7 Hilbert Spaces

The basic concepts of finite-dimensional vector spaces introduced in Chap. 2 can readily be generalized to infinite dimensions. The definition of a vector space and concepts of linear combination, linear independence, subspace, span, and so forth all carry over to infinite dimensions. However, one thing is crucially different in the new situation, and this difference makes the study of infinite-dimensional vector spaces both richer and more nontrivial: In a finite-dimensional vector space we dealt with finite sums; in infinite dimensions we encounter infinite sums. Thus, we have to investigate the convergence of such sums.

7.1 The Question of Convergence

The intuitive notion of convergence acquired in calculus makes use of the idea of closeness. This, in turn, requires the notion of distance.[1] We considered such a notion in Chap. 2 in the context of a norm, and saw that the inner product had an associated norm. However, it is possible to introduce a norm on a vector space without an inner product.

One such norm, applicable to $\mathbb{C}^n$ and $\mathbb{R}^n$, was

$$\|a\|_p \equiv \left(\sum_{i=1}^{n} |\alpha_i|^p\right)^{1/p},$$

where p is an integer. The "natural" norm, i.e., that induced on $\mathbb{C}^n$ (or $\mathbb{R}^n$) by the usual inner product, corresponds to $p = 2$. The distance between two points depends on the particular norm used. For example, consider the "point" (or vector) $|b\rangle = (0.1, 0.1, \dots, 0.1)$ in a 1000-dimensional space ($n = 1000$). One can easily check that the distance of this vector from the origin varies considerably with p: $\|b\|_1 = 100$, $\|b\|_2 = 3.16$, $\|b\|_{10} = 0.2$. This variation may give the impression that there is no such thing as "closeness", and it all depends on how one defines the norm. This is not true,

Closeness is a relative concept!

[1]It is possible to introduce the idea of closeness abstractly, without resort to the notion of distance, as is done in topology. However, distance, as applied in vector spaces, is as abstract as we want to get.

S. Hassani, *Mathematical Physics*, DOI 10.1007/978-3-319-01195-0_7,

because closeness is a relative concept: One always *compares* distances. A norm with large p shrinks *all* distances of a space, and a norm with small p stretches them. Thus, although it is impossible (and meaningless) to say that "$|a\rangle$ is close to $|b\rangle$" because of the dependence of distance on p, one can always say "$|a\rangle$ is closer to $|b\rangle$ than $|c\rangle$ is to $|d\rangle$", regardless of the value of p.

Now that we have a way of telling whether vectors are close together or far apart, we can talk about limits and the convergence of sequences of vectors. Let us begin by recalling the definition of a Cauchy sequence (see Definition 1.3.4):

Cauchy sequence defined

Definition 7.1.1 An infinite sequence of vectors $\{|a_i\rangle\}_{i=1}^{\infty}$ in a normed linear space $\mathcal{V}$ is called a **Cauchy sequence** if $\lim_{\substack{i\to\infty\\ j\to\infty}} \|a_i - a_j\| = 0$.

A convergent sequence is necessarily Cauchy. This can be shown using the triangle inequality (see Problem 7.2). However, there may be Cauchy sequences in a given vector space that do not converge to any vector in that space (see the example below). Such a convergence requires additional properties of a vector space summarized in the following definition.

complete vector space defined

Definition 7.1.2 A **complete vector space** $\mathcal{V}$ is a normed linear space for which every Cauchy sequence of vectors in $\mathcal{V}$ has a limit vector in $\mathcal{V}$. In other words, if $\{|a_i\rangle\}_{i=1}^{\infty}$ is a Cauchy sequence, then there exists a vector $|a\rangle \in \mathcal{V}$ such that $\lim_{i\to\infty} \|a_i - a\| = 0$.

Example 7.1.3 (1) $\mathbb{R}$ is complete with respect to the absolute-value norm $\|\alpha\| = |\alpha|$. In other words, every Cauchy sequence of real numbers has a limit in $\mathbb{R}$. This is proved in real analysis.
(2) $\mathbb{C}$ is complete with respect to the norm $\|\alpha\| = |\alpha| = \sqrt{(\mathrm{Re}\,\alpha)^2 + (\mathrm{Im}\,\alpha)^2}$. Using $|\alpha| \le |\mathrm{Re}\,\alpha| + |\mathrm{Im}\,\alpha|$, one can show that the completeness of $\mathbb{C}$ follows from that of $\mathbb{R}$. Details are left as an exercise for the reader.
(3) The set of rational numbers $\mathbb{Q}$ is *not* complete with respect to the absolute-value norm. In fact, $\{(1 + 1/k)^k\}_{k=1}^{\infty}$ is a sequence of rational numbers that is Cauchy but does not converge to a rational number; it converges to e, the base of the natural logarithm, which is known to be an irrational number. (See also the discussion after Definition 1.3.4.)

Let $\{|a_i\rangle\}_{i=1}^{\infty}$ be a Cauchy sequence of vectors in a finite-dimensional vector space $\mathcal{V}_N$. Choose an orthonormal basis $\{|e_k\rangle\}_{k=1}^{N}$ in $\mathcal{V}_N$ such that[2] $|a_i\rangle = \sum_{k=1}^{N} \alpha_k^{(i)} |e_k\rangle$ and $|a_j\rangle = \sum_{k=1}^{N} \alpha_k^{(j)} |e_k\rangle$. Then

[2]Recall that one can always define an inner product on a finite-dimensional vector space. So, the existence of orthonormal bases is guaranteed.

$$\|a_i - a_j\|^2 = \langle a_i - a_j | a_i - a_j \rangle = \left\| \sum_{k=1}^{N} \bigl(\alpha_k^{(i)} - \alpha_k^{(j)}\bigr) |e_k\rangle \right\|^2$$

$$= \sum_{k,l=1}^{N} \bigl(\alpha_k^{(i)} - \alpha_k^{(j)}\bigr)^* \bigl(\alpha_l^{(i)} - \alpha_l^{(j)}\bigr) \langle e_k | e_l \rangle = \sum_{k=1}^{N} \bigl|\alpha_k^{(i)} - \alpha_k^{(j)}\bigr|^2.$$

The LHS goes to zero, because the sequence is assumed Cauchy. Furthermore, all terms on the RHS are positive. Thus, they too must go to zero as $i, j \to \infty$. By the completeness of $\mathbb{C}$, there must exist $\alpha_k \in \mathbb{C}$ such that $\lim_{n\to\infty} \alpha_k^{(n)} = \alpha_k$ for $k = 1, 2, \dots, N$. Now consider $|a\rangle \in \mathcal{V}_N$ given by $|a\rangle = \sum_{k=1}^{N} \alpha_k |e_k\rangle$. We claim that $|a\rangle$ is the limit of the above sequence of vectors in $\mathcal{V}_N$. Indeed,

$$\lim_{i\to\infty} \|a_i - a\|^2 = \lim_{i\to\infty} \sum_{k=1}^{N} \bigl|\alpha_k^{(i)} - \alpha_k\bigr|^2 = \sum_{k=1}^{N} \lim_{i\to\infty} \bigl|\alpha_k^{(i)} - \alpha_k\bigr|^2 = 0.$$

We have proved the following:

all finite-dimensional vector spaces are complete

Proposition 7.1.4 *Every Cauchy sequence in a finite-dimensional inner product space over $\mathbb{C}$ (or $\mathbb{R}$) is convergent. In other words, every finite-dimensional complex (or real) inner product space is complete with respect to the norm induced by its inner product.*

The next example shows how important the word "finite" is.

Example 7.1.5 Consider $\{f_k\}_{k=1}^{\infty}$, the infinite sequence of *continuous* functions defined in the interval $[-1, +1]$ by

$$f_k(x) = \begin{cases} 1 & \text{if } 1/k \le x \le 1, \\ (kx+1)/2 & \text{if } -1/k \le x \le 1/k, \\ 0 & \text{if } -1 \le x \le -1/k. \end{cases}$$

This sequence belongs to $\mathcal{C}^0(-1, 1)$, the inner product space of continuous functions with its usual inner product: $\langle f|g\rangle = \int_{-1}^{1} f^*(x) g(x)\, dx$. It is straightforward to verify that $\|f_k - f_j\|^2 = \int_{-1}^{1} |f_k(x) - f_j(x)|^2 dx \xrightarrow[k,j\to\infty]{} 0$. Therefore, the sequence is Cauchy. However, the limit of this sequence is (see Fig. 7.1)

$$f(x) = \begin{cases} 1 & \text{if } 0 < x \le 1, \\ 0 & \text{if } -1 \le x < 0, \end{cases}$$

which is discontinuous at $x = 0$ and therefore does not belong to the space in which the original sequence lies.

We see that infinite-dimensional vector spaces are not generally complete. It is a nontrivial task to show whether or not a given infinite-dimensional vector space is complete.

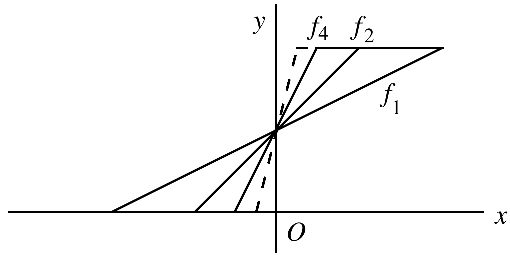

Fig. 7.1 The limit of the sequence of the *continuous* functions f_k is a discontinuous function that is 1 for $x > 0$ and 0 for $x < 0$

Any vector space (finite- or infinite-dimensional) contains all finite linear combinations of the form $\sum_{i=1}^{n} \alpha_i |a_i\rangle$ when it contains all the $|a_i\rangle$'s. This follows from the very definition of a vector space. However, the situation is different when n goes to infinity. For the vector space to contain the infinite sum, firstly, the meaning of such a sum has to be clarified, i.e., a norm and an associated convergence criterion needs to be put in place. Secondly, the vector space has to be complete with respect to that norm. A complete normed vector space is called a **Banach space**. We shall not deal with a general Banach space, but only with those spaces whose norms arise naturally from an inner product. This leads to the following definition:

Banach space

Definition 7.1.6 A complete inner product space, commonly denoted by $\mathcal{H}$, is called a **Hilbert space**.

Hilbert space defined

Thus, all finite-dimensional real or complex vector spaces are Hilbert spaces. However, when we speak of a Hilbert space, we shall usually assume that it is infinite-dimensional.

It is convenient to use orthonormal vectors in studying Hilbert spaces. So, let us consider an infinite sequence $\{|e_i\rangle\}_{i=1}^{\infty}$ of orthonormal vectors all belonging to a Hilbert space $\mathcal{H}$. Next, take any vector $|f\rangle \in \mathcal{H}$, construct the complex numbers $f_i = \langle e_i|f\rangle$, and form the sequence of vectors[3]

$$|f_n\rangle = \sum_{i=1}^{n} f_i |e_i\rangle \quad \text{for } n = 1, 2, \ldots \tag{7.1}$$

For the pair of vectors $|f\rangle$ and $|f_n\rangle$, the Schwarz inequality gives

$$\left|\langle f|f_n\rangle\right|^2 \le \langle f|f\rangle\langle f_n|f_n\rangle = \langle f|f\rangle\left(\sum_{i=1}^{n} |f_i|^2\right), \tag{7.2}$$

[3]We can consider $|f_n\rangle$ as an "approximation" to $|f\rangle$, because both share the same components along the same set of orthonormal vectors. The sequence of orthonormal vectors acts very much as a basis. However, to be a basis, an extra condition must be met. We shall discuss this condition shortly.

where Eq. (7.1) has been used to evaluate $\langle f_n|f_n\rangle$. On the other hand, taking the inner product of (7.1) with $\langle f|$ yields

$$\langle f|f_n\rangle = \sum_{i=1}^{n} f_i \langle f|e_i\rangle = \sum_{i=1}^{n} f_i f_i^* = \sum_{i=1}^{n} |f_i|^2.$$

Substitution of this in Eq. (7.2) yields the **Parseval inequality**:

Parseval inequality

$$\sum_{i=1}^{n} |f_i|^2 \leq \langle f|f\rangle. \tag{7.3}$$

This conclusion is true for arbitrarily large n and can be stated as follows:

Proposition 7.1.7 *Let $\{|e_i\rangle\}_{i=1}^{\infty}$ be an infinite set of orthonormal vectors in a Hilbert space, $\mathcal{H}$. Let $|f\rangle \in \mathcal{H}$ and define complex numbers $f_i = \langle e_i|f\rangle$. Then the* ***Bessel inequality*** *holds*: $\sum_{i=1}^{\infty} |f_i|^2 \leq \langle f|f\rangle$.

Bessel inequality

The Bessel inequality shows that the vector

$$\sum_{i=1}^{\infty} f_i|e_i\rangle \equiv \lim_{n\to\infty} \sum_{i=1}^{n} f_i|e_i\rangle$$

converges; that is, it has a finite norm. However, the inequality does not say whether the vector converges to $|f\rangle$. To make such a statement we need completeness:

Definition 7.1.8 A sequence of orthonormal vectors $\{|e_i\rangle\}_{i=1}^{\infty}$ in a Hilbert space $\mathcal{H}$ is called **complete** if the only vector in $\mathcal{H}$ that is orthogonal to all the $|e_i\rangle$ is the zero vector, in which case $\{|e_i\rangle\}_{i=1}^{\infty}$ is called a **basis** for $\mathcal{H}$.

complete orthonormal sequence of vectors; basis for $\mathcal{H}$

The notion of completeness does not enter the discussion of an N-dimensional vector space, because any N orthonormal vectors form a basis. If you take away some of the vectors, you don't have a basis, because you have less than N vectors. The situation is different in infinite dimensions. If you start with a basis and take away some of the vectors, you still have an *infinite* number of orthonormal vectors. The notion of completeness ensures that no orthonormal vector is taken out of a basis. This completeness property is the extra condition alluded to (in the footnote) above, and is what is required to make a basis.

In mathematics literature, one distinguishes between a general and a *separable* Hilbert space. The latter is characterized by having a *countable* basis. Thus, in the definition above, the Hilbert space is actually a separable one, and from now on, by Hilbert space we shall mean a separable Hilbert space.

Proposition 7.1.9 *Let $\{|e_i\rangle\}_{i=1}^{\infty}$ be an orthonormal sequence in $\mathcal{H}$. Then the following statements are equivalent*:

1. $\{|e_i\rangle\}_{i=1}^{\infty}$ *is complete.*
2. $|f\rangle = \sum_{i=1}^{\infty} |e_i\rangle\langle e_i|f\rangle\ \forall |f\rangle \in \mathcal{H}$.

3. $\sum_{i=1}^{\infty} |e_i\rangle\langle e_i| = \mathbf{1}$.
4. $\langle f|g\rangle = \sum_{i=1}^{\infty} \langle f|e_i\rangle\langle e_i|g\rangle \ \forall |f\rangle, |g\rangle \in \mathcal{H}$.
5. $\|f\|^2 = \sum_{i=1}^{\infty} |\langle e_i|f\rangle|^2 \ \forall |f\rangle \in \mathcal{H}$.

Proof We shall prove the implications $1 \Rightarrow 2 \Rightarrow 3 \Rightarrow 4 \Rightarrow 5 \Rightarrow 1$.

$1 \Rightarrow 2$: It is sufficient to show that the vector $|\psi\rangle \equiv |f\rangle - \sum_{i=1}^{\infty} |e_i\rangle\langle e_i|f\rangle$ is orthogonal to all the $|e_j\rangle$:

$$\langle e_j|\psi\rangle = \langle e_j|f\rangle - \sum_{i=1}^{\infty} \overbrace{\langle e_j|e_i\rangle}^{\delta_{ij}} \langle e_i|f\rangle = 0.$$

$2 \Rightarrow 3$: Since $|f\rangle = \mathbf{1}|f\rangle = \sum_{i=1}^{\infty}(|e_i\rangle\langle e_i|)|f\rangle$ is true for all $|f\rangle \in \mathcal{H}$, we must have $\mathbf{1} = \sum_{i=1}^{\infty} |e_i\rangle\langle e_i|$.

$3 \Rightarrow 4$: $\langle f|g\rangle = \langle f|\mathbf{1}|g\rangle = \langle f|(\sum_{i=1}^{\infty} |e_i\rangle\langle e_i|)|g\rangle = \sum_{i=1}^{\infty} \langle f|e_i\rangle\langle e_i|g\rangle$.

$4 \Rightarrow 5$: Let $|g\rangle = |f\rangle$ in statement 4 and recall that $\langle f|e_i\rangle = \langle e_i|f\rangle^*$.

$5 \Rightarrow 1$: Let $|f\rangle$ be orthogonal to all the $|e_i\rangle$. Then all the terms in the sum are zero implying that $\|f\|^2 = 0$, which in turn gives $|f\rangle = 0$, because only the zero vector has a zero norm. □

Parseval equality; generalized Fourier coefficients

The equality

$$\|f\|^2 = \langle f|f\rangle = \sum_{i=1}^{\infty} \big|\langle e_i|f\rangle\big|^2 = \sum_{i=1}^{\infty} |f_i|^2, \quad f_i = \langle e_i|f\rangle, \tag{7.4}$$

is called the **Parseval equality**, and the complex numbers f_i are called **generalized Fourier coefficients**. The relation

$$\mathbf{1} = \sum_{i=1}^{\infty} |e_i\rangle\langle e_i| \tag{7.5}$$

completeness relation

is called the **completeness relation**.

Historical Notes

David Hilbert 1862–1943

David Hilbert (1862–1943), the greatest mathematician of the twentieth century, received his Ph.D. from the University of Königsberg and was a member of the staff there from 1886 to 1895. In 1895 he was appointed to the chair of mathematics at the University of Göttingen, where he continued to teach for the rest of his life.

Hilbert is one of that rare breed of late 19th-century mathematicians whose spectrum of expertise covered a wide range, with formal set theory at one end and mathematical physics at the other. He did superb work in geometry, algebraic geometry, algebraic number theory, integral equations, and operator theory. The seminal two-volume book *Methoden der mathematische Physik* by R. Courant, still one of the best books on the subject, was greatly influenced by Hilbert.

Hilbert's work in geometry had the greatest influence in that area since Euclid. A systematic study of the axioms of Euclidean geometry led Hilbert to propose 21 such axioms, and he analyzed their significance. He published *Grundlagen der Geometrie* in 1899, putting geometry on a formal axiomatic foundation. His famous 23 Paris problems challenged (and still today challenge) mathematicians to solve fundamental questions.

It was late in his career that Hilbert turned to the subject for which he is most famous among physicists. A lecture by Erik Holmgren in 1901 on Fredholm's work on integral equations, which had already been published in Sweden, aroused Hilbert's interest in the subject. David Hilbert, having established himself as the leading mathematician of his time by his work on algebraic numbers, algebraic invariants, and the foundations of geometry, now turned his attention to **integral equations**. He says that an investigation of the subject showed him that it was important for the theory of definite integrals, for the development of arbitrary functions in series (of special functions or trigonometric functions), for the theory of linear differential equations, for potential theory, and for the calculus of variations. He wrote a series of six papers from 1904 to 1910 and reproduced them in his book *Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen* (1912). During the latter part of this work he applied integral equations to problems of mathematical physics.

It is said that Hilbert discovered the correct field equation for general relativity in 1915 (one year before Einstein) using the variational principle, but never claimed priority.

Hilbert claimed that he worked best out-of-doors. He accordingly attached an 18-foot blackboard to his neighbor's wall and built a covered walkway there so that he could work outside in any weather. He would intermittently interrupt his pacing and his blackboard computations with a few turns around the rest of the yard on his bicycle, or he would pull some weeds, or do some garden trimming. Once, when a visitor called, the maid sent him to the backyard and advised that if the master wasn't readily visible at the blackboard to look for him up in one of the trees.

Highly gifted and highly versatile, David Hilbert radiated over mathematics a catching optimism and a stimulating vitality that can only be called "the spirit of Hilbert." Engraved on a stone marker set over Hilbert's grave in Göttingen are the master's own optimistic words: "Wir müssen wissen. Wir werden wissen." ("We must know. We shall know.")

"Wir müssen wissen. Wir werden wissen."

7.2 The Space of Square-Integrable Functions

Chapter 2 showed that the collection of all continuous functions defined on an interval $[a, b]$ forms a linear vector space. Example 7.1.5 showed that this space is not complete. Can we enlarge this space to make it complete? Since we are interested in an inner product as well, and since a natural inner product for functions is defined in terms of integrals, we want to make sure that our functions are integrable. However, integrability does not require continuity, it only requires *piecewise* continuity. In this section we shall discuss conditions under which the space of functions becomes complete. An important class of functions has already been mentioned in Chap. 2. These functions satisfy the inner product given by

$$\langle g|f\rangle = \int_a^b g^*(x) f(x) w(x)\, dx.$$

If $g(x) = f(x)$, we obtain

$$\langle f|f\rangle = \int_a^b \left|f(x)\right|^2 w(x)\, dx. \tag{7.6}$$

Functions for which such an integral is defined are said to be **square-integrable**.

square-integrable functions

The space of square-integrable functions over the interval $[a, b]$ is denoted by $\mathcal{L}_w^2(a, b)$. In this notation $\mathcal{L}$ stands for *Lebesgue*, who generalized the notion of the ordinary Riemann integral to cases for which the integrand could be highly discontinuous; 2 stands for the power of $f(x)$ in the integral; a and b denote the limits of integration; and w refers to the weight function (a strictly positive real-valued function). When $w(x) = 1$, we use the notation $\mathcal{L}^2(a,b)$. The significance of $\mathcal{L}^2_w(a,b)$ lies in the following theorem (for a proof, see [Reed 80, Chap. III]):

$\mathcal{L}^2_w(a,b)$ is complete

Theorem 7.2.1 (Riesz-Fischer theorem) *The space $\mathcal{L}^2_w(a,b)$ is complete.*

all Hilbert spaces are alike

A complete infinite-dimensional inner product space was earlier defined to be a Hilbert space. The following theorem shows that the number of (separable) Hilbert spaces is severely restricted. (For a proof, see [Frie 82, p. 216].)

Theorem 7.2.2 *All complete inner product spaces with countable bases are isomorphic to $\mathcal{L}^2_w(a,b)$.*

$\mathcal{L}^2_w(a,b)$ is defined in terms of functions that satisfy Eq. (7.6). Yet an inner product involves integrals of the form $\int_a^b g^*(x) f(x) w(x)\,dx$. Are such integrals well-defined and finite? Using the Schwarz inequality, which holds for any inner product space, finite or infinite, one can show that the integral is defined.

The isomorphism of Theorem 7.2.2 makes the Hilbert space more tangible, because it identifies the space with a space of functions, objects that are more familiar than abstract vectors. Nonetheless, a faceless function is very little improvement over an abstract vector. What is desirable is a set of concrete functions with which we can calculate. The following theorem provides such functions (for a proof, see [Simm 83, pp. 154–161]).

Theorem 7.2.3 (Stone-Weierstrass approximation theorem) *The sequence of monomials $\{x^k\}_{k=0}^\infty$ forms a basis of $\mathcal{L}^2_w(a,b)$.*

Thus, any square-integrable function f can be written as $f(x) = \sum_{k=0}^\infty \alpha_k x^k$. This theorem shows that $\mathcal{L}^2_w(a,b)$ is indeed a *separable* Hilbert space as expected in Theorem 7.2.2.

7.2.1 Orthogonal Polynomials

the polynomials $\{C_n(x)\}_{n=0}^\infty$ are orthogonal to each other

The monomials $\{x^k\}_{k=0}^\infty$ are not orthonormal but are linearly independent. If we wish to obtain an orthonormal—or simply orthogonal—linear combination of these vectors, we can use the Gram-Schmidt process. The result will be certain polynomials, denoted by $C_n(x)$, that are orthogonal to one another and span $\mathcal{L}^2_w(a,b)$.

Such orthogonal polynomials satisfy very useful **recurrence relations**, which we now derive. In the following discussion $p_{\le k}(x)$ denotes a generic polynomial of degree less than or equal to k. For example, $3x^5 - 4x^2 + 5$, $2x + 1$, $-2.4x^4 + 3x^3 - x^2 + 6$, and 2 are all denoted by $p_{\le 5}(x)$ or $p_{\le 8}(x)$ or $p_{\le 59}(x)$ because they all have degrees less than or equal to 5, 8, and 59. Since a polynomial of degree less than n can be written as a linear combination of $C_k(x)$ with $k < n$, we have the obvious property

$$\int_a^b C_n(x) p_{\le n-1}(x) w(x)\, dx = 0. \tag{7.7}$$

Let $k_m^{(m)}$ and $k_m^{(m-1)}$ denote, respectively, the coefficients of x^m and x^{m-1} in $C_m(x)$, and let

$$h_m = \int_a^b \left[C_m(x)\right]^2 w(x)\, dx. \tag{7.8}$$

The polynomial $C_{n+1}(x) - (k_{n+1}^{(n+1)}/k_n^{(n)}) x C_n(x)$ has degree less than or equal to n, and therefore can be expanded as a linear combination of the $C_j(x)$:

$$C_{n+1}(x) - \frac{k_{n+1}^{(n+1)}}{k_n^{(n)}} x C_n(x) = \sum_{j=0}^{n} a_j C_j(x). \tag{7.9}$$

Take the inner product of both sides of this equation with $C_m(x)$:

$$\int_a^b C_{n+1}(x) C_m(x) w(x)\, dx - \frac{k_{n+1}^{(n+1)}}{k_n^{(n)}} \int_a^b x C_n(x) C_m(x) w(x)\, dx$$
$$= \sum_{j=0}^{n} a_j \int_a^b C_j(x) C_m(x) w(x)\, dx.$$

The first integral on the LHS vanishes as long as $m \le n$; the second integral vanishes if $m \le n-2$ [if $m \le n-2$, then $xC_m(x)$ is a polynomial of degree $n-1$]. Thus, we have

$$\sum_{j=0}^{n} a_j \int_a^b C_j(x) C_m(x) w(x)\, dx = 0 \quad \text{for } m \le n-2.$$

The integral in the sum is zero unless $j = m$, by orthogonality. Therefore, the sum reduces to

$$a_m \int_a^b \left[C_m(x)\right]^2 w(x)\, dx = 0 \quad \text{for } m \le n-2.$$

Since the integral is nonzero, we conclude that $a_m = 0$ for $m = 0, 1, 2, \dots,$ $n-2$, and Eq. (7.9) reduces to

$$C_{n+1}(x) - \frac{k_{n+1}^{(n+1)}}{k_n^{(n)}} x C_n(x) = a_{n-1} C_{n-1}(x) + a_n C_n(x). \tag{7.10}$$

It can be shown that if we define

$$\alpha_n = \frac{k_{n+1}^{(n+1)}}{k_n^{(n)}}, \qquad \beta_n = \alpha_n \left(\frac{k_{n+1}^{(n)}}{k_{n+1}^{(n+1)}} - \frac{k_n^{(n-1)}}{k_n^{(n)}} \right), \qquad \gamma_n = -\frac{h_n}{h_{n-1}} \frac{\alpha_n}{\alpha_{n-1}}, \tag{7.11}$$

then Eq. (7.10) can be expressed as

$$C_{n+1}(x) = (\alpha_n x + \beta_n)C_n(x) + \gamma_n C_{n-1}(x), \tag{7.12}$$

or

$$xC_n(x) = \frac{1}{\alpha_n}C_{n+1}(x) - \frac{\beta_n}{\alpha_n}C_n(x) - \frac{\gamma_n}{\alpha_n}C_{n-1}(x). \tag{7.13}$$

a recurrence relation for orthogonal polynomials

Other recurrence relations, involving higher powers of x, can be obtained from the one above. For example, a recurrence relation involving x^2 can be obtained by multiplying both sides of Eq. (7.13) by x and expanding each term of the RHS using that same equation. The result will be

$$\begin{aligned} x^2 C_n(x) = {} & \frac{1}{\alpha_n \alpha_{n+1}} C_{n+2}(x) - \left(\frac{\beta_{n+1}}{\alpha_n \alpha_{n+1}} + \frac{\beta_n}{\alpha_n^2}\right) C_{n+1}(x) \\ & - \left(\frac{\gamma_{n+1}}{\alpha_n \alpha_{n+1}} - \frac{\beta_n^2}{\alpha_n^2} + \frac{\gamma_n}{\alpha_n \alpha_{n-1}}\right) C_n(x) \\ & + \left(\frac{\beta_n \gamma_n}{\alpha_n^2} + \frac{\beta_{n-1}\gamma_n}{\alpha_n \alpha_{n-1}}\right) C_{n-1}(x) + \frac{\gamma_{n-1}\gamma_n}{\alpha_n \alpha_{n-1}} C_{n-2}(x). \end{aligned} \tag{7.14}$$

Example 7.2.4 As an application of the recurrence relations above, let us evaluate

$$I_1 \equiv \int_a^b x C_m(x) C_n(x) w(x)\, dx.$$

Substituting (7.13) in the integral gives

$$\begin{aligned} I_1 = {} & \frac{1}{\alpha_n}\int_a^b C_m(x)C_{n+1}(x)w(x)\,dx - \frac{\beta_n}{\alpha_n}\int_a^b C_m(x)C_n(x)w(x)\,dx \\ & - \frac{\gamma_n}{\alpha_n}\int_a^b C_m(x)C_{n-1}(x)w(x)\,dx. \end{aligned}$$

We now use the orthogonality relations among the $C_k(x)$ to obtain

$$\begin{aligned} I_1 &= \frac{1}{\alpha_n}\delta_{m,n+1} \overbrace{\int_a^b C_m^2(x)w(x)\,dx}^{=h_m} - \frac{\beta_n}{\alpha_n}\delta_{mn}\int_a^b C_m^2(x)w(x)\,dx \\ &\quad - \frac{\gamma_n}{\alpha_n}\delta_{m,n-1}\int_a^b C_m^2(x)w(x)\,dx \\ &= \left(\frac{1}{\alpha_{m-1}}\delta_{m,n+1} - \frac{\beta_m}{\alpha_m}\delta_{mn} - \frac{\gamma_{m+1}}{\alpha_{m+1}}\delta_{m,n-1}\right)h_m, \end{aligned}$$

or

$$I_1 = \begin{cases} h_m/\alpha_{m-1} & \text{if } m = n+1, \\ -\beta_m h_m/\alpha_m & \text{if } m = n, \\ -\gamma_{m+1} h_m/\alpha_{m+1} & \text{if } m = n-1, \\ 0 & \text{otherwise.} \end{cases}$$

Example 7.2.5 Let us find the orthogonal polynomials forming a basis of $\mathcal{L}^2(-1,+1)$, which we denote by $P_n(x)$, where n is the degree of the polynomial. Let $P_0(x)=1$. To find $P_1(x)$, write $P_1(x)=ax+b$, and determine a and b in such a way that $P_1(x)$ is orthogonal to $P_0(x)$:

$$0=\int_{-1}^{1}P_1(x)P_0(x)\,dx=\int_{-1}^{1}(ax+b)\,dx=\frac{1}{2}ax^2\bigg|_{-1}^{1}+2b=2b.$$

So one of the coefficients, b, is zero. To find the other one, we need some standardization procedure. We "standardize" $P_n(x)$ by requiring that $P_n(1)=1\ \forall n$. For $n=1$ this yields $a\times 1=1$, or $a=1$, so that $P_1(x)=x$.

We can calculate $P_2(x)$ similarly: Write $P_2(x)=ax^2+bx+c$, impose the condition that it be orthogonal to both $P_1(x)$ and $P_0(x)$, and enforce the standardization procedure. All this will yield

$$0=\int_{-1}^{1}P_2(x)P_0(x)\,dx=\frac{2}{3}a+2c,\qquad 0=\int_{-1}^{1}P_2(x)P_1(x)\,dx=\frac{2}{3}b,$$

and $P_2(1)=a+b+c=1$. These three equations have the unique solution $a=3/2$, $b=0$, $c=-1/2$. Thus, $P_2(x)=\frac{1}{2}(3x^2-1)$. These are the first three Legendre polynomials, which are part of a larger group of polynomials to be discussed in Chap. 8.

7.2.2 Orthogonal Polynomials and Least Squares

The method of least squares is no doubt familiar to the reader. In the simplest procedure, one tries to find a *linear function* that most closely fits a set of data. By definition, "most closely" means that the sum of the squares of the differences between the data points and the corresponding values of the linear function is minimum. More generally, one seeks the best *polynomial* fit to the data.

We shall consider a related topic, namely least-square fitting of a given *function* with polynomials. Suppose $f(x)$ is a function defined on (a,b). We want to find a polynomial that most closely approximates f. Write such a polynomial as $p(x)=\sum_{k=0}^{n}a_kx^k$, where the a_k's are to be determined such that

$$S(a_0,a_1,\dots,a_n)\equiv\int_a^b\big[f(x)-a_0-a_1x-\cdots-a_nx^n\big]^2dx$$

is a minimum. Differentiating S with respect to the a_k's and setting the result equal to zero gives

$$0=\frac{\partial S}{\partial a_j}=\int_a^b 2\big(-x^j\big)\left[f(x)-\sum_{k=0}^{n}a_kx^k\right]dx,$$

or

$$\sum_{k=0}^{n}a_k\int_a^b x^{j+k}dx=\int_a^b f(x)x^j\,dx.$$

One can rewrite this in matrix form as $\mathsf{B}\mathsf{a} = \mathsf{c}$, where a is a column vector with components a_k, and B and c are a matrix and a column vector whose components are

$$\mathsf{B}_{kj} = \frac{b^{j+k+1} - a^{j+k+1}}{j+k+1} \quad \text{and} \quad c_j = \int_a^b f(x)x^j\,dx. \tag{7.15}$$

By solving this matrix equation, one finds the a_k's, which in turn give the best fit.

A drawback of the procedure above is that the desire for a higher-degree polynomial fit entails the implementation of the procedure from scratch and the solution of a completely new matrix equation. One way to overcome this difficulty is to use orthogonal polynomials. Then we would have

$$S(a_0, a_1, \ldots, a_n) \equiv \int_a^b \left[f(x) - \sum_{k=0}^n a_k C_k(x) \right]^2 w(x)\,dx,$$

where we have introduced a weight function $w(x)$ for convenience. The derivative equation becomes

$$0 = \frac{\partial S}{\partial a_j} = \int_a^b 2\bigl[-C_j(x)\bigr]\left[f(x) - \sum_{k=0}^n a_k C_k(x) \right] w(x)\,dx,$$

or

$$\sum_{k=0}^n a_k \underbrace{\int_a^b C_j(x)C_k(x)w(x)\,dx}_{=0 \text{ unless } j=k} = \int_a^b C_j(x)f(x)w(x)\,dx.$$

It follows that

$$a_j = \frac{\int_a^b C_j(x)f(x)w(x)\,dx}{\int_a^b [C_j(x)]^2 w(x)\,dx}, \qquad j = 0, 1, \ldots, n, \tag{7.16}$$

which is true regardless of the number of polynomials in the sum. Hence, once we find $\{a_j\}_{j=0}^m$, we can add the $(m+1)$st polynomial and determine a_{m+1} from Eq. (7.16) without altering the previous coefficients.

Example 7.2.6 Let us find the least-square fit to $f(x) = \cos(\frac{1}{2}\pi x)$ in the interval $(-1, +1)$ using polynomials of second degree. First we use a single polynomial whose coefficients are determined by Eq. (7.15). We can easily calculate the column vector c:

$$c_0 = \int_{-1}^1 \cos\left(\frac{1}{2}\pi x\right) dx = \frac{4}{\pi},$$

$$c_1 = \int_{-1}^1 x\cos\left(\frac{1}{2}\pi x\right) dx = 0,$$

$$c_2 = \int_{-1}^1 x^2\cos\left(\frac{1}{2}\pi x\right) dx = -\frac{32}{\pi^3} + \frac{4}{\pi}.$$

The elements of the matrix B can also be calculated easily. To find the unknown a_k's, we need to solve

$$\begin{pmatrix} 2 & 0 & \frac{2}{3} \\ 0 & \frac{2}{3} & 0 \\ \frac{2}{3} & 0 & \frac{2}{5} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \frac{4}{\pi} \\ 0 \\ -\frac{32}{\pi^3} + \frac{4}{\pi} \end{pmatrix}.$$

The solution is

$$a_0 = \frac{24}{\pi^3}, \qquad a_1 = 0, \qquad a_2 = \frac{6}{\pi} - \frac{72}{\pi^3}.$$

Therefore,

$$\cos\left(\frac{1}{2}\pi x\right) \approx \frac{24}{\pi^3} + \left(\frac{6}{\pi} - \frac{72}{\pi^3}\right)x^2.$$

If we wish to use orthogonal polynomials with $w(x) = 1$, we can employ the polynomials found in Example 7.2.5. Then

$$a_j = \frac{\int_{-1}^{1} P_j(x)\cos(\frac{1}{2}\pi x)\,dx}{\int_{-1}^{1}[P_j(x)]^2\,dx}, \qquad j = 0, 1, 2,$$

which yields

$$a_0 = \frac{2}{\pi}, \qquad a_1 = 0, \qquad a_2 = -\frac{120}{\pi^3} + \frac{20}{\pi}.$$

We can therefore write

$$\cos\left(\frac{1}{2}\pi x\right) \approx \frac{2}{\pi}P_0 + \left(-\frac{120}{\pi^3} + \frac{20}{\pi}\right)P_2.$$

7.3 Continuous Index

Once we allow the number of dimensions to be infinite, we open the door for numerous possibilities that are not present in the finite case. One such possibility arises because of the variety of infinities. We have encountered two types of infinity in Chap. 1, the countable infinity and the uncountable infinity. The paradigm of the former is the "number" of integers, and that of the latter is the "number" of real numbers. The nature of dimensionality of the vector space is reflected in the components of a general vector, which has a finite number of components in a finite-dimensional vector space, a countably infinite number of components in an infinite-dimensional vector space with a *countable basis*, and an uncountably infinite number of components in an infinite-dimensional vector space with no countable basis.

To gain an understanding of the nature of, and differences between, the three types of vector spaces mentioned above, it is convenient to think of components as functions of a "counting set". Thus, the components f_i of a vector $|f\rangle$ in an N-dimensional vector space can be thought of as values of a function f defined on the finite set $\{1, 2, \dots, N\}$, and to emphasize such functional dependence, we write $f(i)$ instead of f_i. Similarly, the components f_i of a vector $|f\rangle$ in a Hilbert space with the countable basis $B = \{|e_i\rangle\}_{i=1}^{\infty}$ can be thought of as values of a function $f : \mathbb{N} \to \mathbb{C}$, where $\mathbb{N}$ is the (infinite) set of natural numbers. The next step is to allow the counting set to be uncountable, i.e., a continuum such as the real numbers or an interval thereof. This leads to a "component" of the form $f(x)$ corresponding to a function $f : \mathbb{R} \to \mathbb{C}$. What about the vectors themselves? What sort of a basis gives rise to such components?

Because of the isomorphism of Theorem 7.2.2, we shall concentrate on $\mathcal{L}_w^2(a, b)$. In keeping with our earlier notation, let $\{|e_x\rangle\}_{x\in\mathbb{R}}$ be a set of vectors and interpret $f(x)$ as $\langle e_x|f\rangle$. The inner product of $\mathcal{L}_w^2(a, b)$ can now be written as

$$\begin{aligned}\langle g|f\rangle &= \int_a^b g^*(x)f(x)w(x)\,dx = \int_a^b \langle g|e_x\rangle\langle e_x|f\rangle w(x)\,dx\\ &= \langle g|\left(\int_a^b |e_x\rangle w(x)\langle e_x|\,dx\right)|f\rangle.\end{aligned}$$

The last line suggests writing

$$\int_a^b |e_x\rangle w(x)\langle e_x|\,dx = \mathbf{1}.$$

completeness relation for a continuous index

In the physics literature the "e" is ignored, and one writes $|x\rangle$ for $|e_x\rangle$. Hence, we obtain the completeness relation for a continuous index:

$$\int_a^b |x\rangle w(x)\langle x|\,dx = \mathbf{1}, \quad \text{or} \quad \int_a^b |x\rangle\langle x|\,dx = \mathbf{1}, \tag{7.17}$$

where in the second integral, $w(x)$ is set equal to unity. We also have

$$|f\rangle = \left(\int_a^b |x\rangle w(x)\langle x|\,dx\right)|f\rangle = \int_a^b f(x)w(x)|x\rangle\,dx, \tag{7.18}$$

which shows how to expand a vector $|f\rangle$ in terms of the $|x\rangle$'s.

Take the inner product of (7.18) with $\langle x'|$ to obtain

$$\langle x'|f\rangle = f(x') = \int_a^b f(x)w(x)\langle x'|x\rangle\,dx,$$

where x' is assumed to lie in the interval (a, b), otherwise $f(x') = 0$ by definition. This equation, which holds for arbitrary f, tells us immediately that $w(x)\langle x'|x\rangle$ is no ordinary function of x and x'. For instance, suppose $f(x') = 0$. Then, the result of integration is always zero, regardless of the behavior of f at other points. Clearly, there is an infinitude of functions that vanish at x', yet all of them give the same integral! Pursuing this line of argument more quantitatively, one can show that $w(x)\langle x'|x\rangle = 0$ if $x \neq x'$, $w(x)\langle x|x\rangle = \infty$, $w(x)\langle x'|x\rangle$ is an even function of $x - x'$, and

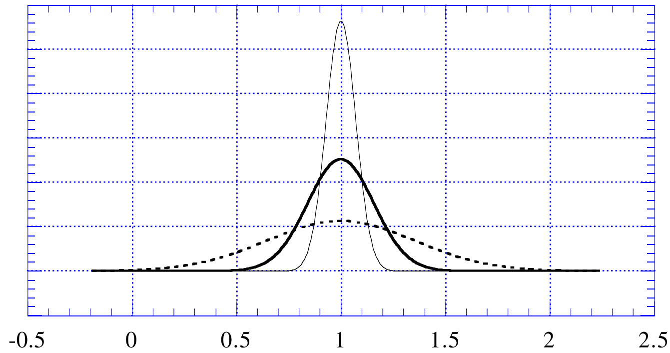

Fig. 7.2 The Gaussian bell-shaped curve approaches the Dirac delta function as the width of the curve approaches zero. The value of ϵ is 1 for the *dashed curve*, 0.25 for the *heavy curve* and 0.05 for the *light curve*

$\int_a^b w(x)\langle x'|x\rangle\, dx = 1$. The proof is left as a problem. The reader may recognize this as the **Dirac delta function**

Dirac delta function

$$\delta(x - x') = w(x)\langle x'|x\rangle, \tag{7.19}$$

which, for a function f defined on the interval (a, b), has the following property:[4]

$$\int_a^b f(x)\delta(x - x')\, dx = \begin{cases} f(x') & \text{if } x' \in (a, b), \\ 0 & \text{if } x' \notin (a, b). \end{cases} \tag{7.20}$$

Written in the form $\langle x'|x\rangle = \delta(x - x')/w(x)$, Eq. (7.19) is the generalization of the orthonormality relation of vectors to the case of a continuous index.

The Dirac delta function is anything but a "function". Nevertheless, there is a well-developed branch of mathematics, called generalized function theory or functional analysis, studying it and many other functions like it in a highly rigorous fashion. We shall only briefly explore this territory of mathematics in the next section. At this point we simply mention the fact that the Dirac delta function can be represented as the limit of certain sequences of ordinary functions. The following three examples illustrate some of these representations.

Example 7.3.1 Consider a Gaussian curve whose width approaches zero at the same time that its height approaches infinity in such a way that its area remains constant. In the infinite limit, we obtain the Dirac delta function. In fact, we have

$$\delta(x - x') = \lim_{\epsilon \to 0} \frac{1}{\sqrt{\epsilon\pi}} e^{-(x-x')^2/\epsilon}.$$

In the limit of $\epsilon \to 0$, the height of this Gaussian goes to infinity while its width goes to zero (see Fig. 7.2). Furthermore, for any nonzero value of ϵ,

[4]For an elementary discussion of the Dirac delta function with many examples of its application, see [Hass 08].

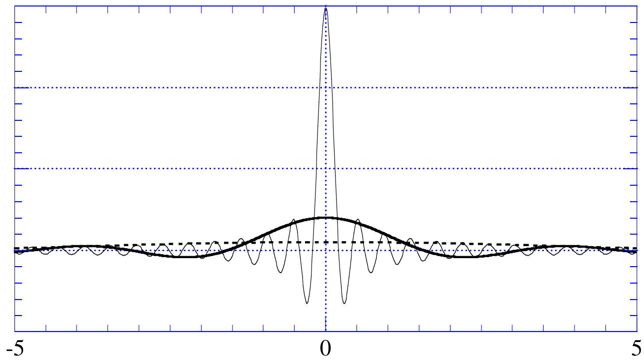

Fig. 7.3 The function $\sin Tx/x$ also approaches the Dirac delta function as the width of the curve approaches zero. The value of T is 0.5 for the *dashed curve*, 2 for the *heavy curve*, and 15 for the *light curve*

we can easily verify that

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{\epsilon\pi}} e^{-(x-x')^2/\epsilon}\,dx = 1.$$

This relation is independent of ϵ and therefore still holds in the limit $\epsilon \to 0$. The limit of the Gaussian behaves like the Dirac delta function.

Example 7.3.2 Consider the function $D_T(x-x')$ defined as

$$D_T(x-x') \equiv \frac{1}{2\pi}\int_{-T}^{T} e^{i(x-x')t}\,dt.$$

The integral is easily evaluated, with the result

$$D_T(x-x') = \frac{1}{2\pi}\frac{e^{i(x-x')t}}{i(x-x')}\bigg|_{-T}^{T} = \frac{1}{\pi}\frac{\sin T(x-x')}{x-x'}.$$

The graph of $D_T(x-0)$ as a function of x for various values of T is shown in Fig. 7.3. Note that the width of the curve decreases as T increases. The area under the curve can be calculated:

$$\int_{-\infty}^{\infty} D_T(x-x')\,dx = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\sin T(x-x')}{x-x'}\,dx = \frac{1}{\pi}\underbrace{\int_{-\infty}^{\infty}\frac{\sin y}{y}\,dy}_{=\pi} = 1.$$

Figure 7.3 shows that $D_T(x-x')$ becomes more and more like the Dirac delta function as T gets larger and larger. In fact, we have

$$\delta(x-x') = \lim_{T\to\infty}\frac{1}{\pi}\frac{\sin T(x-x')}{x-x'}. \qquad (7.21)$$

To see this, we note that for any finite T we can write

$$D_T(x-x') = \frac{T}{\pi}\frac{\sin T(x-x')}{T(x-x')}.$$

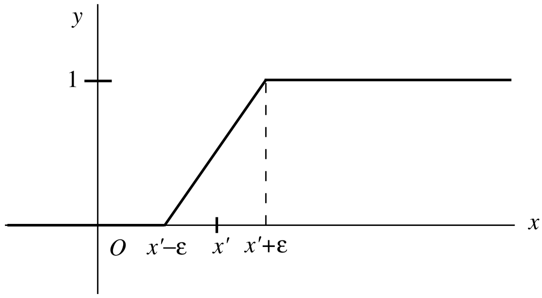

Fig. 7.4 The step function, or θ-function, shown in the figure has the Dirac delta function as its derivative

Furthermore, for values of x that are very close to x',

$$T(x - x') \to 0 \quad \text{and} \quad \frac{\sin T(x - x')}{T(x - x')} \to 1.$$

Thus, for such values of x and x', we have $D_T(x - x') \approx (T/\pi)$, which is large when T is large. This is as expected of a delta function: $\delta(0) = \infty$. On the other hand, the width of $D_T(x - x')$ around x' is given, roughly, by the distance between the points at which $D_T(x - x')$ drops to zero: $T(x - x') = \pm\pi$, or $x - x' = \pm\pi/T$. This width is roughly $\Delta x = 2\pi/T$, which goes to zero as T grows. Again, this is as expected of the delta function.

The preceding example suggests another representation of the Dirac delta function:

$$\delta(x - x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(x-x')t}\,dt. \tag{7.22}$$

step function or θ function

Example 7.3.3 A third representation of the Dirac delta function involves the **step function** $\theta(x - x')$, which is defined as

$$\theta(x - x') \equiv \begin{cases} 0 & \text{if } x < x', \\ 1 & \text{if } x > x' \end{cases}$$

and is discontinuous at $x = x'$. We can approximate this step function by a variety of continuous functions. One such function is $T_\epsilon(x - x')$ defined by

$$T_\epsilon(x - x') \equiv \begin{cases} 0 & \text{if } x \le x' - \epsilon, \\ \frac{1}{2\epsilon}(x - x' + \epsilon) & \text{if } x' - \epsilon \le x \le x' + \epsilon, \\ 1 & \text{if } x \ge x' + \epsilon, \end{cases}$$

where ϵ is a small positive number as shown in Fig. 7.4. It is clear that

$$\theta(x - x') = \lim_{\epsilon \to 0} T_\epsilon(x - x').$$

Now let us consider the derivative of $T_\epsilon(x-x')$ with respect to x:

$$\frac{dT_\epsilon}{dx}(x-x') = \begin{cases} 0 & \text{if } x < x'-\epsilon, \\ \frac{1}{2\epsilon} & \text{if } x'-\epsilon < x < x'+\epsilon, \\ 0 & \text{if } x > x'+\epsilon. \end{cases}$$

We note that the derivative is not defined at $x = x'-\epsilon$ and $x = x'+\epsilon$, and that dT_ϵ/dx is zero everywhere except when x lies in the interval $(x'-\epsilon, x'+\epsilon)$, where it is equal to $1/(2\epsilon)$ and goes to infinity as $\epsilon \to 0$. Here again we see signs of the delta function. In fact, we also note that

$$\int_{-\infty}^{\infty}\left(\frac{dT_\epsilon}{dx}\right)dx = \int_{x'-\epsilon}^{x'+\epsilon}\left(\frac{dT_\epsilon}{dx}\right)dx = \int_{x'-\epsilon}^{x'+\epsilon}\frac{1}{2\epsilon}dx = 1.$$

It is not surprising, then, to find that $\lim_{\epsilon\to 0}\frac{dT_\epsilon}{dx}(x-x') = \delta(x-x')$. Assuming that the interchange of the order of differentiation and the limiting process is justified, we obtain the important identity

δ function as derivative of θ function

$$\frac{d}{dx}\theta(x-x') = \delta(x-x'). \tag{7.23}$$

Now that we have some understanding of one continuous index, we can generalize the results to several continuous indices. In the earlier discussion we looked at $f(x)$ as the xth component of some abstract vector $|f\rangle$. For functions of n variables, we can think of $f(x_1,\dots,x_n)$ as the component of an abstract vector $|f\rangle$ along a basis vector $|x_1,\dots,x_n\rangle$.[5] This basis is a direct generalization of one continuous index to n. Then $f(x_1,\dots,x_n)$ is defined as $f(x_1,\dots,x_n) = \langle x_1,\dots,x_n|f\rangle$. If the region of integration is denoted by Ω, and we use the abbreviations

$$\mathbf{r} \equiv (x_1, x_2, \dots, x_n), \qquad d^n x = dx_1 dx_2 \dots dx_n,$$

$$|x_1, x_2, \dots, x_n\rangle = |\mathbf{r}\rangle, \qquad \delta(x_1-x_1')\dots\delta(x_n-x_n') = \delta(\mathbf{r}-\mathbf{r}'),$$

then we can write

$$\begin{aligned} |f\rangle &= \int_\Omega d^n x f(\mathbf{r})w(\mathbf{r})|\mathbf{r}\rangle, & \int_\Omega d^n x |\mathbf{r}\rangle w(\mathbf{r})\langle\mathbf{r}| = \mathbf{1}, \\ f(\mathbf{r}') &= \int_\Omega d^n x f(\mathbf{r})w(\mathbf{r})\langle\mathbf{r}'|\mathbf{r}\rangle, & \langle\mathbf{r}'|\mathbf{r}\rangle w(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}'), \end{aligned} \tag{7.24}$$

where $d^n x$ is the "volume" element and Ω is the region of integration of interest.

For instance, if the region of definition of the functions under consideration is the surface of the unit sphere, then [with $w(\mathbf{r}) = 1$], one gets

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta |\theta,\phi\rangle\langle\theta,\phi| = \mathbf{1}. \tag{7.25}$$

[5] Do not confuse this with an n-dimensional vector. In fact, the dimension is n-fold infinite: each x_i counts one infinite set of numbers!

This will be used in our discussion of spherical harmonics in Chap. 13.

An important identity using the three-dimensional Dirac delta function comes from potential theory. This is (see [Hass 08] for a discussion of this equation)

$$\nabla^2\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right) = -4\pi\delta(\mathbf{r}-\mathbf{r}'). \tag{7.26}$$

7.4 Generalized Functions

Paul Adrian Maurice Dirac discovered the delta function in the late 1920s while investigating scattering problems in quantum mechanics. This "function" seemed to violate most properties of other functions known to mathematicians at the time. However, later, when mathematicians found a rigorous way of studying this and other functions similar to it, a new vista in higher mathematics opened up.

The derivative of the delta function, $\delta'(x-x')$ is such that for any ordinary function $f(x)$,

$$\int_{-\infty}^{\infty} f(x)\delta'(x-a)\,dx = -\int_{-\infty}^{\infty} f'(x)\delta(x-a)\,dx = -f'(a).$$

We can *define* $\delta'(x-a)$ by this relation. In addition, we can define the derivative of any function, including discontinuous functions, at any point (including points of discontinuity, where the usual definition of derivative fails) by this relation. That is, if $\varphi(x)$ is a "bad" function whose derivative is not defined at some point(s), and $f(x)$ is a "good" function, we can define the derivative of $\varphi(x)$ by

$$\int_{-\infty}^{\infty} f(x)\varphi'(x)\,dx \equiv -\int_{-\infty}^{\infty} f'(x)\varphi(x)\,dx.$$

The integral on the RHS is well-defined.

Functions such as the Dirac delta function and its derivatives of all orders are not functions in the traditional sense. What is common among all of them is that in most applications they appear inside an integral, and we saw in Chap. 2 that integration can be considered as a linear functional on the space of continuous functions. It is therefore natural to describe such functions in terms of linear functionals. This idea was picked up by Laurent Schwartz in the 1950s who developed it into a new branch of mathematics called **generalized functions**, or **distributions**.

A distribution is a mathematical entity that appears inside an integral in conjunction with a well-behaved **test function**—which we assume to depend on n variables—such that the result of integration is a well-defined number. Depending on the type of test function used, different kinds of distributions can be defined. If we want to include the Dirac delta function and its derivatives of all orders, then the test functions must be infinitely differentiable, that is, they must be $\mathcal{C}^\infty$ functions on $\mathbb{R}^n$ (or $\mathbb{C}^n$). Moreover, in

test function

order for the theory of distributions to be mathematically feasible, all the test functions must be of **compact support**, i.e., they must vanish outside a finite "volume" of $\mathbb{R}^n$ (or $\mathbb{C}^n$). One common notation for such functions is $\mathcal{C}_F^\infty(\mathbb{R}^n)$ or $\mathcal{C}_F^\infty(\mathbb{C}^n)$ (F stands for "finite"). The definitive property of distributions concerns the way they combine with test functions to give a number. The test functions used clearly form a vector space over $\mathbb{R}$ or $\mathbb{C}$. In this vector-space language, distributions are linear functionals. The linearity is a simple consequence of the properties of the integral. We therefore have the following definition of a distribution.

generalized functions and distributions defined

Definition 7.4.1 A **distribution**, or **generalized function**, is a continuous[6] linear functional on the space $\mathcal{C}_F^\infty(\mathbb{R}^n)$ or $\mathcal{C}_F^\infty(\mathbb{C}^n)$. If $f \in \mathcal{C}_F^\infty$ and φ is a distribution, then $\varphi[f] = \int_{-\infty}^{\infty} \varphi(\mathbf{r}) f(\mathbf{r})\, d^n x$.

Another notation used in place of $\varphi[f]$ is $\langle \varphi, f \rangle$. This is more appealing not only because φ is linear, in the sense that $\varphi[\alpha f + \beta g] = \alpha\varphi[f] + \beta\varphi[g]$, but also because the set of all such linear functionals forms a vector space; that is, the linear combination of the φ's is also defined. Thus, $\langle \varphi, f \rangle$ suggests a mutual "democracy" for both f's and φ's.

We now have a shorthand way of writing integrals. For instance, if δ_a represents the Dirac delta function $\delta(x - a)$, with an integration over x understood, then $\langle \delta_a, f \rangle = f(a)$. Similarly, $\langle \delta'_a, f \rangle = -f'(a)$, and for linear combinations, $\langle \alpha\delta_a + \beta\delta'_a, f \rangle = \alpha f(a) - \beta f'(a)$.

Example 7.4.2 An ordinary (continuous) function g can be thought of as a special case of a distribution. The linear functional $g : \mathcal{C}_F^\infty(\mathbb{R}) \to \mathbb{R}$ is simply defined by $\langle g, f \rangle \equiv g[f] = \int_{-\infty}^{\infty} g(x) f(x)\, dx$.

Example 7.4.3 An interesting application of distributions (generalized functions) occurs when the notion of density is generalized to include not only (smooth) volume densities, but also point-like, linear, and surface densities.

A point charge q located at $\mathbf{r}_0$ can be thought of as having a charge density $\rho(\mathbf{r}) = q\delta(\mathbf{r} - \mathbf{r}_0)$. In the language of linear functionals, we interpret ρ as a distribution, $\rho : \mathcal{C}_F^\infty(\mathbb{R}^3) \to \mathbb{R}$, which for an arbitrary function f gives

$$\rho[f] = \langle \rho, f \rangle = q f(\mathbf{r}_0). \tag{7.27}$$

The delta function character of ρ can be detected from this equation by recalling that the LHS is

$$\int \rho(\mathbf{r}) f(\mathbf{r})\, d^3x = \lim_{\substack{N \to \infty \\ \Delta V_i \to 0}} \sum_{i=1}^{N} \rho(\mathbf{r}_i) f(\mathbf{r}_i) \Delta V_i.$$

[6] See [Zeid 95, pp. 27, 156–160] for a formal definition of continuity for linear functionals.

On the RHS of this equation, the only volume element that contributes is the one that contains the point $\mathbf{r}_0$; all the rest contribute zero. As $\Delta V_i \to 0$, the only way that the RHS can give a nonzero number is for $\rho(\mathbf{r}_0)f(\mathbf{r}_0)$ to be infinite. Since f is a well-behaved function, $\rho(\mathbf{r}_0)$ must be infinite, implying that $\rho(\mathbf{r})$ acts as a delta function. This shows that the definition of Eq. (7.27) leads to a delta-function behavior for ρ. Similarly for linear and surface densities.

The example above and Problems 7.12 and 7.13 suggest that a distribution that confines an integral to a lower-dimensional space must have a delta function in its definition.

We have seen that the delta function can be thought of as the limit of an ordinary function. This idea can be generalized.

Definition 7.4.4 Let $\{\varphi_n(x)\}$ be a sequence of functions such that

$$\lim_{n\to\infty}\int_{-\infty}^{\infty}\varphi_n(x)f(x)\,dx$$

exists *for all* $f \in \mathcal{C}_F^\infty(\mathbb{R})$. Then the sequence is said to converge to the distribution φ, defined by

$$\langle\varphi, f\rangle = \lim_{n\to\infty}\int_{-\infty}^{\infty}\varphi_n(x)f(x)\,dx \quad \forall f.$$

This convergence is denoted by $\varphi_n \to \varphi$.

For example, it can be verified that

$$\frac{n}{\sqrt{\pi}}e^{-n^2x^2} \to \delta(x) \quad \text{and} \quad \frac{1-\cos nx}{n\pi x^2} \to \delta(x)$$

and so on. The proofs are left as exercises.

Historical Notes

"Physical Laws should have mathematical beauty." This statement was Dirac's response to the question of his philosophy of physics, posed to him in Moscow in 1955. He wrote it on a blackboard that is still preserved today.

Paul Adrien Maurice Dirac (1902–1984), was born in 1902 in Bristol, England, of a Swiss, French-speaking father and an English mother. His father, a taciturn man who refused to receive friends at home, enforced young Paul's silence by requiring that only French be spoken at the dinner table. Perhaps this explains Dirac's later disinclination toward collaboration and his general tendency to be a loner in most aspects of his life. The fundamental nature of his work made the involvement of students difficult, so perhaps Dirac's personality was well-suited to his extraordinary accomplishments.


Paul Adrien Maurice Dirac 1902–1984

Dirac went to Merchant Venturer's School, the public school where his father taught French, and while there displayed great mathematical abilities. Upon graduation, he followed in his older brother's footsteps and went to Bristol University to study electrical engineering. He was 19 when he graduated Bristol University in 1921. Unable to find a suitable engineering position due to the economic recession that gripped post-World War I England, Dirac accepted a fellowship to study mathematics at Bristol University. This fellowship, together with a grant from the Department of Scientific and Industrial Research, made it possible for Dirac to go to Cambridge as a research student in 1923. At Cambridge Dirac was exposed to the experimental activities of the Cavendish Laboratory, and he became a member of the intellectual circle over which Rutherford and Fowler presided. He took his Ph.D. in 1926 and was elected in 1927 as a fellow. His appointment as university lecturer came in 1929. He assumed the Lucasian professorship following Joseph Larmor in 1932 and retired from it in 1969. Two years later he accepted a position at Florida State University where he lived out his remaining years. The FSU library now carries his name.

"The amount of theoretical ground one has to cover before being able to solve problems of real practical value is rather large, but this circumstance is an inevitable consequence of the fundamental part played by transformation theory and is likely to become more pronounced in the theoretical physics of the future." P.A.M. Dirac (1930)

In the late 1920s the relentless march of ideas and discoveries had carried physics to a generally accepted relativistic theory of the electron. Dirac, however, was dissatisfied with the prevailing ideas and, somewhat in isolation, sought for a better formulation. By 1928 he succeeded in finding an equation, the *Dirac equation*, that accorded with his own ideas and also fit most of the established principles of the time. Ultimately, this equation, and the physical theory behind it, proved to be one of the great intellectual achievements of the period. It was particularly remarkable for the internal beauty of its mathematical structure, which not only clarified previously mysterious phenomena such as **spin** and the **Fermi-Dirac** statistics associated with it, but also predicted the existence of an electron-like particle of negative energy, the antielectron, or *positron*, and, more recently, it has come to play a role of great importance in modern mathematics, particularly in the interrelations between topology, geometry, and analysis. Heisenberg characterized the discovery of antimatter by Dirac as "the most decisive discovery in connection with the properties or the nature of elementary particles.... This discovery of particles and antiparticles by Dirac ... changed our whole outlook on atomic physics completely." One of the interesting implications of his work that predicted the positron was the prediction of a *magnetic monopole*. Dirac won the Nobel Prize in 1933 for this work.

Dirac is not only one of the chief authors of quantum mechanics, but he is also the creator of *quantum electrodynamics* and one of the principal architects of *quantum field theory*. While studying the scattering theory of quantum particles, he invented the (Dirac) *delta function*; in his attempt at quantizing the general theory of relativity, he founded *constrained Hamiltonian dynamics*, which is one of the most active areas of theoretical physics research today. One of his greatest contributions is the invention of *bra* $\langle\,|$ and *ket* $|\,\rangle$.

While at Cambridge, Dirac did not accept many research students. Those who worked with him generally thought that he was a good supervisor, but one who did not spend much time with his students. A student needed to be extremely independent to work under Dirac. One such student was Dennis Sciama, who later became the supervisor of Stephen Hawking, the current holder of the Lucasian chair. Salam and Wigner, in their preface to the Festschrift that honors Dirac on his seventieth birthday and commemorates his contributions to quantum mechanics succinctly assessed the man:

> Dirac is one of the chief creators of quantum mechanics.... Posterity will rate Dirac as one of the greatest physicists of all time. The present generation values him as one of its greatest teachers.... On those privileged to know him, Dirac has left his mark ... by his human greatness. He is modest, affectionate, and sets the highest possible standards of personal and scientific integrity. He is a legend in his own lifetime and rightly so.

(Taken from Schweber, S.S. "Some chapters for a history of quantum field theory: 1938-1952", in *Relativity, Groups, and Topology II* vol. 2, B.S. DeWitt and R. Stora, eds., North-Holland, Amsterdam, 1984.)

derivative of a distribution

Definition 7.4.5 The **derivative** of a distribution φ is another distribution φ' defined by $\langle\varphi', f\rangle = -\langle\varphi, f'\rangle\ \forall f \in \mathcal{C}_F^\infty$.

Example 7.4.6 We can combine the last two definitions to show that if the functions θ_n are defined as

$$\theta_n(x) \equiv \begin{cases} 0 & \text{if } x \le -\frac{1}{n}, \\ (nx+1)/2 & \text{if } -\frac{1}{n} \le x \le \frac{1}{n}, \\ 1 & \text{if } x \ge \frac{1}{n}, \end{cases}$$

then $\theta_n'(x) \to \delta(x)$.

We write the definition of the derivative, $\langle \theta_n', f\rangle = -\langle \theta_n, f'\rangle$, in terms of integrals:

$$\begin{aligned}
&\int_{-\infty}^{\infty} \theta_n'(x) f(x)\, dx \\
&= -\int_{-\infty}^{\infty} \theta_n(x) \frac{df}{dx}\, dx = -\int_{-\infty}^{\infty} \theta_n(x)\, df \\
&= -\left(\int_{-\infty}^{-1/n} \theta_n(x)\, df + \int_{-1/n}^{1/n} \theta_n(x)\, df + \int_{1/n}^{\infty} \theta_n(x)\, df\right) \\
&= -\left(0 + \int_{-1/n}^{1/n} \frac{nx+1}{2}\, df + \int_{1/n}^{\infty} df\right) \\
&= -\frac{n}{2} \int_{-1/n}^{1/n} x\, df - \frac{1}{2} \int_{-1/n}^{1/n} df - \int_{1/n}^{\infty} df \\
&= -\frac{n}{2} \left(x f(x)\Big|_{-1/n}^{1/n} - \int_{-1/n}^{1/n} f(x)\, dx \right) \\
&\quad - \frac{1}{2}\big(f(1/n) - f(-1/n)\big) - f(\infty) + f(1/n).
\end{aligned}$$

For large n, we have $1/n \approx 0$ and $f(\pm 1/n) \approx f(0)$. Thus,

$$\begin{aligned}
\int_{-\infty}^{\infty} \theta_n'(x) f(x)\, dx &\approx -\frac{n}{2}\left(\frac{1}{n} f\left(\frac{1}{n}\right) + \frac{1}{n} f\left(-\frac{1}{n}\right) - \frac{2}{n} f(0)\right) + f(0) \\
&\approx f(0).
\end{aligned}$$

The approximation becomes equality in the limit $n \to \infty$. Thus,

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} \theta_n'(x) f(x)\, dx = f(0) = \langle \delta_0, f\rangle \quad \Rightarrow \quad \theta_n' \to \delta.$$

Note that $f(\infty) = 0$ because of the assumption that all functions must vanish outside a finite volume.

7.5 Problems

7.1 Show that $|\|a\| - \|b\|| \le \|a \pm b\| \le \|a\| + \|b\|$.

7.2 Show that a convergent sequence is necessarily Cauchy.

7.3 Verify that the sequence of functions $\{f_k(x)\}$ defined in Example 7.1.5 is a Cauchy sequence.

7.4 Prove the completeness of $\mathbb{C}$, using the completeness of $\mathbb{R}$.

7.5 Let $\mathcal{L}^1(\mathbb{R})$ be the set of all functions f such that $\|f\| \equiv \int_{-\infty}^{\infty} |f(x)|\, dx$ is finite. This is clearly a normed vector space. Let f and g be nonzero functions such that at no x are $f(x)$ and $g(x)$ both nonzero. Verify that

(a) $\|f \pm g\| = \|f\| + \|g\|$.
(b) $\|f + g\|^2 + \|f - g\|^2 = 2(\|f\| + \|g\|)^2$.
(c) Using parts (a), (b), and Theorem 2.2.9, show that $\mathcal{L}^1(\mathbb{R})$ is not an inner product space.

This construction shows that not all norms arise from an inner product.

7.6 Use Eq. (7.10) to derive Eq. (7.12). Hint: To find a_n, equate the coefficients of x^n on both sides of Eq. (7.10). To find a_{n-1}, multiply both sides of Eq. (7.10) by $C_{n-1}w(x)$ and integrate, using the definitions of $k_n^{(n)}$, $k_n^{(n-1)}$, and h_n.

7.7 Evaluate the integral $\int_a^b x^2 C_m(x) C_n(x) w(x)\, dx$.

7.8 Write a density function for two point charges q_1 and q_2 located at $\mathbf{r} = \mathbf{r}_1$ and $\mathbf{r} = \mathbf{r}_2$, respectively.

7.9 Write a density function for four point charges $q_1 = q$, $q_2 = -q$, $q_3 = q$ and $q_4 = -q$, located at the corners of a square of side $2a$, lying in the xy-plane, whose center is at the origin and whose first corner is at (a, a).

7.10 Show that $\delta(f(x)) = \frac{1}{|f'(x_0)|}\delta(x - x_0)$, where x_0 is a root of f and x is confined to values close to x_0. Hint: Make a change of variable to $y = f(x)$.

7.11 Show that

$$\delta\big(f(x)\big) = \sum_{k=1}^{m} \frac{1}{|f'(x_k)|}\delta(x - x_k),$$

where the x_k's are all the roots of f in the interval on which f is defined.

7.12 Define the distribution $\rho : \mathcal{C}^\infty(\mathbb{R}^3) \to \mathbb{R}$ by

$$\langle \rho, f \rangle = \iint_S \sigma(\mathbf{r}) f(\mathbf{r})\, da(\mathbf{r}),$$

where $\sigma(\mathbf{r})$ is a smooth function on a smooth surface S in $\mathbb{R}^3$. Show that $\rho(\mathbf{r})$ is zero if $\mathbf{r}$ is not on S and infinite if $\mathbf{r}$ is on S.

7.13 Define the distribution $\rho : \mathcal{C}^\infty(\mathbb{R}^3) \to \mathbb{R}$ by

$$\langle \rho, f \rangle = \int_C \lambda(\mathbf{r}) f(\mathbf{r})\, d\ell(\mathbf{r}),$$

where $\lambda(\mathbf{r})$ is a smooth function on a smooth curve C in $\mathbb{R}^3$. Show that $\rho(\mathbf{r})$ is zero if $\mathbf{r}$ is not on C and infinite if $\mathbf{r}$ is on C.

7.14 Express the three-dimensional Dirac delta function as a product of three one-dimensional delta functions involving the coordinates in

(a) cylindrical coordinates,
(b) spherical coordinates,
(c) general curvilinear coordinates.

Hint: The Dirac delta function in $\mathbb{R}^3$ satisfies $\iiint \delta(\mathbf{r}) d^3x = 1$.

7.15 Show that $\int_{-\infty}^{\infty} \delta'(x) f(x)\, dx = -f'(0)$ where $\delta'(x) \equiv \frac{d}{dx}\delta(x)$.

7.16 Evaluate the following integrals:

$$\text{(a)} \quad \int_{-\infty}^{\infty} \delta\big(x^2 - 5x + 6\big)\big(3x^2 - 7x + 2\big)\, dx.$$

$$\text{(b)} \quad \int_{-\infty}^{\infty} \delta\big(x^2 - \pi^2\big) \cos x\, dx.$$

$$\text{(c)} \quad \int_{0.5}^{\infty} \delta(\sin \pi x) \left(\frac{2}{3}\right)^x dx.$$

$$\text{(d)} \quad \int_{-\infty}^{\infty} \delta\big(e^{-x^2}\big) \ln x\, dx.$$

Hint: Use the result of Problem 7.11.

7.17 Consider $|x|$ as a generalized function and find its derivative.

7.18 Let $\eta \in \mathcal{C}^\infty(\mathbb{R}^n)$ be a smooth function on $\mathbb{R}^n$, and let φ be a distribution. Show that $\eta\varphi$ is also a distribution. What is the natural definition for $\eta\varphi$? What is $(\eta\varphi)'$, the derivative of $\eta\varphi$?

7.19 Show that each of the following sequences of functions approaches $\delta(x)$ in the sense of Definition 7.4.4.

$$\text{(a)} \quad \frac{n}{\sqrt{\pi}} e^{-n^2x^2}.$$

$$\text{(b)} \quad \frac{1 - \cos nx}{\pi n x^2}.$$

$$\text{(c)} \quad \frac{n}{\pi} \frac{1}{1 + n^2x^2}.$$

$$\text{(d)} \quad \frac{\sin nx}{\pi x}.$$

Hint: Approximate $\varphi_n(x)$ for large n and $x \approx 0$, and then evaluate the appropriate integral.

7.20 Show that $\frac{1}{2}(1 + \tanh nx) \to \theta(x)$ as $n \to \infty$.

7.21 Show that $x\delta'(x) = -\delta(x)$.