{\langle u \,|\, Au\rangle}{\|u\|^2} = \frac{\langle Au \,|\, u\rangle}{\|u\|^2} = \frac{\overline{\langle u \,|\, Au\rangle}}{\|u\|^2} = \overline{\lambda}.$$

If $Au = \lambda u$ and $Av = \mu v$, then

$$0 = \langle Au \,|\, v\rangle - \langle u \,|\, Av\rangle = (\lambda - \mu)\langle u \,|\, v\rangle$$

whence $\langle u \,|\, v\rangle = 0$ whenever $\lambda \neq \mu$.

For each complex number define Δ_λ to be the domain of the *resolvent operator* $(A - \lambda I)^{-1}$,

$$\Delta_\lambda = D_{(A-\lambda I)^{-1}} = R_{A-\lambda I}.$$

The operator $(A - \lambda I)^{-1}$ is well-defined with domain Δ_λ provided λ is not an eigenvalue. For, if λ is not an eigenvalue then $\ker(A - \lambda I) = \{0\}$ and for every $y \in R_{A-\lambda I}$ there exists a unique $x \in D_A$ such that $y = (A - \lambda I)x$.

Exercise: Show that for all complex numbers λ, the operator $A - \lambda I$ is closed.

As for bounded operators a complex number λ is said to be a **regular value** for A if $\Delta_\lambda = \mathcal{H}$. The resolvent operator $(A - \lambda I)^{-1}$ can then be shown to be a bounded (continuous) operator. The set of complex numbers that are not regular are again known as the **spectrum** of A.

Theorem 13.24 *λ is an eigenvalue of a self-adjoint operator (A, D_A) if and only if the resolvent set Δ_λ is not dense in $\mathcal{H}$.*

Proof: If $Ax = \lambda x$ where $x \neq 0$, then

$$0 = \langle (A - \lambda I)x \,|\, u\rangle = \langle x \,|\, (A - \lambda I)u\rangle$$

for all $u \in D_A$. Hence $\langle x \,|\, v\rangle = 0$ for all $v \in \Delta_\lambda = R_{A-\lambda I}$. If Δ_λ is dense in $\mathcal{H}$ then, by Lemma 13.20, this can only be true for $x = 0$, contrary to assumption.

Conversely if Δ_λ is not dense then by Theorem 13.8 there exists a non-zero vector $x \in \big(\overline{\Delta_\lambda}\big)^\perp$. This vector has the property

$$0 = \langle x \,|\, (A - \lambda I)u\rangle = \langle (A - \lambda I)x \,|\, u\rangle$$

for all $u \in D_A$. Since D_A is a dense domain, x must be an eigenvector, $Ax = \lambda x$. ■

It is natural to classify the spectrum into two parts – the **point spectrum** consisting of eigenvalues, where the resolvent set Δ_λ is not dense in $\mathcal{H}$, and the **continuous spectrum** consisting of those values λ for which Δ_λ is not closed. Note that these are not mutually exclusive; it is possible to have eigenvalues λ for which the resolvent set is neither closed nor dense. The entire spectrum of a self-adjoint operator can, however, be shown to consist of real numbers. The spectral theorem 13.19 generalizes for self-adjoint operators as follows:

Theorem 13.25 *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$. There exists an increasing family of projection operators E_λ $(\lambda \in \mathbb{R})$, with $E_\lambda \le P_{\lambda'}$ for $\lambda \le \lambda'$, such that*

$$E_{-\infty} = 0 \quad \textit{and} \quad E_\infty = I$$

such that

$$A = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}E_\lambda,$$

where the integral is interpreted as the Lebesgue–Stieltjes integral

$$\langle u \,|\, Au\rangle = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}\langle u \,|\, E_\lambda u\rangle$$

valid for all $u \in D_A$

The proof is difficult and can be found in [7]. Its main use is that it permits us to define functions $f(A)$ of a self-adjoint operator A for a very wide class of functions. For example if $f : \mathbb{R} \to \mathbb{C}$ is a Lebesgue integrable function then we set

$$f(A) = \int_{-\infty}^{\infty} f(\lambda) \, \mathrm{d}E_\lambda.$$

This is shorthand for

$$\langle u \,|\, f(A)v\rangle = \int_{-\infty}^{\infty} f(\lambda) \, \mathrm{d}\langle u \,|\, E_\lambda v\rangle$$

for arbitrary vectors $u \in \mathcal{H}$, $v \in D_A$. One of the most useful of such functions is $f = \mathrm{e}^{ix}$, giving rise to a unitary transformation

$$U = \mathrm{e}^{iA} = \int_{-\infty}^{\infty} \mathrm{e}^{i\lambda} \, \mathrm{d}E_\lambda.$$

This relation between unitary and self-adjoint operators has its main expression in Stone's theorem, which generalizes the result for finite dimensional vector spaces, discussed in Example 6.12 and Problem 6.12.

Theorem 13.26 *Every one-parameter unitary group of transformations U_t on a Hilbert space, such that $U_t U_s = U_{t+s}$, can be expressed in the form*

$$U_t = \mathrm{e}^{iAt} = \int_{-\infty}^{\infty} \mathrm{e}^{i\lambda t}\, \mathrm{d}E_\lambda.$$

Problems

Problem 13.29 For unbounded operators, show that

(a) $(AB)C = A(BC)$.
(b) $(A + B)C = AC + BC$.
(c) $AB + AC \subseteq A(B + C)$. Give an example where $A(B + C) \neq AB + AC$.

Problem 13.30 Show that a densely defined bounded operator A in $\mathcal{H}$ has a unique extension to an operator $\hat{A}$ defined on all of $\mathcal{H}$. Show that $\|\hat{A}\| = \|A\|$.

Problem 13.31 If A is self-adjoint and B a bounded operator, show that $B^* AB$ is self-adjoint.

Problem 13.32 Show that if (A, D_A) and (B, D_B) are operators on dense domains in $\mathcal{H}$ then $B^* A^* \subseteq (AB)^*$.

Problem 13.33 For unbounded operators, show that $A^* + B^* \subseteq (A + B)^*$.

Problem 13.34 If (A, D_A) is a densely defined operator and D_{A^*} is dense in $\mathcal{H}$, show that $A \subseteq A^{**}$.

Problem 13.35 If A is a symmetric operator, show that A^* is symmetric if and only if it is self-adjoint, $A^* = A^{**}$.

Problem 13.36 If $A_1, A_2, \dots, A_n$ are operators on a dense domain such that

$$\sum_{i=1}^{n} A_i^* A_i = 0,$$

show that $A_1 = A_2 = \cdots = A_n = 0$.

Problem 13.37 If A is a self-adjoint operator show that

$$\|(A + iI)u\|^2 = \|Au\|^2 + \|u\|^2$$

and that the operator $A + iI$ is invertible. Show that the operator $U = (A - iI)(A + iI)^{-1}$ is unitary (called the *Cayley transform* of A).

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