4

Function Vector Spaces and Fourier Series

Vector spaces of functions can be infinite-dimensional. This implies a non-trivial extension of many of the concepts developed for finite-dimensional spaces. Section 4.1 is meant to provide a general picture of the location and depth of these extensions, introducing an infinite orthonormal set of functions $(2\pi)^{-1/2} \exp(inx)$, for $n = 0, \pm 1, \pm 2, \ldots$, periodic in x with period 2π. A large class of functions can be expanded in a series, called Fourier series, involving this orthonormal set. In Section 4.2 we prove one version of the Dirichlet conditions which give a sufficiency definition for this set, while in Sections 4.3 and 4.4 we explore several properties of series expansions related to each other by translation, inversion, complex conjugation, and differentiation and examine their convergence rates and the Gibbs phenomenon. The next two sections, 4.5 and 4.6, enter into the field of generalized functions and their divergent series representation. Although the complete mathematical treatment of this subject is by no means elementary, we have followed a "middle path" in the spirit of a physicist's use of quantum mechanics. Section 4.7 collects some results to be used in Chapter 5 and establishes a link with Part III.

4.1. Notions on Function Vector Spaces

The defining properties of complex vector spaces were given in Section 1.1. These comprise the operations of sum of vectors, multiplication by complex numbers, and the distributivity of one with respect to the other. The largest number of linearly independent vectors one can find in the space defines the *dimension* of that space. When this number is not bounded, the space is said to be infinite-dimensional. In this section we shall see that sets of *functions* over some interval constitute such spaces. While intuition based on ordinary finite-dimensional spaces is a reliable guide, the concepts must be sharpened. Here we shall present the main ideas but gloss over the considerable mathematical sophistication needed to fully justify them.

4.1.1. The Vector Space Axioms

Let $f(x), g(x), \ldots \in \mathscr{F}_{\mathscr{I}}$ denote functions whose domain $\mathscr{I}$ is an interval in the real line $\mathscr{R}$ and whose range is the field of complex numbers $\mathscr{C}$ (i.e., $f\colon \mathscr{I} \to \mathscr{C}, \mathscr{I} \subseteq \mathscr{R}$). Then $af(x) + bg(x)$, where $a, b \in \mathscr{C}$ is another such function, an element of $\mathscr{F}_{\mathscr{I}}$. The defining properties of vector spaces (Section 1.1) are satisfied, and $\mathscr{F}_{\mathscr{I}}$ is thus a vector space whose elements, functions, are the vectors in the space.

4.1.2. Linear Independence

The statement of *linear independence* of a finite set of functions $\{f_n(x)\}_{n=1}^N := \{f_1(x), f_2(x), \ldots, f_N(x)\}, f_k(x) \in \mathscr{F}_{\mathscr{I}}$, can be phrased as

$$\sum_{n=1}^{N} c_n f_n(x) = 0 \Leftrightarrow c_n = 0, \qquad n = 1, 2, \ldots, N. \tag{4.1}$$

[This is a direct translation of Eq. (1.1).] When the functions $f_n(x)$ of our chosen set are $N - 1$ times differentiable, linear independence can be tested in principle by constructing the system of equations formed by (4.1) and its $N - 1$ derivatives:

$$\sum_{n=1}^{N} c_n f_n^{(p)}(x) = 0, \qquad p = 0, 1, 2, \ldots, N - 1. \tag{4.2}$$

If the c_n are zero, (4.2) is clearly satisfied. Now, for (4.2) to imply that all $c_n = 0$, the *determinant* of the system (4.2) must be *different* from zero. This is the *Wronskian* of the set:

$$W(\{f_n\}, x) := \det\|d^{p-1}f_n(x)/dx^{p-1}\|, \qquad p, n = 1, 2, \ldots, N. \tag{4.3}$$

4.1.3. Spaces of Polynomials

Consider as a first example the set of *power* functions in $\mathscr{F}_{\mathscr{I}}$:

$$t_n(x) := x^{n-1}/(n - 1)!, \qquad n = 1, 2, \ldots, N. \tag{4.4}$$

These are, of course, differentiable to any order as $d^p t_n(x)/dx^p = t_{n-p}(x)$, $t_1(x) = 1$, $t_n(x) := 0$ for $n \leqslant 0$. The Wronskian (4.3) will then be the determinant of a triangular matrix whose diagonal elements are $d^{n-1}t_n(x)/dx^{n-1} = 1$, and hence $W(\{t_n\}, x) = 1$ for any value of N. Now, linear combinations of the vectors (4.4),

$$f(x) = \sum_{n=1}^{N} c_n t_n(x) = \sum_{n=1}^{N} c_n x^{n-1}/(n-1)!, \tag{4.5}$$

can easily be seen to constitute a vector space of dimension N with a basis (4.4). In fact, they are the set of *polynomials* up to degree $N-1$.

What happens when we let N grow without bound? The basis vectors will remain linearly independent, and the set (4.5) will become the space of all formal power series

$$f(x) = \sum_{n=1}^{\infty} c_n x^{n-1}/(n-1)! \tag{4.6}$$

characterized by the set of coefficients $\{c_n\}_{n=1}^{\infty}$, $c_n \in \mathscr{C}$. There are several observations to be made here: (a) If the series (4.6) converges for all x in the interval $\mathscr{I}$, it represents the Taylor expansion of $f(x)$. This is the case, in particular, when the set $\{c_n\}_{n=1}^{\infty}$ has a finite number of nonzero coefficients so that $f(x)$ is actually a polynomial. (b) The series (4.6), when evaluated, may well diverge within $\mathscr{I}$. The formal power series (4.6) can still be handled, however, in terms of the *coordinates* $\{c_n\}_{n=1}^{\infty}$ and subjected to the formal operations of sum and multiplication by a number. (c) We have no guarantee that the space of functions (4.6) is the set of *all* functions in $\mathscr{F}_{\mathscr{I}}$. In fact, it is clearly not.

4.1.4. Inner Product and Norm

To have a better grasp of function vector spaces, it is convenient to introduce an *inner product* in $\mathscr{F}_{\mathscr{I}}$. For $\mathbf{f}$ and $\mathbf{g} \in \mathscr{F}_{\mathscr{I}}$ representing the functions $f(x)$ and $g(x)$, respectively, we define this (in analogy to Section 1.2) as

$$(\mathbf{f}, \mathbf{g}) := \int_{\mathscr{I}} dx f(x)^* g(x). \tag{4.7}$$

In the process of introducing such an inner product, we shall be losing those functions in $\mathscr{F}_{\mathscr{I}}$ whose integral is not defined. This inner product (4.7) is *sesquilinear*, i.e., linear in the second argument and antilinear in the first [Eqs. (1.4) and (1.5)]. From (4.7) we can also define a *norm* as

$$\|\mathbf{f}\| := (\mathbf{f}, \mathbf{f})^{1/2} = \left[\int_{\mathscr{I}} dx |f(x)|^2\right]^{1/2}. \tag{4.8}$$

On the question of whether the inner product (4.7) is positive definite, note that we may have functions $z(x)$ which are zero *almost everywhere* in $\mathscr{I}$, i.e., except on at most a denumerable number of isolated points, where they can take finite values. All such functions will have $\|\mathbf{z}\| = 0$ under (*Lebesgue*) integration. We shall consider all such functions to be *equivalent* to the null function ($\mathbf{z} = \mathbf{0}$). We shall similarly speak of $\mathbf{f}$ and any $\mathbf{f} + \mathbf{z}$ being equivalent. In this context, the inner product (4.7) is positive definite, as *only* for $\mathbf{f} = \mathbf{0}$, i.e., equivalent to the null function, do we have $\|\mathbf{f}\| = 0$. The space of the (*Lebesgue*) square-integrable functions plays a central role in much of mathematical physics and will be denoted by $\mathscr{L}^2(\mathscr{I})$.

One important property of vector spaces with positive inner products is that their elements satisfy the *Schwartz inequality*, which was seen in Section 1.2 and which takes the same form as in Eq. (1.13): $|(\mathbf{f}, \mathbf{g})|^2 \leqslant \|\mathbf{f}\| \cdot \|\mathbf{g}\|$. There, the proof did not require the dimension of the space to be finite. In this part we consider the case when $\mathscr{I}$ is a *finite* interval within $\mathscr{R}$. By translations and changes of scale in x we can always transform $\mathscr{I}$ onto the interval extending from $-\pi$ to π.

4.1.5. A Set of Orthonormal Oscillating Exponential Functions

A set of functions $\{f_n(x)\}$ which satisfy $(\mathbf{f}_n, \mathbf{f}_m) = 0$ for $n \neq m$ will be said to be *orthogonal*. Moreover, if $\|\mathbf{f}_n\| = 1$, the set is *orthonormal*. The functions

$$\varphi_n(x) := (2\pi)^{-1/2} \exp(inx), \qquad n = 0, \pm 1, \pm 2, \ldots, x \in (-\pi, \pi], \tag{4.9}$$

can be seen to constitute such an orthonormal set since

$$\begin{aligned}(\boldsymbol{\varphi}_n, \boldsymbol{\varphi}_m) &= (2\pi)^{-1} \int_{-\pi}^{\pi} dx [\exp(inx)]^* \exp(imx) \\ &= (2\pi)^{-1} \int_{-\pi}^{\pi} dx \exp[i(m-n)x] \\ &= \begin{cases} [2\pi i(m-n)]^{-1} \exp[i(m-n)x]|_{-\pi}^{\pi} = 0, & n \neq m, \\ (2\pi)^{-1} \displaystyle\int_{-\pi}^{\pi} dx = 1, & n = m. \end{cases}\end{aligned} \tag{4.10}$$

We shall henceforth denote by $\mathscr{Z}$ the set of all integers. A set of orthogonal functions is also linearly independent in a space with a positive inner product, since $\sum_{n \in \mathscr{Z}} c_n \boldsymbol{\varphi}_n = 0$ when placed in inner product with any one $\boldsymbol{\varphi}_m$ leads to $c_m(\boldsymbol{\varphi}_m, \boldsymbol{\varphi}_m) = 0$, which implies $c_m = 0$ for $m \in \mathscr{Z}$.

Exercise 4.1. Show that the set of power functions (4.4) does *not* form an orthonormal set under (4.7). The implementation of the Schmidt orthogonalization procedure leads to the basis of orthogonal *Legendre* polynomials $P_n(\pi x)$. [See, for instance, the book by Dennery and Krzywicki (1967, Chapter III).]

4.1.6. The Space of Formal Fourier Series

We construct now the space of all formal series involving (4.9):

$$f(x) = \sum_{n \in \mathscr{Z}} f_n \varphi_n(x), \qquad f_n \in \mathscr{C}. \tag{4.11a}$$

Performing the inner product of the above equation with $\varphi_m(x)$ and assuming that the sum and the integration in the inner product can be exchanged, we can use the linearity of the product and the orthonormality of the set $\{\boldsymbol{\varphi}_n\}_{n \in \mathscr{Z}}$ in order to find the *coordinates* of $\mathbf{f}$ in the $\boldsymbol{\varphi}$-basis as

$$f_n = (\boldsymbol{\varphi}_n, \mathbf{f}). \tag{4.11b}$$

The inner product can then be written as

$$(\mathbf{f}, \mathbf{g}) = \Big(\sum_{n \in \mathscr{Z}} f_n \boldsymbol{\varphi}_n, \mathbf{g}\Big) = \sum_{n \in \mathscr{Z}} f_n^* (\boldsymbol{\varphi}_n, \mathbf{g}) = \sum_{n \in \mathscr{Z}} f_n^* g_n. \tag{4.12}$$

Written out, Eqs. (4.11) read

$$f(x) = (2\pi)^{-1/2} \sum_{n \in \mathscr{Z}} f_n \exp(inx), \tag{4.13a}$$

$$f_n = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) \exp(-inx). \tag{4.13b}$$

These are referred to, respectively, as the *Fourier series* and *partial-wave decomposition* or as the Fourier partial-wave *synthesis* and *analysis*. Equation (4.12) is the generalized *Parseval identity*

$$(\mathbf{f}, \mathbf{g}) = \int_{-\pi}^{\pi} dx f(x)^* g(x) = \sum_{n \in \mathscr{Z}} f_n^* g_n. \tag{4.14}$$

This is a relation between the integral of the product of two functions and the sum of their partial-wave products.

4.1.7. Further Comments

Before pointing out the mathematical difficulties we have glossed over in deriving (4.13) and (4.14), let us interpret these formulas as they stand. Equations (4.13) tell us that an arbitrary function (in a class still to be determined) on the interval from $-\pi$ to π can be expanded in a series of exponential functions quite similar to the Taylor expansion (4.6). This result might appear rather surprising, and indeed, historically, although Euler and Lagrange worked with series of the type (4.13a), they assumed that $f(x)$ had to be infinitely differentiable, since the summands of the series are. It was Fourier who in 1822 first dealt with series of the type (4.13a) to expand functions which were composed of an arbitrary (but finite) number of segments of different continuous functions. Sufficiency conditions for the convergence of the series were found later by Dirichlet (Section 4.2). In contrast with the Taylor series (4.6), where the coefficients $c_n = d^{n-1}f(x)/dx^{n-1}|_{x=0}$ depend on the *local* properties of the function, i.e., the value of $f(x)$ and its derivatives at the single point $x = 0$, say, the Fourier partial-wave coefficients (4.13b) depend on the *global* characteristics of the function throughout the integration interval and not at all on the value of the function at any single ordinary point. Fourier series have been used extensively for generations in problems connected with wave and diffusion phenomena, some of which will appear in subsequent chapters.

Not until the 1930s, however, did physicists start making use of the formal Fourier series (4.13a) when convergence in the classical sense was *not* assured or expected. The work of Dirac (1935) in quantum mechanics, fundamental as it is, was not considered mathematically sound until it was fully justified by the distribution theory of L. Schwartz in the early 1950s. Although divergent series within integrals had been properly treated by Fejér and Cesàro, Dirac performed many of the dubious steps we have followed in deriving (4.13), particularly the exchange of infinite summations and integrals [leading from (4.10) and (4.11a) to (4.11b) and (4.12)], neither of which need exist. In presenting our results in the way we shall, we are not engaging in violence with existing mathematics but are rather exploiting the fact that the notation and "naïve" concepts used in classical analysis can be considerably stretched to include deeper results in an operationally well-defined way. In the following sections we shall find several instances where, with the appropriate warning signs, such an approach leads to profitable shortcuts.

Exercise 4.2. Explore the relation between the Taylor and Fourier series as follows. Let $F(z)$ be a function of the complex variable z, analytic in a disk with center at the origin and radius α. The coefficients in the Taylor expansion

$$F(z) = \sum_{n=0}^{\infty} F_n z^n/n! \tag{4.15a}$$

can be written, using Cauchy's theorem [see Ahlfors (1953, Chapter 4)], as

$$F_n = F^{(n)}(0) = \frac{n!}{2\pi i}\oint_C dz F(z) z^{-n-1}, \tag{4.15b}$$

where the contour C encircles the origin in a counterclockwise direction inside the region of analyticity of F. (See Fig. 4.1.) Let $z = \rho e^{i\phi}$, and consider the circular integration contour C with center at the origin and radius $\gamma < \alpha$, the contour line element being $dz = i\gamma e^{i\phi}\, d\phi$. Let $f_\rho(\phi) := (2\pi)^{-1/2}F(\rho e^{i\phi})$. Equations (4.15) then become

$$f_\rho(\phi) = (2\pi)^{-1/2}\sum_{n=0}^{\infty} F_n\rho^n \exp(in\phi)/n! \tag{4.16a}$$

$$(n!)^{-1}\gamma^n F^n = (2\pi)^{-1/2}\int_{-\pi}^{\pi} d\phi f_\gamma(\phi)\exp(-in\phi). \tag{4.16b}$$

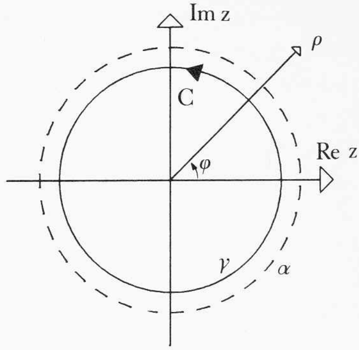

Fig. 4.1. Integration contour for Eq. (4.15b).

For $\rho = \gamma$ and $f_n := \gamma^n F_n/n!$ these are the Fourier series formulas ($n \geqslant 0$). The delicate point in this analysis (which is *not* an exercise) is the consideration of *all* functions for which this is valid, i.e., the limit $\gamma \to \alpha$. Note that (4.16a) involves only summation over nonnegative partial waves. These functions lie in *Hardy* spaces [see Dym and McKean (1972, Section 38.8)]. To obtain the full Fourier series, one has to consider Laurent expansions of functions analytic in an annulus.

4.2. The Dirichlet Conditions

The construction of the Fourier partial-wave analysis and synthesis as the "limit" of a succession of vector spaces of growing dimension (Sections 3.4 and 4.1), for all its suggestiveness, did not provide us with an unambiguous characterization of the class of functions which can be expanded in the set of functions $\{\varphi_n(x)\}_{n\in\mathscr{Z}}$ in Eq. (4.9). As a minimal condition, we saw that this could be done for functions $f(x)$ which are trigonometric polynomials, as then they are a finite sum of $\varphi_n(x)$'s and the orthogonality of the φ's alone guarantees the validity of the pair of equations (4.13)–(4.14).

4.2.1. Statement of the Theorem

A classic theorem by Dirichlet states that if a function $f(x)$ is periodic with period 2π and is *piecewise differentiable*, the succession of truncated sums

$$f_k(x) := (2\pi)^{-1/2} \sum_{|n|\leqslant k} f_n \exp(inx), \qquad k = 1, 2, \ldots, \tag{4.17a}$$

where

$$f_n := (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) \exp(-inx), \tag{4.17b}$$

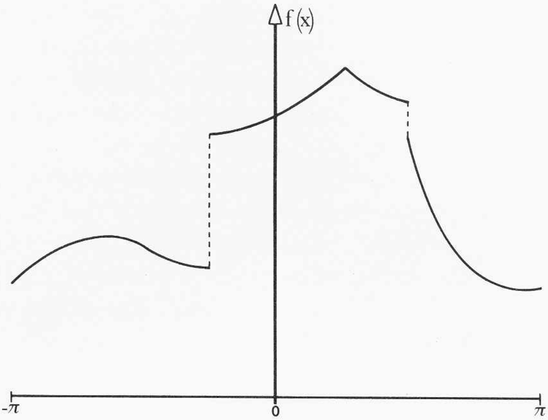

Fig. 4.2. A piecewise differentiable function has bounded derivatives everywhere, except at most at a finite number of points, where it may have bounded discontinuities. Even at these points, however, the limits of the derivatives are defined and bounded as we approach the discontinuity points from the right or from the left.

converges to $f(x)$ at all points of continuity of the function. At the points of discontinuity, if any, the succession converges to the midpoint, i.e.,

$$\lim_{k\to\infty} f_k(x) = \tfrac{1}{2}[f(x^+) + f(x^-)] := \lim_{\substack{\varepsilon\to 0 \\ (\varepsilon > 0)}} \tfrac{1}{2}[f(x+\varepsilon) + f(x-\varepsilon)]. \quad (4.17c)$$

Moreover, in any subinterval where $f(x)$ is free of discontinuities, the convergence of the sequence $f_k(x)$ to $f(x)$ is *uniform*, that is, the bound on $|f_k(x) - f(x)|$ is independent of x.

We remind the reader that a piecewise differentiable function is one which has a bounded left and right derivative everywhere except at most at a finite number of isolated points. Specifically, $f'(x^\pm) := \lim_{\varepsilon\to 0} df(y)/dy\,|_{y=x\pm\varepsilon}$, $\varepsilon > 0$, must have a finite value for every x, although in case $f(x)$ or $f'(x)$ has a discontinuity at x_0, $f'(x_0{}^+)$ and $f'(x_0{}^-)$ may be different. See Fig. 4.2. The discontinuity must thus be bounded, and therefore $f(x)$ itself is bounded. Since the interval is finite, the function is absolutely integrable.

We shall call the space of functions which satisfy the Dirichlet conditions $\mathscr{V}^D$. Note that any *finite* linear combination of functions in $\mathscr{V}^D$ is a function in $\mathscr{V}^D$.

4.2.2. Alternative Versions

The Dirichlet conditions, as stated above, are *sufficient* conditions for the *pointwise uniform* convergence (for every x in the interval) of the Fourier series. They are not necessary, however, and several weaker (and harder to prove) sets of conditions lead to similar results. A second commonly stated set of conditions is the following: Let $f(x)$ be a periodic function of period 2π which (a) is piecewise continuous, i.e., continuous at all but a finite set of points; (b) has a finite number of bounded discontinuities; (c) has a finite number of maxima and minima; and (d) is absolutely integrable. Then the succession of truncated sums (4.17a) converges as described above. The convergence is uniform for subintervals free of discontinuities of $f(x)$. Conditions (b) and (c) are asking for *bounded total variation*. Further weakening of the conditions can be achieved if these are required to hold only inside a subinterval of $[-\pi, \pi]$. [See, for example, Bary (1964, Chapter 1) and Dym and McKean (1972, Sections 1.4 and 1.5).]

4.2.3. Proof

Due to the transparency of the proof, we shall tackle the first version of the theorem. First substitute (4.17b) into (4.17a). As the sum is finite, it can be interchanged with integration, yielding

$$f_k(x) = (2\pi)^{-1} \int_{-\pi}^{\pi} dy f(y) \sum_{|n| \leqslant k} \exp[in(x - y)] =: \int_{-\pi}^{\pi} dy f(y) D_k(x - y), \tag{4.18}$$

where the *Dirichlet kernel* $D_k(x - y)$ can be calculated using the geometric progression formula (1.50) for $x = \exp[i(x - y)]$, $a = -k$, $b = 2k$:

$$\begin{aligned} D_k(z) &= (2\pi)^{-1} \sum_{|n| \leqslant k} \exp(inz) \\ &= (2\pi)^{-1}[1 - \exp(iz)]^{-1} \exp(-ikz)\{1 - \exp[i(2k + 1)z]\} \\ &= (2\pi)^{-1} \sin[(k + \tfrac{1}{2})z]/\sin(z/2). \end{aligned} \tag{4.19}$$

We note that the Dirichlet kernel is a real *even* function and that

$$D_k(0) = (2\pi)^{-1}(2k + 1), \tag{4.20a}$$

$$\int_{-\pi}^{\pi} dy D_k(x - y) = 1. \tag{4.20b}$$

The last relation is due to (4.10), as all but the $n = 0$ summand in (4.19) integrate to zero. The Dirichlet kernel (Fig. 4.3) oscillates strongly throughout the interval; at the midpoint it has its maximum at a peak which is roughly double the width of that of other oscillations. When integrated as in (4.18), in company with a differentiable or continuous function, this peak for large k is expected essentially to "punch out" the value of the function at $y = x$, the rapid oscillations beside the main peak giving a vanishing contribution due to the Riemann-Lebesgue lemma [see Apostol (1975, Section 15-6)].

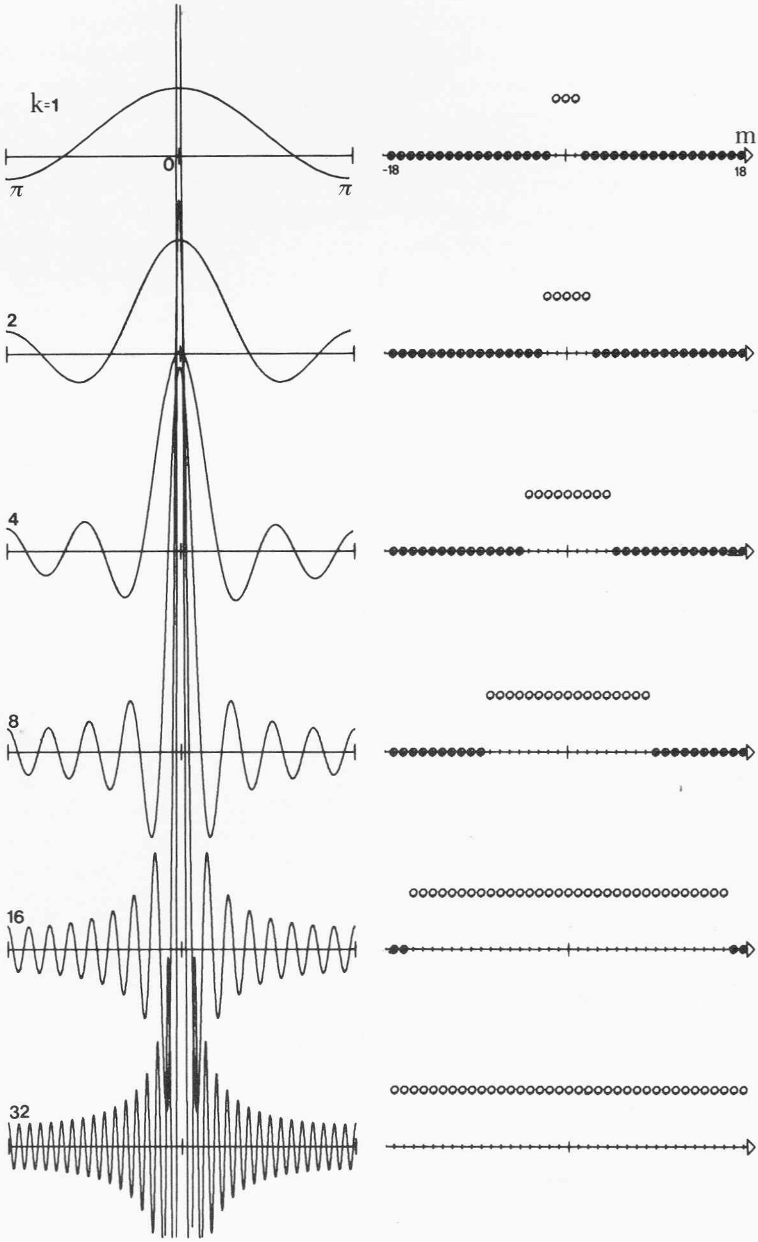

Fig. 4.3. Dirichlet kernel functions $D_k(x)$ for increasing values of k (left). These functions have constant partial-wave coefficients $(2\pi)^{-1/2}$ for $|m| \leqslant k$ (right). For increasing k, the central peak grows without bound.

Consider now the difference between the kth truncated sum $f_k(x)$ and $\frac{1}{2}[f(x^+) + f(x^-)]$, where $f(x^\pm) := \lim_{\varepsilon \to 0} f(x \pm \varepsilon)$, $\varepsilon > 0$. This allows us to work with points where the function is continuous, the last expression then being simply $f(x)$, or points where it is discontinuous but differentiable for points arbitrarily close at either side of the discontinuity. Using (4.18), (4.20b), the evenness of $D_k(x - y)$, and the periodicity of the functions involved, we write

$$f_k(x) - \tfrac{1}{2}[f(x^+) + f(x^-)] = \int_0^\pi dy[f(x + y) - f(x^+)]D_k(y) + \int_0^\pi dy[f(x - y) - f(x^-)]D_k(y). \quad (4.21)$$

The integrals have the form

$$\int_0^\pi dy g_\pm(x, y) \sin[(k + \tfrac{1}{2})y], \qquad g_\pm(x, y) = \tfrac{1}{2}[f(x \pm y) - f(x^\pm)]/\sin(y/2), \quad (4.22)$$

and they exist because the kernel and, by assumption, $f(x)$ are absolutely integrable. The only point which might seem troublesome is $y = 0$, but clearly $g_\pm(x, 0^\pm) = f'(x^\pm)$, which is bounded.

We can now integrate (4.22) by parts:

$$(k + \tfrac{1}{2})^{-1}\left\{ g_\pm(x, y) \cos[(k + \tfrac{1}{2})y]|_{y=0}^{\pi} - \int_0^\pi dy \frac{\partial g_\pm(x, y)}{\partial y} \cos[(k + \tfrac{1}{2})y] \right\}. \quad (4.23)$$

As the difference (4.21) is proportional to $(k + \frac{1}{2})^{-1}$ times a bounded function of x (see Exercise 4.3), when $k \to \infty$ this difference tends toward zero, and the succession of truncated sums $f_k(x)$ approaches $\frac{1}{2}[f(x^+) + f(x^-)]$. In particular, when x is a point where $f(x)$ is continuous, the bound of the function in (4.23) provides a bound on the difference (4.21) which is *independent* of x. The convergence of the succession of truncated sums will thus be *uniform* for the intervals of continuity of the function.

Exercise 4.3. Prove that $\partial g_\pm(x, y)/\partial y$ is a bounded function in the interval $[0, \pi]$. In particular, at the problematic point $y = 0$ this function is zero.

Exercise 4.4. Verify that the Parseval identity, Eq. (4.14), is a direct consequence of the validity of (4.17).

To provide working examples of Fourier series expansions which will be used later on, we shall consider some specific cases which satisfy the Dirichlet conditions.

4.2.4. Example: The Rectangle Function

The *rectangle function* of width ε and height η centered at the origin is

$$R^{(\varepsilon,\eta)}(x) := \begin{cases} \eta, & -\varepsilon/2 < x \leqslant \varepsilon/2 < \pi, \\ 0, & \text{otherwise.} \end{cases} \tag{4.24}$$

See Fig. 4.4. The rectangle function is assumed to be periodic as are all functions in $\mathscr{V}^D$, so we require $\varepsilon < 2\pi$. The partial-wave coefficients can be found by direct substitution in (4.17b):

$$R_0^{(\varepsilon,\eta)} = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx R^{(\varepsilon,\eta)}(x) = \eta(2\pi)^{-1/2} \int_{-\varepsilon/2}^{\varepsilon/2} dx = \eta\varepsilon(2\pi)^{-1/2}, \tag{4.25a}$$

$$R_n^{(\varepsilon,\eta)} = \eta(2\pi)^{-1/2} \int_{-\varepsilon/2}^{\varepsilon/2} dx \exp(-inx) = 2\eta \sin(\tfrac{1}{2}n\varepsilon)/(2\pi)^{1/2}n, \quad n \neq 0. \tag{4.25b}$$

Note that for $n = 0$ Eq. (4.25b) yields formally (4.25a).

Partial-wave synthesis for the truncated sums (4.17a) defines the functions

$$\begin{aligned} R_k^{(\varepsilon,\eta)}(x) &= (2\pi)^{-1/2} R_0^{(\varepsilon,\eta)} + (2\pi)^{-1/2} \sum_{0 \neq |n| \leqslant k} R_n^{(\varepsilon,\eta)} \exp(inx) \\ &= \eta(2\pi)^{-1}\Big(\varepsilon + 4 \sum_{0 \neq |n| \leqslant k} n^{-1} \sin \tfrac{1}{2}n\varepsilon \cos nx\Big) \\ &= \eta(2\pi)^{-1}\Big\{\varepsilon + 2 \sum_{n=1}^{k} n^{-1} \sin[n(x + \varepsilon/2)] \\ &\qquad - 2 \sum_{n=1}^{k} n^{-1} \sin[n(x - \varepsilon/2)]\Big\}. \end{aligned} \tag{4.26a}$$

These truncated sums have been plotted for a few values of k in Fig. 4.5. In this figure it appears that the truncated sums indeed converge to the original function. The oscillations near the edges of the discontinuity do not decrease in amplitude, however, as the number of terms increases. This is the *Gibbs phenomenon*, which we shall discuss further in Section 4.4. The result we have proved in this section tells us that, as the rectangle function (4.24) satisfies the Dirichlet conditions,

$$\lim_{k \to \infty} R_k^{(\varepsilon,\eta)}(x) = \begin{cases} R^{(\varepsilon,\eta)}(x), & x \neq \pm\varepsilon/2, \\ \eta/2, & x = \pm\varepsilon/2. \end{cases} \tag{4.26b}$$

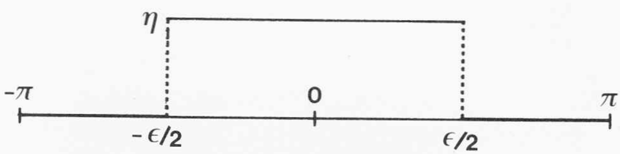

Fig. 4.4. The rectangle function.

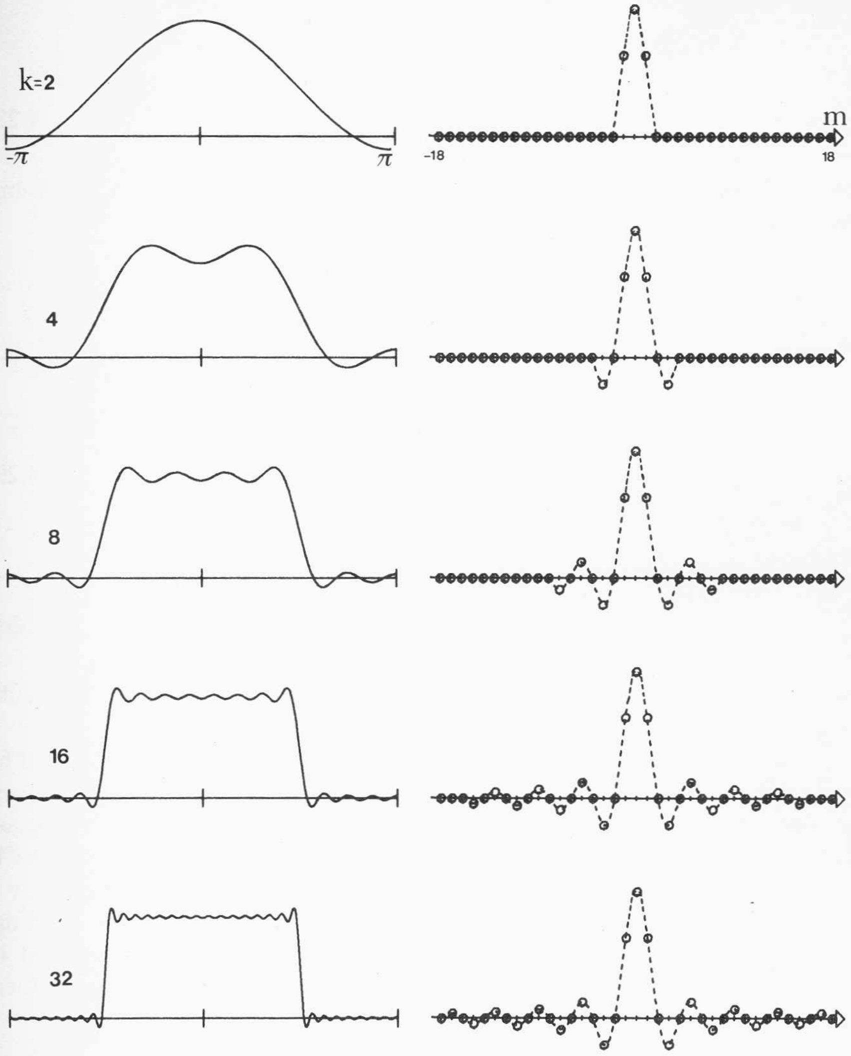

Fig. 4.5. Succession of truncated Fourier sums approximating the rectangle function (left) with k summands. The Fourier coefficients (right) are zero for $|m| > k$.

Exercise 4.5. Prove the trigonometric series identity

$$\sum_{n=1}^{\infty} n^{-1} \sin n\theta = \begin{cases} (\pi - \theta)/2, & 0 < \theta < 2\pi, \\ 0, & \theta = 0, 2\pi \end{cases} \tag{4.27}$$

using Fourier series. Note that to prove this identity *without* this technique is quite difficult. [See, for instance, the book by Bromwich (1926, p. 188).]

4.2.5. Example: The Triangle Function

Consider now the *triangle function* of height h:

$$T^h(x) = \begin{cases} h(x+\pi)/\pi, & -\pi < x \leqslant 0, \\ h(\pi - x)/\pi, & 0 \leqslant x \leqslant \pi. \end{cases} \tag{4.28}$$

See Fig. 4.6. Again, the Fourier partial-wave coefficients can be found without further ado as

$$\begin{aligned} T_n^h &= (2\pi)^{-1/2}\left[\pi^{-1}\int_{-\pi}^{0} dx h(x+\pi)\exp(-inx) \right. \\ &\qquad \left. + \pi^{-1}\int_0^{\pi} dx h(\pi - x)\exp(-inx)\right] \\ &= \begin{cases} \pi h(2\pi)^{-1/2}, & n = 0, \\ 4h(2\pi)^{-1/2}/\pi n^2, & n \text{ odd}, \\ 0, & \text{otherwise}. \end{cases} \end{aligned} \tag{4.29}$$

The Fourier synthesis is then given by the limit of the truncated sums

$$T_k^h(x) = h\Big(\tfrac{1}{2} + 4\pi^{-2} \sum_{|n| \text{odd} \leqslant k} n^{-2}\cos nx\Big), \tag{4.30a}$$

$$\lim_{k\to\infty} T_k^h(x) = T^h(x). \tag{4.30b}$$

The convergence of (4.30) as $k \to \infty$ to the triangle function is guaranteed by the easily verifiable fact that $T^h(x)$ satisfies the Dirichlet conditions. Moreover, it converges faster than the truncated sum succession of the rectangle function (4.26). While an upper bound of the partial-wave coefficients of the latter is $\sim |n|^{-1}$, those of (4.30) decrease as $\sim |n|^{-2}$. Thus it suffices to keep only a few terms to reproduce the original function down to the limit of visual acuity in Fig. 4.7. The question of convergence rate will be explored in Section 4.4. The two functions we have introduced here as examples and others which will appear later on have been collected in Table 4.4.

Exercise 4.6. Prove that $f(x)$ is a *positive* function if and only if its Fourier coefficients f_n are a *positive-definite* set, i.e.,

$$f(x) > 0 \Leftrightarrow \sum_{n,n' \in \mathscr{Z}} f_{n-n'} g_n^* g_{n'} > 0 \tag{4.31a}$$

for an arbitrary set of coefficients $\{g_n\}_{n\in\mathscr{Z}}$. You can show first that the second member of (4.31a) equals $(2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) |g(x)|^2$. Refer to Eq. (1.56). Similarly, for all $g(x) \in \mathscr{L}^2(-\pi, \pi)$,

$$f_n > 0 \Leftrightarrow \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dx' f(x - x') g(x)^* g(x') > 0. \tag{4.31b}$$

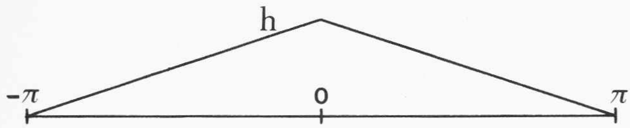

Fig. 4.6. The triangle function.

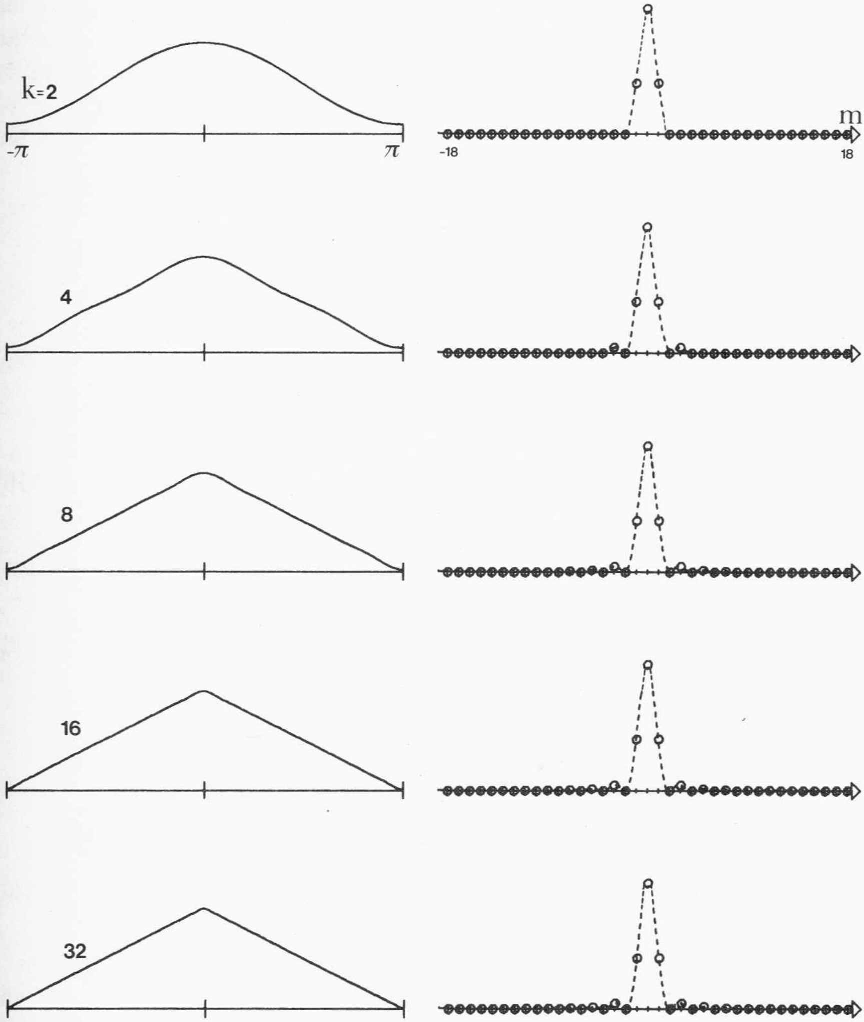

Fig. 4.7. Succession of truncated sums approximating the triangle function (left) and Fourier coefficients (right). The latter are zero for $|m| > k$.

4.3. Alternative Representations, Transformations, and Symmetries

The Fourier series

$$f(x) = (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n \exp(inx), \qquad x \in (-\pi, \pi], \tag{4.32a}$$

$$f_n = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) \exp(-inx), \qquad n \in \mathscr{Z}, \tag{4.32b}$$

expands the function $f(x) \in \mathscr{V}^D$ in terms of imaginary exponential functions. When the function is real or has certain symmetry properties, it may be more convenient to use the trigonometric functions, sine and cosine, for the same purpose. The rectangle and triangle functions which served as examples in Section 4.2 have been given alternative series representations in terms of the trigonometric functions [Eqs. (4.26a) and (4.30a)]. At a glance, these tell us (among other things) that the series are *even* functions in x.

4.3.1. The Sine and Cosine Fourier Series

Using Euler's formula, we can rewrite (4.32) as

$$f(x) = (2\pi)^{-1/2} f_0{}^+ + \pi^{-1/2} \sum_{n=1}^{\infty} (f_n{}^+ \cos nx + f_n{}^- \sin nx) \tag{4.33a}$$

with

$$f_0{}^+ := f_0 = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x), \tag{4.33b}$$

$$f_n{}^+ := 2^{-1/2}(f_n + f_{-n}) = \pi^{-1/2} \int_{-\pi}^{\pi} dx f(x) \cos nx, \qquad n = 1, 2, \ldots, \tag{4.33c}$$

$$f_n{}^- := 2^{-1/2} i(f_n - f_{-n}) = \pi^{-1/2} \int_{-\pi}^{\pi} dx f(x) \sin nx, \qquad n = 1, 2, \ldots. \tag{4.33d}$$

This is sometimes called the Fourier *sine and cosine series.*

4.3.2. Moduli and Phase Shifts

A further alternative representation can be set up from (4.33) as

$$f(x) = (2\pi)^{-1/2} F_0 + \pi^{-1/2} \sum_{n=1}^{\infty} F_n \cos(nx + \phi_n), \tag{4.34a}$$

$$F_0 := f_0{}^+, \qquad F_n \cos \phi_n := f_n{}^+, \qquad F_n \sin \phi_n := -f_n{}^-, \qquad n = 1, 2, \ldots, \tag{4.34b}$$

which expresses $f(x)$ in a cosine series with *phase shifts*. Note that if $f_n{}^+$ and $f_n{}^-$ are complex, so are F_n and ϕ_n.

Exercise 4.7. Find the analogue of (4.34) in terms of *sine* functions with phase shifts. Relate these to (4.33) and (4.34b).

4.3.3. Linear Operators

Part of the task of finding the Fourier partial-wave coefficients of a function is obviated if we know how to build, from known ones, new Fourier series for related functions. The first and most obvious correspondence is the one obtained under *linear combination* of functions. Let $f(x)$ and $g(x)$ be two functions satisfying the Dirichlet conditions, with partial-wave coefficients $\{f_n\}_{n\in\mathscr{Z}}$ and $\{g_n\}_{n\in\mathscr{Z}}$. Then clearly the linear combination function $h(x) = af(x) + bg(x)$, $a, b \in \mathscr{C}$, will also satisfy the Dirichlet conditions and will have Fourier coefficients $h_n = af_n + bg_n$, $n \in \mathscr{Z}$. The proof of this result uses elementary results on the differentiability and integrability of linear combinations of functions.

Exercise 4.8. Show that the coefficients of the Fourier sine and cosine series (4.33) of the above sum of two functions are $h_n{}^{\pm} = af_n{}^{\pm} + bg_n{}^{\pm}$.

We shall now introduce *linear operators* $\mathbb{A}$ as mappings in the space of functions $\mathscr{V}^D$ which satisfy the Dirichlet conditions. This follows closely the finite-dimensional concepts introduced in Section 1.3, except that we have no *a priori* guarantee that any given operator will be a one-to-one mapping of $\mathscr{V}^D$ on $\mathscr{V}^D$. In this section we shall consider only operators which *do* map this space into itself, i.e., if $\mathbf{f} \in \mathscr{V}^D$, then $\mathbb{A}\mathbf{f} \in \mathscr{V}^D$. Moreover, these mappings are to be *linear*, i.e.,

$$\mathbb{A}(a\mathbf{f} + b\mathbf{g}) = a(\mathbb{A}\mathbf{f}) + b(\mathbb{A}\mathbf{g}) \tag{4.35}$$

for $\mathbf{f}, \mathbf{g} \in \mathscr{V}^D$ and $a, b \in \mathscr{C}$.

4.3.4. The Translation Operator

Let $\mathbb{T}_a$ stand for the linear operator which translates the reference coordinates of the real line to the left by a, i.e.,

$$(\mathbb{T}_a\mathbf{f})(x) = f(x + a), \qquad a \equiv a \bmod 2\pi,\ x \equiv x \bmod 2\pi. \tag{4.36a}$$

It is clear that $\mathbb{T}_a\mathbf{f}$ satisfies the Dirichlet conditions if $\mathbf{f}$ does. If the Fourier coefficients of the latter are $\{f_n\}_{n\in\mathscr{Z}}$, then those of $\mathbb{T}_a\mathbf{f}$ will be

$$\begin{aligned}(\mathbb{T}_a\mathbf{f})_n &= (2\pi)^{-1/2}\int_{-\pi}^{\pi} dx(\mathbb{T}_a\mathbf{f})(x)\exp(-inx)\\ &= (2\pi)^{-1/2}\int_{-\pi}^{\pi} dx f(x + a)\exp(-inx)\\ &= (2\pi)^{-1/2}\int_{-\pi}^{\pi} dx' f(x')\exp[-in(x' - a)] = \exp(ina)f_n. \qquad (4.36\text{b})\end{aligned}$$

Note that in $\mathscr{V}^D$, $\mathbb{T}_{2\pi}$ is equivalent to the identity operator.

In terms of the alternative representations (4.33) and (4.34) the transformations of the coefficients (4.36b) take the forms

$$\begin{aligned}(\mathbb{T}_a\mathbf{f})_n{}^{+} &= 2^{-1/2}[(\mathbb{T}_a\mathbf{f})_n + (\mathbb{T}_a\mathbf{f})_{-n}]\\ &= 2^{-1/2}[\exp(ina)f_n + \exp(-ina)f_{-n}]\\ &= 2^{-1/2}[\cos na(f_n + f_{-n}) + i\sin na(f_n - f_{-n})]\\ &= \cos(na)f_n{}^{+} + \sin(na)f_n{}^{-}, \qquad n = 1, 2, \ldots. \end{aligned} \tag{4.37a}$$

Similarly,

$$(\mathbb{T}_a\mathbf{f})_n{}^{-} = -\sin naf_n{}^{+} + \cos naf_n{}^{-}, \qquad n = 1, 2, \ldots, \tag{4.37b}$$

while

$$(\mathbb{T}_a\mathbf{f})_0{}^{+} = f_0, \tag{4.37c}$$

which is formally contained in (4.37a) for $n = 0$. These relations can be also obtained as in (4.36b) using (4.33b)–(4.33d). In Table 4.1 we summarize the results of this section.

Exercise 4.9. Show that if $\mathbf{g} = \mathbb{T}_a\mathbf{f}$ with shifted Fourier cosine coefficients G_n, γ_n and F_n, ϕ_n, respectively, then

$$G_n = F_n, \qquad n = 0, 1, 2, \ldots, \tag{4.38a}$$

$$\gamma_n = \phi_n + na, \qquad n = 1, 2, \ldots, \tag{4.38b}$$

which simply tells us that under translations only the phase shifts are changed, while the amplitudes of the constituent waves remain the same.

Exercise 4.10. Build a *square wave* of height η with P pulses (Fig. 4.8) from the rectangle function (4.24) as

$$S^{(P,\eta)}(x) = -\eta + \sum_{l=1}^{P} R^{(\pi/P,2\eta)}(x - x_l), \qquad x_l = (2l + 1)\pi/2P. \tag{4.39a}$$

Since we know the Fourier coefficients of the undisplaced rectangle function (4.25), using (4.36), linear combination, and Eq. (1.50), show that the Fourier coefficients of (4.39a) are

$$S_n^{(P,\eta)} = \begin{cases} 4i\eta P(2\pi)^{-1/2}/n, & n = (2k + 1)P, k \in \mathscr{Z},\\ 0, & \text{otherwise},\end{cases} \tag{4.39b}$$

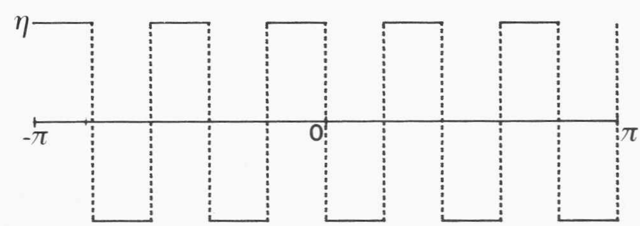

Fig. 4.8. Square wave with five pulses.

or

$$S_n^{(P,\eta)-} = \begin{cases} -4\eta P\pi^{-1/2}/n, & n = (2k+1)P,\ k \in \mathscr{Z}, \\ 0, & \text{otherwise}, \end{cases} \tag{4.39c}$$

$$S_n^{(P,\eta)+} = 0. \tag{4.39d}$$

Exercise 4.11. Let $\tilde{\mathbb{T}}_k$ stand for an operator which translates the Fourier coefficient labels k units to the left:

$$(\tilde{\mathbb{T}}_k\mathbf{f})_n = f_{n+k}. \tag{4.40a}$$

Show that the action on the corresponding functions is

$$(\tilde{\mathbb{T}}_k\mathbf{f})(x) = \exp(-ikx)f(x). \tag{4.40b}$$

4.3.5. The Inversion Operator

Now let $\mathbb{I}_0$ be the operator which inverts the coordinate axis through the origin:

$$(\mathbb{I}_0\mathbf{f})(x) = f(-x). \tag{4.41a}$$

Then, by reasoning parallel to (4.36b), we obtain the relation between the Fourier coefficients of $\mathbf{f}$ and $\mathbb{I}_0\mathbf{f}$ as

$$(\mathbb{I}_0\mathbf{f})_n = f_{-n}, \tag{4.41b}$$

i.e., f_n as a function of $n \in \mathscr{Z}$ also suffers reflection through the origin.

Exercise 4.12. Show that the coefficients in the sine and cosine Fourier series transform under inversions in the way given by the corresponding entries in Table 4.1. Do the same for the amplitude and phase-shift coefficients.

Exercise 4.13. Verify that the Fourier coefficients of the square wave in Fig. 4.8 [Eqs. (4.39b)–(4.39d)] imply the oddness of the function as $S_n = -S_{-n}$. The rectangle and triangle functions of Section 4.2 are even. Verify this property by means of their Fourier coefficients.

Exercise 4.14. In the spirit of Section 3.4, where Fourier series were seen as the infinite-dimensional limit of the finite Fourier transforms, show that $\mathbb{T}_a$ and $\mathbb{I}_0$ are the corresponding "limits" of the rotation and reflection operators $\mathbb{R}^k$ and $\mathbb{I}_0$ for finite-dimensional spaces in Section 1.5. The operators introduced here also form a *group*, as

$$\mathbb{T}_a\mathbb{T}_b = \mathbb{T}_{a+b}, \qquad \mathbb{T}_0 = \mathbb{1} = \mathbb{T}_{2\pi}, \qquad \mathbb{T}_a^{-1} = \mathbb{T}_{-a}, \tag{4.42a}$$

$$\mathbb{I}_0^2 = \mathbb{1}, \qquad \mathbb{I}_a := \mathbb{T}_a\mathbb{I}_0\mathbb{T}_{-a}, \qquad \mathbb{I}_a\mathbb{I}_b = \mathbb{T}_{2(b-a)}, \tag{4.42b}$$

which is the infinite-dimensional version of the dihedral group. As these consist of reflections and rotations by any angle in a two-dimensional plane and conserve angles between vectors, the group they constitute is called the two-dimensional *orthogonal* group O_2.

Exercise 4.15. Show that $\mathbb{T}_a$ and $\mathbb{I}_a$ map $\mathscr{V}^D$ into itself and moreover that

$$(\mathbf{g}, \mathbb{T}_a\mathbf{f}) = (\mathbb{T}_{-a}\mathbf{g}, \mathbf{f}), \tag{4.43a}$$

$$(\mathbf{g}, \mathbb{I}_a\mathbf{f}) = (\mathbb{I}_a\mathbf{g}, \mathbf{f}) \tag{4.43b}$$

on any pair of square-integrable functions **f**, **g**.

Exercise 4.16. Define the *dilatation operator* $\mathbb{D}_k$ for k an integer that has the following effect on periodic functions $f(x)$ of period 2π:

$$(\mathbb{D}_k\mathbf{f})(x) = f(kx), \tag{4.44a}$$

i.e., they are transformed into functions of period $2\pi/k$ (which are *also* of period 2π), repeating k times the form of **f** in $(-\pi, \pi]$. Show that the Fourier coefficients of $\mathbb{D}_k\mathbf{f}$ are related to those of **f** as

$$(\mathbb{D}_k\mathbf{f})_n = \begin{cases} f_m & \text{if } n = km,\ m \in \mathscr{Z}, \\ 0 & \text{otherwise.} \end{cases} \tag{4.44b}$$

In particular, we have $\mathbb{D}_1 = \mathbb{1}$ and $\mathbb{D}_{-1} = \mathbb{I}_0$. Show that this works with the square wave with P pulses (Fig. 4.8) in Exercise 4.10. Note that the group axioms of Section 1.4 we can satisfy are (a) $\mathbb{D}_k\mathbb{D}_l = \mathbb{D}_{kl}$, (b) associativity, and (c) existence of an identity $\mathbb{D}_1 = \mathbb{1}$. Axiom (d), the existence of an inverse for every $\mathbb{D}_k$, is *not* satisfied. Such an operator would take us *out* of the space of periodic functions of period 2π and hence does not exist in the space. A group minus axiom (d) constitutes a structure called a *semigroup with identity*.

4.3.6. Complex Conjugation

Now consider the function $f^*(x)$ which is the *complex conjugate* of a given $f(x) \in \mathscr{V}^D$. The Fourier partial-wave coefficients of the former can be related to those of the latter by

$$\begin{aligned}(\mathbf{f}^*)_n &= (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f^*(x)\exp(inx) \\ &= \left[(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f(x)\exp(-inx)\right]^* = (f_{-n})^*. \end{aligned}\tag{4.45}$$

Exercise 4.17. Show that the coefficients in the alternative representations of the Fourier series of the complex conjugate of a given function are those in the corresponding entries in Table 4.1.

4.3.7. Eigenfunctions and Eigenvalues

When a function $f(x)$ is mapped into a multiple of itself under the action of a given operator $\mathbb{A}$, i.e., when

$$(\mathbb{A}\mathbf{f})(x) = \lambda f(x), \tag{4.46}$$

we shall say that $f(x)$ is an *eigenfunction* of $\mathbb{A}$ with *eigenvalue* λ. Equation (4.46) describes those directions in the function vector space which are preserved under the action of $\mathbb{A}$. In the context of transformations, an $f(x)$ satisfying (4.46) is also said to exhibit *definite* symmetry under the action of $\mathbb{A}$. The functions which satisfy (4.46) with $\lambda = 1$ are said to be *invariant* under that transformation.

Let us investigate the eigenvalues and functions of the operators introduced in this section from the point of view of the possible symmetries they can exhibit.

4.3.8. Definite Symmetry under Inversion

Consider first the inversion operator $\mathbb{I}_0$ in (4.41a). As $\mathbb{I}_0^2 = \mathbb{1}$, $(\mathbb{I}_0^2\mathbf{f})(x) = \lambda(\mathbb{I}_0\mathbf{f})(x) = \lambda^2 f(x) = f(x)$; hence the eigenvalues of $\mathbb{I}_0$ in $\mathscr{V}^D$ can only be $\lambda = 1$ or $\lambda = -1$. Functions which are *even* $[f(x) = f(-x)]$ will be eigenfunctions of $\mathbb{I}_0$ with eigenvalue $\lambda = 1$, while *odd* functions $[f(x) = -f(-x)]$ will correspond to the eigenvalue $\lambda = -1$. Definite symmetry under inversions is called *parity*, so eigenfunctions of the inversion operator are those of even or odd parity. Any function can be decomposed uniquely into a sum of an even- and an odd-parity function; however, superpositions have *no definite* parity. The inversion operator thus divides the space of functions into two subspaces, each of definite parity, whose union is the full space and whose intersection is only the null function. Now, Eq. (4.41b) gives us the same information but in terms of the Fourier coefficients: even (respectively odd) functions will have partial-wave coefficients which are even: $f_n = f_{-n}$ (respectively odd: $f_n = -f_{-n}$). Table 4.2 shows the implied relations for the alternative representations. From (4.33c)–(4.33d) we can see quite simply that for even (respectively odd) functions, $f_n^- = 0$ (respectively $f_n^+ = 0$), while (4.34b) shows that all $\phi_n = 0$ (respectively $\phi_n = \pi/2$).

4.3.9. Definite Symmetry under Translations

Regarding functions with definite symmetry under translations, Eqs. (4.36), we first note that any function consisting of a *single* partial wave $\varphi_l(x) = (2\pi)^{-1/2} \exp(ilx)$ [Eq. (4.9)], i.e., with Fourier coefficients $\sim \delta_{n,l}$, will be an eigenfunction of *all* translation operators $\mathbb{T}_a$, with eigenvalue $\exp(ila)$. Indeed, they are the *only* functions to have this property and could have been constructed asking for it to hold. Let us consider now a *fixed* operator $\mathbb{T}_a$ and look for all partial waves which correspond to the *same* eigenvalue λ_0. Since any function in $\mathscr{V}^D$ consisting only of such partial waves will be an eigenfunction of $\mathbb{T}_a$ with eigenvalue λ_0, we shall generate *eigenspaces* of $\mathbb{T}_a$ labeled by λ_0 whose properties will be then explored. Let the translation be by $a = 2\pi/k$, where k is a positive integer. The eigenvalue of $\varphi_l(x)$ will then be $\exp(2\pi il/k)$, which is the same for all $n \equiv l \bmod k$ (that is, for $n = l + km$, m an integer). If l is chosen in the range $0, 1, \ldots, k - 1$, we can divide $\mathscr{V}^D$

into k eigenspaces $\mathscr{V}_l^D$, any element of which has eigenvalue $\exp(2\pi il/k)$ under $\mathbb{T}_a$. In particular, $\mathscr{V}_0^D$ is the space of all *k-fold periodic functions* in $(-\pi, \pi]$, i.e., with period $2\pi/k$, and consists only of linear combinations of $\varphi_n(x)$ with n an integer multiple of k. Only these partial-wave coefficients can be nonzero. (See Exercises 4.10 and 4.16 for $k = P$, where indeed we found that $S_n = 0$ when n is not a multiple of P.) For other values of l translation by $2\pi/k$ will produce a function identical with the original one but for a phase factor $\exp(2\pi il/k)$. In particular, if k is even, the space $\mathscr{V}_{k/2}^D$ will consist of all functions which change sign under such a translation.

Exercise 4.18. Consider Fig. 4.8. The square wave changes sign under translation by π/P. By the above argument show that for $k = 2P$ the only partial-wave coefficients which can be nonzero are S_n for $n = (2m + 1)P$, $m \in \mathscr{Z}$, i.e., the *odd* multiples of P. In this way we are predicting *all* the zeros which appear on the Fourier partial wave expansion of the square wave.

Exercise 4.19. Show that the only periodic function with definite symmetry under dilatations is the constant function.

4.3.10. Real and Imaginary Functions

Last, we turn to complex conjugation. As the application of this operation twice is equivalent to the identity, we can have only $f^*(x) = f(x)$ when the function is *real* or $f^*(x) = -f(x)$ when it is *pure imaginary*. The simplest description of these two subspaces of functions is in terms of the coefficients of the sine and cosine Fourier series, which are constrained to be purely real or imaginary, respectively. See Table 4.2.

Exercise 4.20. Verify that the Fourier partial-wave coefficients in all representations for the rectangle, triangle, and square-wave function indeed have the property of Table 4.2 corresponding to real functions. For the case of the square wave in Fig. 4.8, we can see that the function is real; hence $S_n = (S_{-n})^*$. It also has odd parity, which means that $S_n = -S_{-n}$. The conclusion therefore is that all Fourier coefficients must be pure imaginary, while the zeros are inferred from the multiple-periodicity argument. We note, moreover, that the overall convergence behavior of the Fourier series can be characterized by $S_n \sim |n|^{-1}$. This feature and its generalization will be studied in Section 4.4.

The results in this section allow us to use the symmetry properties of a function under inversion, translation, and complex conjugation in order to predict corresponding properties of the Fourier partial-wave coefficients, in particular, to know which are equal to each other and which are *zero*. This usually results in a drastic simplification of the problem at hand and is widely used, for instance, in quantum mechanics in order to reduce the—generalized—partial-wave decomposition of the allowed states of a system where the symmetry properties are inferred from physical considerations.

Table 4.1 Transformations of the Function $f(x)$ and Corresponding Transformations of the Fourier Partial-Wave Coefficients

		Fourier Partial-Wave Coefficients		
Operation	Function	Eq. (4.32)	Eq. (4.33)	Eq. (4.34)
Identity	$f(x)$	$f_n, n \in \mathscr{Z}$	$f_n^+, n = 0, 1, 2, \ldots$ $f_n^-, n = 1, 2, 3, \ldots$	$F_n, n = 0, 1, 2, \ldots$ $\phi_n, n = 1, 2, 3, \ldots$
Translation	$(\mathbb{T}_a\mathbf{f})(x) = f(x + a)$	$\exp(ina)f_n$	$\cos(na)f_n^+ + \sin(na)f_n^-$ $-\sin(na)f_n^+ + \cos(na)f_n^-$	F_n $\phi_n + na$
	$\exp(-ikx)f(x)$	f_{n+k}		
Inversion	$(\mathbb{I}_0\mathbf{f})(x) = f(-x)$	f_{-n}	f_n^+ $-f_n^-$	F_n $-\phi_n$
Dilatation	$(\mathbb{D}_k\mathbf{f})(x) = f(kx), k \in \mathscr{Z}$	f_{kn} (all others zero)	f_{kn}^+ f_{kn}^-	F_{kn} ϕ_{kn}
Complex conjugation	$f^*(x)$	$(f_{-n})^*$	$(f_n^+)^*$ $(f_n^-)^*$	F_n^* ϕ_n^*

Table 4.2 Functions with Definite Symmetry under a Transformation and the Corresponding Restrictions on Their Fourier Partial-Wave Coefficients

Transformation	Function property	Restrictions on the Fourier partial-wave coefficients		
Translation by $2\pi/k$ (k integer)	k-fold periodic in $(-\pi, \pi]$	$f_n = 0$ for $n \not\equiv 0 \bmod k$ (n not multiple of k)		
	Changes phase by $\exp(2\pi il/k)$	$f_n = 0$ for $n \not\equiv l \bmod k$ (similarly for alternative representations)		
Inversion	Even	$f_n = f_{-n}$	$f_n^- = 0$	$\phi_n = 0$
	Odd	$f_n = -f_{-n}$	$f_n^+ = 0$	$\phi_n = \pi/2$
Complex conjugation	Real	$f_n = (f_{-n})^*$	$f_n^\pm$ real	F_n, ϕ_n real
	Pure imaginary	$f_n = -(f_{-n})^*$	$f_n^\pm$ imag.	F_n imag., ϕ_n real

4.4. Differential Properties and Convergence

In this section we shall explore the relations between Fourier series and differentiation. This will lead to a better understanding of the rapidity of convergence of these series, the Gibbs phenomenon, and some of the "smoothing" techniques used to circumvent it. Finally, we shall mention the meanings of "best approximation" and the Bessel inequality.

4.4.1. Fourier Series, Integration, and Convergence

Consider a function $f(x)$ which satisfies the Dirichlet conditions and its integral

$$f^{(-1)}(x) := \int_c^x dy f(y). \tag{4.47}$$

It is easy to see that $f^{(-1)}(x)$ will also satisfy the Dirichlet continuity conditions since the integral of a differentiable (or continuous) function with at most bounded discontinuities is differentiable at all but a finite number of points. So that $f^{(-1)}(x)$ will be *periodic* with period 2π, we must require that a shift in the integration limits by 2π, each independently, leave the value unchanged. This means that

$$\int_x^{x+2\pi} dy f(y) = (2\pi)^{1/2} f_0 = 0,$$

i.e., $f_0 = 0$. If this is satisfied, we can consider the Fourier coefficients of $f(x)$ and $f^{(-1)}(x)$, $\{f_n\}_{n\in\mathscr{Z}}$ and $\{f_n^{(-1)}\}_{n\in\mathscr{Z}}$, writing

$$\begin{aligned}(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n^{(-1)} \exp(inx) = f^{(-1)}(x) &= (2\pi)^{-1/2} \int_c^x dy \sum_{n\in\mathscr{Z}} f_n \exp(iny) \\ &= (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n \int_c^x dy \exp(iny) \\ &= (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n (in)^{-1} \exp(inx) \\ &\quad - (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n (in)^{-1} \exp(inc). \end{aligned} \tag{4.48}$$

We have been able to exchange integration and infinite summation, as they both exist and converge uniformly. The last sum in (4.48) is the arbitrary integration constant $f_0^{(-1)}$. The equality of the coefficients of the (independent) partial waves yields

$$f_n^{(-1)} = (in)^{-1} f_n, \qquad 0 \neq n \in \mathscr{Z}. \tag{4.49}$$

In relating the Fourier coefficients of $f(x)$ with those of its antiderivative $f^{(-1)}(x)$ we see that the latter give rise to a more rapidly converging Fourier series than the former. In fact, uniform convergence of the former guarantees that of the latter.

4.4.2. Differentiation

Turning the tables, suppose now that we know the Fourier coefficients of a piecewise differentiable function $f(x)$ satisfying the Dirichlet conditions. The Fourier coefficients of its *derivative* $f'(x)$, $\{f_n'\}_{n\in\mathscr{Z}}$, which we must assume also satisfies Dirichlet, can be found from (4.49), replacing $f^{(-1)}$ by f and f by f', as

$$f_n' = inf_n, \qquad n \in \mathscr{Z}. \tag{4.50}$$

We can perform differentiation repeatedly and—Dirichlet allowing—express the Fourier coefficients of the pth derivative of $f(x)$, $f^{(p)}(x)$, as

$$f_n^{(p)} = (in)^p f_n, \qquad n \in \mathscr{Z}. \tag{4.51}$$

The Fourier series with coefficients (4.51) will converge to the pth derivative of $f(x)$. In fact this allows us to define *fractional derivatives* for *complex p*. In Fig. 4.9 we have plotted the fractional derivatives of the triangle function, minus a constant so that its integral will be a periodic function, for real p between -1 and 1.75. In Table 4.3 we have collected some of the useful facts found in this section. An extensive table of Fourier coefficients and trigonometric series has been compiled by Oberhettinger (1973a).

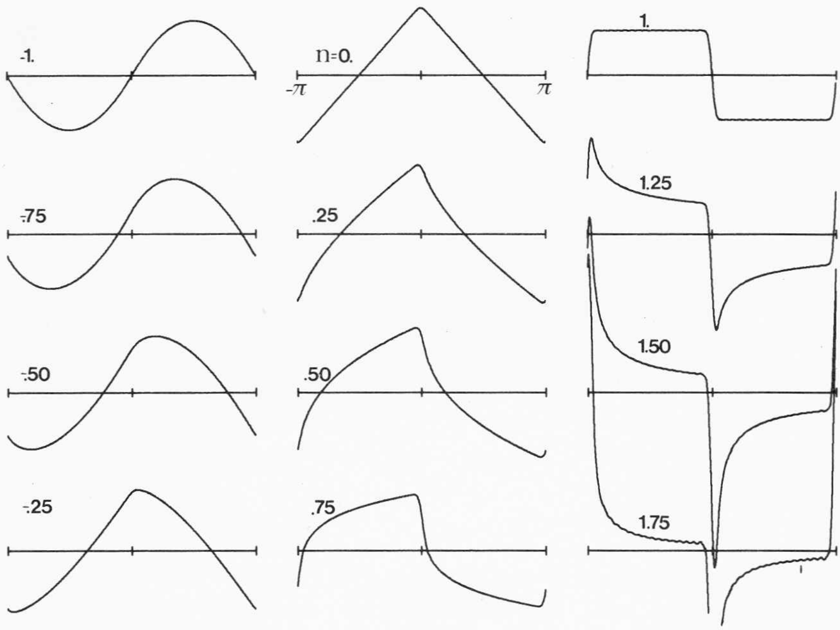

Fig. 4.9. Fractional derivatives of order n of the triangle function. The latter has been slightly smoothed so as to avoid the appearance of the Gibbs phenomenon for positive derivatives in the finite computed series; still, spurious oscillations appear in the highest derivatives.

Exercise 4.21. Assume $f(x)$ is a trigonometric polynomial. Verify the validity of (4.51).

4.4.3. A Theorem on the Convergence of Fourier Series

One feature which is apparent in the relation (4.51) is that the rapidity of convergence of the *infinite* Fourier series of $f^{(p)}(x)$ gets worse with each successive derivative. It is to be expected that we may reach a p where the Fourier series diverges. In fact, we shall prove the following statement: *If the* pth *derivative of a function* $f(x)$ *is a square-integrable, its Fourier coefficients must decrease as* $|f_n| \leqslant c|n|^{-p}$ *for* $c = \|\mathbf{f}^{(p)}\|^{1/2}$.

4.4.4. Proof

The proof proceeds by use of the Schwartz inequality [Eq. (1.13)], noting that, since

$$f_n = (in)^{-p} f_n^{(p)} = (in)^{-p}(\boldsymbol{\varphi}_n, \mathbf{f}^{(p)}) \tag{4.52}$$

[see Eqs. (4.7), (4.9), and (4.17b)], we have

$$|f_n| = |n|^{-p}|(\boldsymbol{\varphi}_n, \mathbf{f}^{(p)})| \leqslant |n|^{-p}\|\boldsymbol{\varphi}_n\|^{1/2}\|\mathbf{f}^{(p)}\|^{1/2}. \tag{4.53}$$

Now, the functions $\varphi_n(x)$ have unit norm, and $\|\mathbf{f}^{(p)}\|$ exists by assumption.

One can immediately draw an important corollary to this result: if a function $f(x)$ is *infinitely* differentiable (and thus integrable, as the interval is finite), then its Fourier coefficients f_n must decrease with increasing n faster than *any power* of $|n|$. Clearly, this result is satisfied when $f_n = 0$ for $|n|$ larger than some fixed M, since then $f(x)$ is only a trigonometric polynomial. It also holds for more general cases, an example being the Jacobi theta function, which will be discussed below.

4.4.5. An Example

We can verify the workings of these results graphically. Consider the triangle function, Eq. (4.28), whose Fourier coefficients are

$$T_n{}^h = \begin{cases} (2\pi)^{-1/2}\pi h, & n = 0, \\ 4(2\pi)^{-1/2}h/\pi n^2, & n \text{ odd}, \\ 0, & \text{otherwise}. \end{cases} \tag{4.54}$$

In Fig. 4.10(a) we show a few truncated sums and note that for the sixteenth one the original function is already "well" reproduced. The derivative of the triangle function of height h is a function with value h/π in $(-\pi, 0)$ and $-h/\pi$ in $(0, \pi)$. This is a square wave [Eqs. (4.39)] with one pulse ($P = 1$) of height $\eta = h/\pi$, whose Fourier coefficients are

$$S_n^{(1,h/\pi)} = \left.\begin{cases} 4i(2\pi)^{-1/2}h/\pi n, & n \text{ odd} \\ 0, & n \text{ even} \end{cases}\right\} = inT_n{}^h. \tag{4.55}$$

The Fourier series with coefficients (4.55) converges slower than (4.54), with the speed of the alternating harmonic series. In Fig. 4.10(b) we have plotted the derivatives of the truncated sums of Fig. 4.10(a). Finally, in Fig. 4.10(c) we have drawn the derivatives of Fig. 4.10(b). This corresponds formally to a Fourier series with coefficients

$$S_n^{(1,h/\pi)\prime} = inS_n^{(1,h/\pi)} = \begin{cases} -4(2\pi)^{-1/2}h\pi^{-1}, & n \text{ odd}, \\ 0, & n \text{ even}. \end{cases} \tag{4.56}$$

The set of coefficients (4.56) cannot give rise to a convergent Fourier series as the terms have the same absolute value for all n. Figure 4.10(c) and the divergent series represented by (4.56), however, are not without meaning, as we shall see in Section 4.5. The point here is to note how the result on convergence applies here. The first derivative of the triangle function is the one-pulse square wave, which is square-integrable; hence the Fourier coefficients

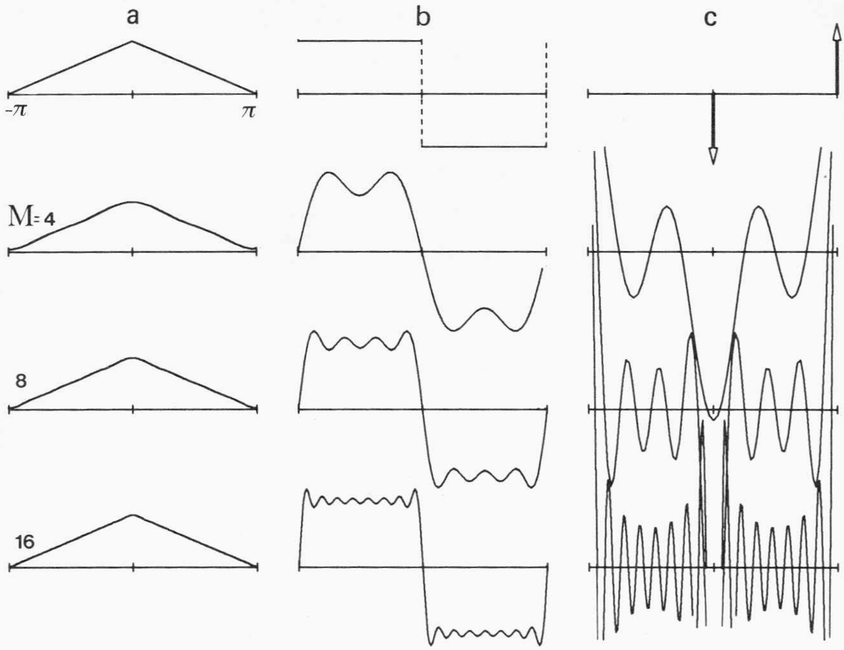

Fig. 4.10. Relation between differentiability and convergence. (a) The triangle function and its first few truncated Fourier sums; (b) and (c) are their first and second derivatives.

of the former, Eq. (4.54), must decrease faster or at least as $|n|^{-1}$, and so they do.

4.4.6. Contrapositive of the Theorem

The *contrapositive* of the result on differentiability and convergence $[(A \Rightarrow B) \Leftrightarrow (\text{not } B \Rightarrow \text{not } A)]$ states that if the Fourier coefficients of a function $f(x)$ decrease *more slowly* than $|n|^{-p}$ (i.e., $|f_n| \geqslant c|n|^{-p}$), then $f^{(p)}(x)$ is *not* square-integrable (i.e., $\|\mathbf{f}^{(p)}\|$ does not exist).

Applied to the example at hand, $|T_n| > c|n|^{-2-\varepsilon}$ for any positive ε, and hence $T^{(2+\varepsilon)}(x)$ is not square-integrable. In fact, $T^{(2)}(x)$ is already outside $\mathscr{L}^2(-\pi, \pi)$, as we can see using the Parseval identity [Eq. (4.14)] for the coefficients (4.56). This relation between differentiability and convergence is not very constraining but, on the other hand, is quite general. Its formulation for arbitrary orthonormal bases can be seen in a short article by Schneider (1971). The convergence properties of trigonometric series constitutes a broad field indeed. The two-volume treatises by Zygmund (1952) and Bary

(1964) cover this ground in due detail. We have collected some of the results of this section in Table 4.3.

4.4.7. The Gibbs Phenomenon

Returning to Fig. 4.10(b) and the Fourier series of the one-pulse square wave with coefficients (4.55), we note that the convergence is particularly poor near the edge of the discontinuities. In Fig. 4.11 we have amplified the oscillations which take place. There is a characteristic *overshoot* in the kth-term truncated series on the order of 9% which is called the *Gibbs phenomenon.* As k increases, the oscillations do not die out but move closer to the discontinuity. The uniform convergence guaranteed by Dirichlet's result holds, of course, but refers to any subinterval which excludes the discontinuity points, and by taking sufficiently high-order truncations we can move the oscillations as near to the edge as we please. In designing an electronic square-pulse generator, for example, which builds this waveform through Fourier synthesis (i.e., by truncated sums of simple sinusoidal waves), one is generally interested in reproducing the overall shape of the pulses and having a more rapid convergence. To achieve this, some kind of *smoothing* has to be applied to the function so as to replace it by a similar-looking function with

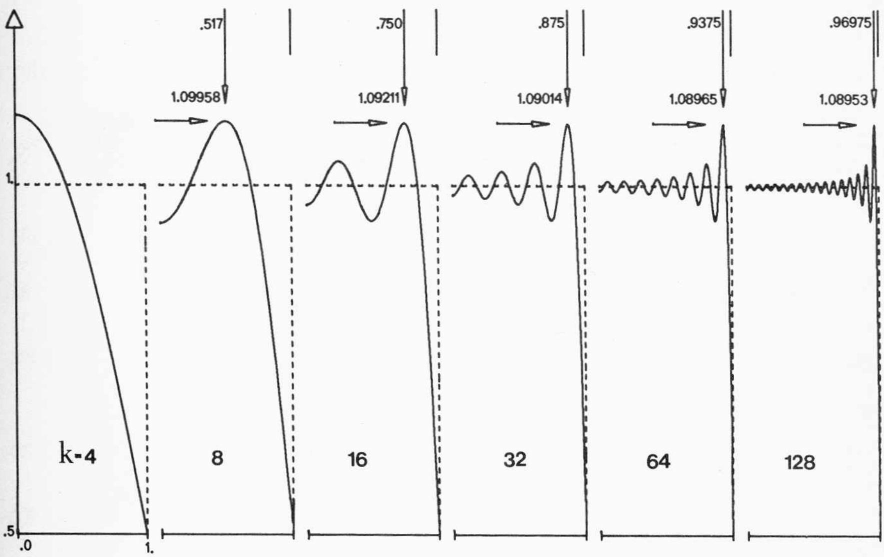

Fig. 4.11. The Gibbs phenomenon. This is an amplification of Fig. 4.5 extending from $x = \pi/4$ to $\pi/2$ over the upper half of the rectangle height. The vertical arrows indicate the position of the maxima as they approach the discontinuity edge and the horizontal ones, their values. The numbers beside the arrows give their location in units of figure width and discontinuity height.

no discontinuities and as highly differentiable as possible. We could also replace the Fourier coefficients f_n by $f_n s_n$, where $\{s_n\}_{n\in\mathscr{Z}}$ is a set of coefficients which fall off to zero for large n, thereby improving the convergence rate of the Fourier series. In fact, the two approaches are equivalent, and they bring in the concept of *convolution* on which we shall briefly digress.

4.4.8. Product and Convolution

Let $\{f_n\}_{n\in\mathscr{Z}}$ and $\{s_n\}_{n\in\mathscr{Z}}$ be the Fourier coefficients of two functions $f(x)$ and $s(x)$ satisfying (for the moment) the Dirichlet conditions. Consider now

$$g_n = s_n f_n, \qquad n \in \mathscr{Z}, \tag{4.57}$$

to be the Fourier coefficients of a new function $g(x)$. The kth truncated sum of this function will be (Section 4.2)

$$\begin{aligned} g_k(x) &= (2\pi)^{-1/2} \sum_{|n|\leqslant k} s_n f_n \exp(inx) \\ &= (2\pi)^{-3/2} \int_{-\pi}^{\pi} dz s(z) \int_{-\pi}^{\pi} dy f(y) \sum_{|n|\leqslant k} \exp[in(x-y-z)] \\ &= (2\pi)^{-1/2} \int_{-\pi}^{\pi} dz s(z) \int_{-\pi}^{\pi} dy f(y) D_k(x-y-z), \end{aligned} \tag{4.58}$$

where we have introduced the Dirichlet kernel (4.19). As we let $k \to \infty$, the integral in y becomes $f(x - z)$ by Dirichlet's result, and hence

$$\begin{aligned} g(x) &= (2\pi)^{-1/2} \int_{-\pi}^{\pi} dz s(z) f(x-z) = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dz s(x-z) f(z) \\ &=: (2\pi)^{-1/2}(s * f)(x). \end{aligned} \tag{4.59}$$

This defines the *convolution* of the functions $s(x)$ and $f(x)$ on the interval $(-\pi, \pi]$. Its structure is analogous to the *finite* convolution of Section 3.1. We have also shown by (4.57)–(4.59) that if $s(x)$ and $f(x)$ satisfy the Dirichlet conditions, so does $(s * f)(x)$.

Exercise 4.22. Assume $f(x)$ and $g(x)$ are two functions satisfying the Dirichlet conditions. Show that their *product*

$$h(x) = f(x)g(x) \tag{4.60}$$

will also satisfy them. Show that the Fourier coefficients of $h(x)$ are

$$h_n = (2\pi)^{-1/2} \sum_{m\in\mathscr{Z}} f_m g_{n-m} = (2\pi)^{-1/2} \sum_{m\in\mathscr{Z}} f_{n-m} g_m. \tag{4.61}$$

This is the *discrete* convolution between the two sets of Fourier coefficients. These relations have been collected in Table 4.3.

4.4.9. Function Smoothing by the Lanczos σ-Factors

The graphical meaning of the convolution between two functions (4.59) can be brought out and applied to the problem of eliminating the Gibbs phenomenon by a particular example. Let $s(x)$ be a rectangle function (4.24) of area $(2\pi)^{1/2}$, so that $\eta = (2\pi)^{1/2}/\varepsilon$. The convolution of this with an arbitrary $f(x)$ is

$$f^R(x) := (2\pi)^{-1/2}(f * R^{(\varepsilon,\eta)}(x)) = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dy f(x-y) R^{(\varepsilon,\eta)}(y)$$

$$= \varepsilon^{-1} \int_{-\varepsilon/2}^{\varepsilon/2} dy f(x-y), \tag{4.62}$$

a function which represents at each point x the *integrated mean* of $f(x)$ *in an interval of width* ε. If $f(x)$ is a rectangle function, say, $f^R(x)$ will be a *trapezium*: the discontinuities of the original function have been smoothed over an interval ε. In terms of the Fourier coefficients, using the rectangle function coefficients (4.25), we obtain

$$f_n^R = f_n R_n^{(\varepsilon,\eta)} = f_n \sin(n\varepsilon/2)/(n\varepsilon/2) =: f_n \sigma_n. \tag{4.63}$$

The coefficients σ_n in (4.63) have thus the same effect on the Fourier coefficients as the integrated mean on the functions. They are called the *Lanczos σ-factors* (Fig. 4.5). Their effect on the improvement of convergence for the function in Fig. 4.11 is given in Fig. 4.12. The sequence of truncated sums is seen to converge to a trapezoidal shape.

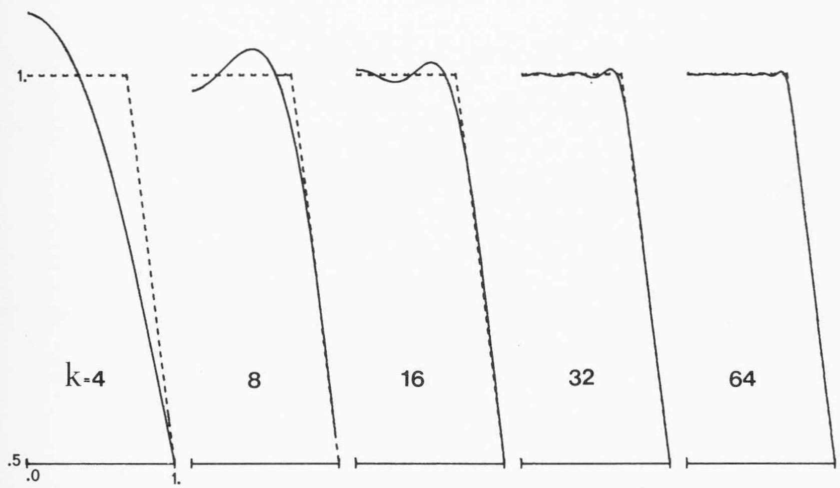

Fig. 4.12. Convergence improvement through the Lanczos σ-factors. Convoluting the function of Figure 4.11 with a rectangle function of width $\varepsilon = \pi/6$ [Eq. (4.63)], the truncated sums approach the trapezium limit with decreasing overshoot.

4.4.10. The θ-Function Smoothing

Another particularly useful function for the process of smoothing discontinuous functions by convolution is one which we can define through its Fourier series as

$$\begin{aligned}\theta(x, \tau) &:= (2\pi)^{-1} \sum_{n\in\mathscr{Z}} \exp(-n^2\tau + inx) \\ &= (2\pi)^{-1}\left[1 + 2\sum_{n=1}^{\infty} \exp(-n^2\tau)\cos nx\right] \\ &= (2\pi)^{-1}\vartheta_3(x/2, e^{-\tau}), \qquad \tau > 0, \end{aligned} \tag{4.64}$$

where ϑ_3 is one of the *Jacobi theta functions* [see Whittaker and Watson (1903, Chapter XXI) and the mathematical function tables of Abramowitz and Stegun (1964, Eq. 16.273)].

The theta function, as defined above, will be seen in Section 5.1 to be a solution to the problem of heat diffusion in a ring. It has been plotted in Fig. 4.13(a). It resembles a Gaussian bell function [$\exp(-x^2/\tau)$, $x \in R$] exhibiting a peak at $x = 0$ and falling off sharply for small values of τ. The Fourier coefficients of (4.64),

$$\theta_n(\tau) = (2\pi)^{-1/2}\exp(-n^2\tau), \tag{4.65}$$

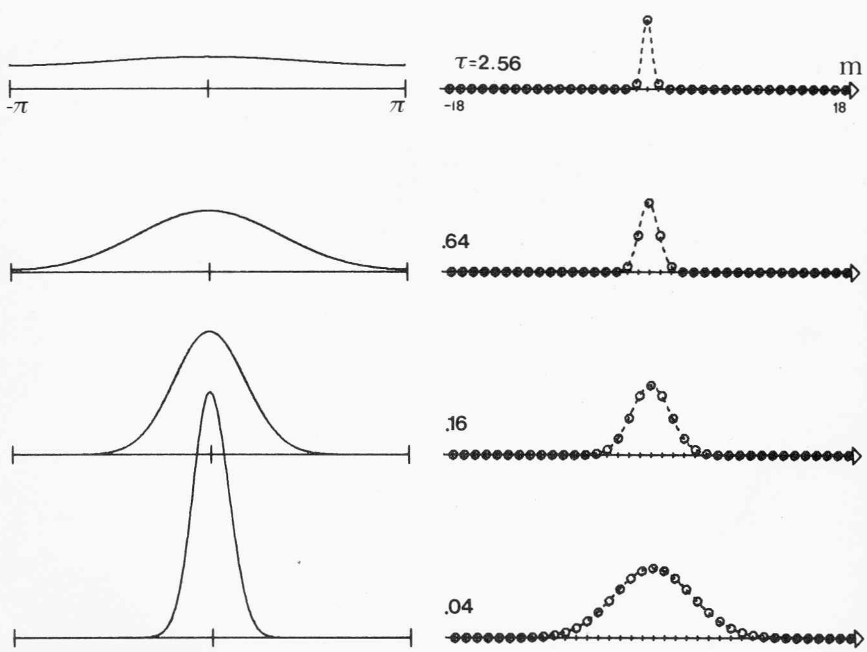

Fig. 4.13. The Jacobi theta function in Eq. (4.64) for (left) various values of the width parameter τ and (right) their Fourier coefficients.

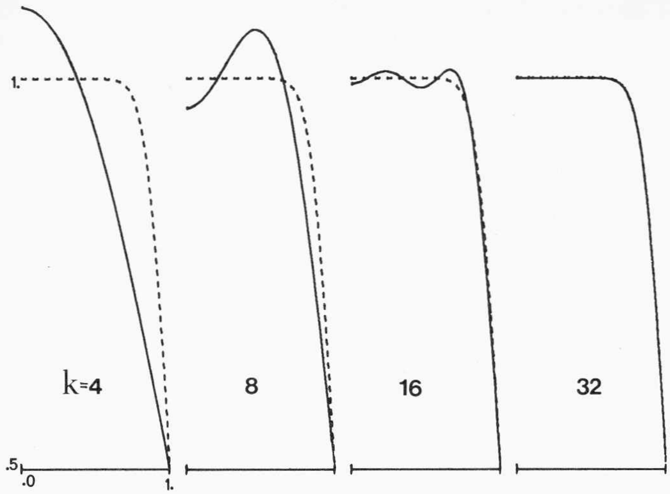

Fig. 4.14. Convergence improvement by the θ-factors of Eq. (4.65) for a value of $\tau = 0.005$.

for growing n, decrease faster than any negative power of $|n|$; indeed, they are discrete points on a Gaussian bell. See Fig. 4.13. It follows that $\theta(x, \tau)$ is infinitely differentiable in x. If (4.64) is placed in convolution with an arbitrary function $f(x)$ which we assume (here) to satisfy the Dirichlet conditions,

$$f^{\theta(\tau)}(x) := (2\pi)^{-1/2}[f * \theta(\cdot, \tau)](x) = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dy f(y)\theta(x - y, \tau), \quad (4.66)$$

the $f(x)$ is smoothed into an $f^{\theta(\tau)}(x)$ which is *infinitely differentiable* in x. The Fourier coefficients of (4.66) are then

$$f_n^{\theta(\tau)} = f_n \exp(-n^2\tau), \quad (4.67)$$

which indeed decrease faster than any negative power of $|n|$. In Fig. 4.14 we have plotted the convergence of the truncated sums of a function with a discontinuity (the same as Figs. 4.11 and 4.12) with θ-smoothing. Further characteristics of the Gibbs phenomenon can be found in the books by Carslaw (1930, Chapter 9) and Dym and McKean (1972, Section 1.6).

Exercise 4.23. Prove that the θ-function (4.64) tends toward infinity at $x = 0$ as $\tau \to 0^+$. Nevertheless, it encloses the unit area

$$\int_{-\pi}^{\pi} dx \theta(x, \tau) = 1 \quad (4.68)$$

independently of the value of τ. In this respect it has two properties in common with the Dirichlet kernel: Eq. (4.20). Particularly, Eq. (4.68) will lead to the total conservation of heat in a ring (Section 5.1). Compare with Eq. (1.73).

Exercise 4.24. Compare Figs. 4.12 and 4.14. Note that for τ small, a narrow peak for $\theta(x, \tau)$ corresponds to a broad Gaussian bell for θ_n, while for large τ, the situation is reversed. This suggests a *complementarity* between the "width" of function and that of its Fourier coefficients. A rough measure of the former is the *equivalent width*

$$W_f := \int_{-\pi}^{\pi} dx f(x)/f(0), \tag{4.69a}$$

which gives the width of a rectangle function with the same area as $f(x)$ and of height $f(0)$. This has been contrived mainly for "peak-like" functions and can be meaningless for others. Correspondingly, we can define the equivalent width for a set of discrete points as

$$\hat{W}_f := \sum_{n \in \mathscr{Z}} f_n/f_0 \tag{4.69b}$$

with a similar interpretation and purpose. Prove the equality

$$W_f \hat{W}_f = 2\pi \tag{4.69c}$$

which accounts for the complementarity of widths in Fig. 4.13. Note that this is akin—but not identical—to the mathematical statement of Heisenberg's uncertainty relation in Section 7.6.

Exercise 4.25. Using the Schwartz inequality, show that

$$|(f * g)(x)| \leqslant \|\mathbf{f}\| \, \|\mathbf{g}\|, \qquad \|\mathbf{f} * \mathbf{g}\| \leqslant (2\pi)^{1/2} \|\mathbf{f}\| \, \|\mathbf{g}\|, \tag{4.70}$$

i.e., the analogue of Eq. (3.10). The result in Exercise 4.26 may be handy.

Exercise 4.26. Show that the convolution $(f * g)(x)$ can be written as an inner product between $\mathbf{f}^*$—the function $f^*(x')$—and a translated, inverted $(\mathbb{I}_0 \mathbb{T}_x \mathbf{g})(x')$, i.e.,

$$(f * g)(x) = (\mathbf{f}^*, \mathbb{I}_0 \mathbb{T}_x \mathbf{g}) = (\mathbb{T}_{-x} \mathbb{I}_0 \mathbf{f}^*, \mathbf{g}). \tag{4.71}$$

Exercise 4.27. In this section we have differentiated functions and found their Fourier coefficients. Now consider applying the *second-difference* operator of Part I to the Fourier coefficients, i.e., let $\mathbf{g} = \Delta \mathbf{f}$, defined as

$$g_n = f_{n+1} - 2f_n + f_{n-1}, \qquad n \in \mathscr{Z}. \tag{4.72a}$$

Show by (4.40) that this corresponds to

$$g(x) = -4 \sin^2(x/2) f(x). \tag{4.72b}$$

4.4.11. Sum Truncation and Best Approximation

In the preceding part of this section we have been concerned with the *smoothing* of discontinuous functions $f(x)$ to a $f^S(x)$ [$S = R$ in (4.62) and $S = \theta(\tau)$ in (4.66)] in order to *improve the convergence rate* of the succession of truncated sums $f_k^S(x)$. The smoothed function *is not* the original function, however. This obvious remark is made in order to emphasize that when the criterion of "best approximation" of $f_k^S(x)$ to $f(x)$ is that the *norm* of the residue vector $r(x) := f(x) - f_k^S(x)$ be minimal, *the best approximation is obtained when only truncation is applied.* To prove this, we generalize slightly the concept of truncated approximations, letting $\mathscr{K}$ be the set of partial waves unaffected by truncation, i.e., $f_n^S = 0$ for $n \notin \mathscr{K}$. We now calculate straightforwardly the norm of the residue vector:

$$\begin{aligned} 0 \leqslant \|\mathbf{r}\|^2 &= (\mathbf{f} - \mathbf{f}_k^S, \mathbf{f} - \mathbf{f}_k^S) \\ &= (\mathbf{f}, \mathbf{f}) - \sum_{n \in \mathscr{K}} f_n^* f_n^S - \sum_{n \in \mathscr{K}} f_n^{S*} f_n + \sum_{n \in \mathscr{K}} |f_n^S|^2 \\ &= (\mathbf{f}, \mathbf{f}) + \sum_{n \in \mathscr{K}} |f_n^S - f_n|^2 - \sum_{n \in \mathscr{K}} |f_n|^2. \end{aligned} \tag{4.73}$$

The last equality can be verified by expanding the last two summands. Now, the f_n's are fixed and so is $\mathscr{K}$. The minimum value of the norm of the residue vector $\|\mathbf{r}\|$ is thus achieved when in (4.73) we set $f_n^S = f_n$ for all $n \in \mathscr{K}$. We thus conclude that in any truncation set $\mathscr{K}$ the best approximation to $f(x)$ in the norm is provided by $f_k(x)$ constructed with the original Fourier coefficients. We also conclude from (4.73) that

$$(\mathbf{f}, \mathbf{f}) \geqslant \sum_{n \in \mathscr{K}} |f_n|^2. \tag{4.74}$$

This is called *Bessel's inequality*. When the truncation set $\mathscr{K}$ becomes the whole of $\mathscr{Z}$, (4.74) becomes Parseval's identity. Otherwise, it provides an upper bound to the norms of the truncated sums.

Table 4.3 Various Operations and Properties Connected with Differentiation and Convolution of Functions and Their Fourier Coefficients

Operation	Function $f(x)$	Fourier coefficients f_n
Differentiation order p	$\dfrac{d^p}{dx^p} f(x)$	$(in)^p f_n$
Integration ($f_0 = 0$)	$\int_c^x dy f(y)$	$(in)^{-1} f_n$, $n \neq 0$ $f_0^{(-1)}$, arbitrary
Second difference	$-4 \sin^2 x f(x)$	$f_{n+1} - 2f_n + f_{n-1}$
Convolution	$(f * g)(x) := \int_{-\pi}^{\pi} dy f(y) g(x - y)$	$(2\pi)^{1/2} f_n g_n$
Product	$f(x) g(x)$	$(2\pi)^{-1/2} \sum_{m \in \mathscr{Z}} f_m g_{n-m}$
Convergence	$\|f^{(p)}\| < \infty$	$\|f_n\| \leqslant c\|n\|^{-p}$

Table 4.4 A Short List of Functions and Their Fourier Coefficients

Function $f(x)$	Fourier coefficients f_n
Single partial wave $\varphi_{n_0}(x)$ [Eq. (4.9)]	δ_{n,n_0}
Dirichlet kernel $D_k(x)$ [Eq. (4.19), Fig. 4.3]	$(2\pi)^{-1/2}$, $\lvert n\rvert \leqslant k$ 0, otherwise
Rectangle function $R^{(\varepsilon,\eta)}(x)$ of width ε and height η [Eq. (4.24), Fig. 4.4]	$(2\pi)^{-1/2}\varepsilon\eta\ (n\varepsilon/2)^{-1}\sin(n\varepsilon/2)$
Triangle function $T^h(x)$ of height h [Eq. (4.28), Fig. 4.6]	$(2\pi)^{1/2}4h/\pi n^2$, n odd $(2\pi)^{-1/2}\pi h$, $n = 0$ 0, otherwise
Square wave $S^{(P,\eta)}(x)$ of P pulses of height η [Eq. (4.39a), Fig. 4.8]	$(2\pi)^{-1/2}4iP\eta/n$, $n = (2k+1)P$, $k \in \mathscr{Z}$ 0, otherwise
Polygonal function $P(x)$ passing through $(x_k, P(x_k))$, $k = 1, \ldots, N$, with slopes m_k and $\varepsilon_k := x_{k+1} - x_k$ [Eq. (4.88), Fig. 4.15(a)]	$-(2\pi)^{-1/2}n^{-2}\sum_{k=1}^{N}(m_{k+1} - m_k)\exp(-inx_{k+1})$, $n \neq 0$ $\frac{1}{2}(2\pi)^{-1/2}\sum_{k=1}^{N}\varepsilon_k[P(x_{k+1}) + P(x_k)]$, $n = 0$
Theta function $\theta\,(x, \tau)$ [Eq. (4.64), Fig. 4.13]	$(2\pi)^{-1/2}\exp(-n^2\tau)$

4.5. The Dirac δ and Divergent Series

Among the functions we have come across, three of them, the Dirichlet kernel, the rectangle function, and the Jacobi theta function [Eqs. (4.19), (4.24), and (4.64)], will now be used to introduce the subject of generalized functions such as the Dirac δ, its derivatives, and the divergent Fourier series which they represent. We shall also provide some concepts from functional analysis so as to outline the proper framework for these objects.

4.5.1. Three Functions and a Limit

We shall be interested in the behavior of the Dirichlet kernel $D_k(x)$ as $k \to \infty$, of the rectangle function of unit area $R^{(\varepsilon,1/\varepsilon)}(x)$ as the width $\varepsilon \to 0$, and of the theta function $\theta(x, \tau)$ as τ tends toward zero from positive values.

To focus on their common properties we shall denote them by

$$\delta^k(x) := D_k(x), \qquad R^{(1/k,k)}(x), \qquad \theta(x, 1/k), \tag{4.75}$$

respectively, noting that they are all real and even and enclose unit area. Their Fourier coefficients are, correspondingly (Table 4.4),

$$\delta_n{}^k = \begin{Bmatrix} (2\pi)^{-1/2}, & |n| \leqslant k \\ 0, & |n| > k \end{Bmatrix}, \quad (2\pi)^{-1/2}2kn^{-1}\sin(n/2k), \quad (2\pi)^{-1/2}\exp(-n^2/k). \tag{4.76}$$

Now, if $f(x)$ is a function satisfying the Dirichlet conditions with Fourier coefficients f_n, then

$$\bar{f}_n^{\,k} := (2\pi)^{1/2} f_n \delta_n^{\,k}, \qquad n \in \mathscr{Z}, \tag{4.77}$$

will be the Fourier coefficients of the convolution (Section 4.4) of $f(x)$ with $\delta^k(x)$:

$$\begin{aligned} \bar{f}^k(y) &= (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} \bar{f}_n^{\,k} \exp(iny) := (\mathbf{f} * \boldsymbol{\delta}^k)(y) \\ &= \int_{-\pi}^{\pi} dx f(x)\delta^k(y-x) = \int_{-\pi}^{\pi} dx f(y-x)\delta^k(x) \\ &= (\boldsymbol{\delta}^k, \mathbb{T}_y \mathbf{f}) = (\mathbb{T}_{-y}\boldsymbol{\delta}^k, \mathbf{f}), \end{aligned} \tag{4.78}$$

where we have also written the expression as an inner product [see Eq. (4.71)]. As $k \to \infty$, $D_k(x)$ behaves peculiarly: it converges nowhere, oscillating faster as k increases. The rectangle and θ-function become high and narrow, and all grow without bound at $x = 0$. Yet (4.77) and (4.78) have a well-defined limit: since $\delta_n^{\,k} \to (2\pi)^{-1/2}$ for $k \to \infty$, $\bar{f}_n^{\,k} \to f_n$ and $\bar{f}^k(y) \to f(y)$.

4.5.2. The Dirac δ Symbol

We can write symbolically

$$\lim_{k\to\infty} \delta^k(x) =: \delta(x) \tag{4.79}$$

and will call this the *Dirac* δ. It has the property

$$(\boldsymbol{\delta}, \mathbb{T}_y \mathbf{f}) = \int_{-\pi}^{\pi} dx f(x+y)\delta(x) = \int_{-\pi}^{\pi} dx f(x)\delta(y-x) = f(y). \tag{4.80}$$

This is to be interpreted as the limit of (4.78) as $k \to \infty$, the symbol δ being replaced by the limit of the integral of any of the sequences of functions (4.75). The Dirac δ assigns to every *continuous* "*test*" function $f(x)$ the number $f(0)$ [$\delta: \mathbf{f} \mapsto (\boldsymbol{\delta}, \mathbf{f}) := f(0) \in \mathscr{C}$]. It is thus a mapping from the space of continuous functions onto the complex field. Such generalized mappings are called *distributions*. Following the mathematical physics usage, we shall speak of them as *generalized functions* since, as we shall see, the Dirac $\delta(y - x)$ and other objects of that kind can be handled as if they were ordinary functions in almost every case.

4.5.3. Divergent Series Representation

The δ Fourier coefficients can be found by their usual definition and (4.80) as

$$\delta_n = (\boldsymbol{\varphi}_n, \boldsymbol{\delta}) = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx \delta(x) \exp(-inx) = (2\pi)^{-1/2} = \lim_{k\to\infty} \delta_n^{\,k}. \tag{4.81}$$

The Fourier series *representing* the Dirac δ is thus

$$\delta(x) = (2\pi)^{-1} \sum_{n\in\mathscr{Z}} \exp(inx). \tag{4.82}$$

Although the actual sum of (4.82) is meaningless since the series diverges, the equation is consistent with the symbolic notation (4.79) and should be interpreted as the equality of the Fourier series for $\delta^k(x)$ in (4.75) and (4.76)—or any other such sequence we may produce—when $k \to \infty$. The divergent series representation can be handled consistently by exchanging sums and integrals while leaving the limit $k \to \infty$ out of sight. One verifies in this way that

$$\begin{aligned} f(y) &= \int_{-\pi}^{\pi} dx f(x)\delta(y-x) = \int_{-\pi}^{\pi} dx f(x)\Big\{(2\pi)^{-1} \sum_{n\in\mathscr{Z}} \exp[in(y-x)]\Big\} \\ &= (2\pi)^{-1} \sum_{n\in\mathscr{Z}} \exp(iny)\left[\int_{-\pi}^{\pi} dx f(x) \exp(inx)\right] \\ &= (2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} f_n \exp(iny). \end{aligned} \tag{4.83}$$

4.5.4. Derivative of a Function at a Point of Discontinuity

We can gain confidence in the use of this convenient shorthand by applying it to the relation between the Fourier coefficients of the triangle function and its first two derivatives [Eqs. (4.54)–(4.56)]. In Section 4.4 we stopped short of analyzing the sequence of truncated sums [Fig. 4.10(c) and Eq. (4.56)] which gave rise to a divergent series. We can now tackle this question. The Fourier coefficients of the derivative of the one-pulse square wave of height $D/2 := h/\pi$ are

$$S_n^{(1,h/\pi)'} = \begin{cases} -2D(2\pi)^{-1/2}, & n \text{ odd} \\ 0, & n \text{ even} \end{cases} = D[-\delta_n + \exp(-in\pi)\delta_n]. \tag{4.84}$$

The corresponding series should then represent the derivative of the one-pulse function with discontinuity D as

$$\frac{d}{dx} S^{(1,D/2)}(x) = D[-\delta(x) + \delta(x-\pi)], \tag{4.85}$$

where we have translated the argument of the second δ [see Eq. (4.36)]. A glance at Fig. 4.10b, c tells us that as the sequence of truncated sums approaches a function with a discontinuity at some point x_d the derivatives of these constitute a sequence of functions which grow at $x = x_d$. At the limit, intuitively, *the derivative of a step function with discontinuity D at x_d is $D\delta(x - x_d)$.*

We verify the validity of (4.85) by introducing both members of the equality into an inner product with a continuous test function $g(x)$, element of $\mathscr{V}^D$, with Fourier coefficients g_n. One can proceed in two ways, either by using (4.84),

$$\begin{aligned}(\mathbf{S}', \mathbf{g}) &= \sum_{n\in\mathscr{Z}} S_n'^* g_n = D \sum_{n\in\mathscr{Z}} [-\delta_n + \exp(-in\pi)\delta_n] g_n \\ &= -D(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} g_n + D(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} g_n \exp(-in\pi) \\ &= -Dg(0) + Dg(-\pi), \end{aligned} \tag{4.86a}$$

or alternatively by integration by parts and recalling the periodicity of all functions involved,

$$\begin{aligned}(\mathbf{S}', \mathbf{g}) &= \int_{-\pi}^{\pi} dx \left[\frac{d}{dx} S(x)\right]^* g(x) \\ &= S(x)g(x)|_{-\pi}^{\pi} - \int_{-\pi}^{\pi} dx S(x) \frac{d}{dx} g(x) \\ &= 0 - (D/2)\left[\int_{-\pi}^{0} - \int_{0}^{\pi}\right] dx\, dg(x)/dx \\ &= -(D/2)[g(0) - g(-\pi) - g(\pi) + g(0)] = -Dg(0) + Dg(\pi). \end{aligned} \tag{4.86b}$$

We thus find

$$(\mathbf{S}^{(1,D/2)\prime}, \mathbf{g}) = \big(D(-\boldsymbol{\delta} + \mathbb{T}_{-\pi}\boldsymbol{\delta}), \mathbf{g}\big) \tag{4.87}$$

for arbitrary continuous $\mathbf{g} \in \mathscr{V}^D$. We can thus state that the equality (4.85) between generalized functions represented by divergent series holds *in the sense* (4.87).

4.5.5. The Polygonal Function

We shall use the relation between derivatives of discontinuous functions and Dirac δ's in order to find the Fourier coefficients of a *polygonal function* [Fig. 4.15(a)] whose graph joins the ordered set of points $\{x_k, P(x_k)\}$, $k = 1, 2, \ldots, N$, with straight lines. This function can be described in terms of the rectangle function (4.24) as

$$P(x) := \sum_{k=1}^{N} (m_k x + b_k) R^{(\varepsilon_k, 1)}(x - x_{k+1/2}), \tag{4.88a}$$

where

$$\varepsilon_k := x_{k+1} - x_k, \qquad x_{k+1/2} := (x_k + x_{k+1})/2, \tag{4.88b}$$

$$m_k := [P(x_{k+1}) - P(x_k)]/\varepsilon_k, \tag{4.88c}$$

$$b_k := P(x_k) - m_k x_k, \qquad k = 1, 2, \ldots, N, \tag{4.88d}$$

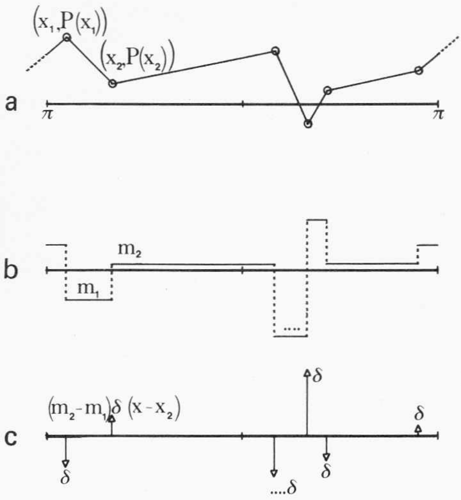

Fig. 4.15. (a) The polygonal function joining the points $[x_k, P(x_k)]$, $k = 1, 2, \ldots, N$, by straight lines; (b) and (c) are its first and second derivatives.

and we identify

$$x_0 \coloneqq x_N - 2\pi, \qquad x_{N+1} \coloneqq x_1 + 2\pi. \tag{4.88e}$$

To find the Fourier series, we differentiate (4.88) repeatedly [Figs. 4.15(b) and (c)]:

$$P'(x) = \sum_{k=1}^{N} m_k R^{(\varepsilon_k, 1)}(x - x_{k+1/2}), \tag{4.89}$$

$$P''(x) = \sum_{k=1}^{N} (m_{k+1} - m_k)\delta(x - x_{k+1}). \tag{4.90}$$

The Fourier coefficients of (4.90) can now be computed easily using the translation relation (4.36). We find

$$P''_n = (2\pi)^{-1/2} \sum_{k=1}^{N} (m_{k+1} - m_k) \exp(-inx_{k+1}). \tag{4.91}$$

The Fourier coefficients of the original function (4.88) are thus (4.91) multiplied by $(in)^{-2}$, $n \neq 0$, i.e.,

$$P_n = -(2\pi)^{-1/2} n^{-2} \sum_{k=1}^{N} (m_{k+1} - m_k) \exp(-inx_{k+1}), \tag{4.92a}$$

while by direct integration of (4.84) we supply the coefficient

$$P_0 = (2\pi)^{-1/2} \cdot \tfrac{1}{2} \sum_{k=1}^{N} \varepsilon_k [P(x_{k+1}) + P(x_k)]. \tag{4.92b}$$

Exercise 4.28. Prove by direct calculation that (4.92) are indeed the Fourier coefficients of the polygonal function (4.88).

Exercise 4.29. Examining the limits of (4.75), show that the Dirac δ is *not* an element of $\mathscr{L}^2(-\pi, \pi)$.

Exercise 4.30. Show that the *convolution* of two Dirac δ's is a Dirac δ, i.e.,

$$(\mathbb{T}_{-y}\boldsymbol{\delta}, \mathbb{T}_{-z}\boldsymbol{\delta}) = \int_{-\pi}^{\pi} dx\delta(x - y)\delta(x - z) = \delta(y - z). \tag{4.93}$$

This can be done either rigorously from (4.75), directly from (4.93) and exchange of integrals, or by the Fourier coefficients.

Exercise 4.31. Assume you have a function $f(x)$ whose Fourier coefficients repeat themselves modulo N, i.e., $f_n = f_{n+N}$. Show that $f(x)$ will be a sum of N Dirac δ's "sitting" on equidistant points in $(-\pi, \pi]$. This is called a "picket-fence" or "Dirac comb" generalized function. In fact, finite-dimensional Fourier transforms can be obtained in this way from Fourier series.

4.5.6. The Derivatives of the Dirac δ

Once we have lost qualms in handling the divergent series representing the Dirac δ, we can proceed with other such generalized functions. Recalling that differentiation of a function $f(x)$ multiplies its Fourier coefficients f_n by in, we can formally differentiate Eq. (4.82) p times and define the pth *derivative of the Dirac* δ as represented by

$$\delta^{(p)}(x) = d^p\delta(x)/dx^p = (2\pi)^{-1} \sum_{n\in\mathscr{Z}} (in)^p \exp(inx), \tag{4.94a}$$

with Fourier coefficients

$$\delta_n^{(p)} = (2\pi)^{-1/2}(in)^p. \tag{4.94b}$$

The validity and use of (4.94) are essentially the same as for the Dirac δ except that we must now *restrict* the space of test functions to $\mathscr{C}^{(p)}$: p-times differentiable functions whose pth derivative is continuous. If $g(x)$ is a $\mathscr{C}^{(p)}$-function with Fourier coefficients g_n,

$$\begin{aligned}(\boldsymbol{\delta}^{(p)}, \mathbb{T}_y\mathbf{g}) &= \sum_{n\in\mathscr{Z}} \delta_n^{(p)*}\, g_n \exp(iny)\\ &= (-1)^p(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} (in)^p g_n \exp(iny)\\ &= (-1)^p \frac{d^p}{dy^p}\left[(2\pi)^{-1/2} \sum_{n\in\mathscr{Z}} g_n \exp(iny)\right] = (-1)^p g^{(p)}(y),\end{aligned} \tag{4.95a}$$

i.e., the pth derivative of $g(x)$ at y. This can be verified formally using integration by parts in the inner product

$$(\boldsymbol{\delta}^{(p)}, \mathbb{T}_y\mathbf{g}) = \int_{-\pi}^{\pi} dx[d^p\delta(x)/dx^p]g(x+y)$$
$$= (-1)^p \int_{-\pi}^{\pi} dx\delta(x)[d^pg(x+y)/dx^p]$$
$$= (-1)^p \frac{d^p}{dy^p}\left[\int_{-\pi}^{\pi} dx\delta(x)g(x+y)\right], \tag{4.95b}$$

which reproduces the result in (4.95a).

Exercise 4.32. The steps taken in Eqs. (4.95) involve reckless exchange of infinite series, integrals, and derivatives. The proper way to justify them is to define a sequence of functions $d^p\delta^k(x)/dx^p$ with the property that

$$\lim_{k\to\infty} \int_{-\pi}^{\pi} dx[d^p\delta^k(x)/dx^p]f(x+y) = (-1)^p d^pf(y)/dy^p. \tag{4.96}$$

The pth derivative of the Dirichlet kernel and of the theta-function provide such sequences. The symbol $\delta^{(p)}(x)$ follows the convention (4.79) on limits and integral. Again, $\boldsymbol{\delta}^{(p)}$ can be seen as a mapping of $\mathbf{f}$ on $(-1)^p f^{(p)}(0) \in \mathscr{C}$.

Exercise 4.33. Show that

$$\delta^{(p)}(-x) = (-1)^p\delta^{(p)}(x) \tag{4.97}$$

by means of its integral properties and its Fourier coefficients.

Exercise 4.34. Prove that

$$(\mathbb{T}_{-y}\boldsymbol{\delta}, \mathbb{T}_{-z}\boldsymbol{\delta}^{(p)}) = \int_{-\pi}^{\pi} dx\delta(x-y)\delta^{(p)}(x-z) = \delta^{(p)}(y-z). \tag{4.98}$$

Exercise 4.35. Prove that a "Taylor expansion" of the Dirac δ

$$\delta(x+y) = \mathbb{T}_y\delta(x) = \exp\left(y\frac{d}{dx}\right)\delta(x) := \sum_{p=0}^{\infty}\frac{y^p}{p!}\delta^{(p)}(x) \tag{4.99}$$

is meaningful. Place the extreme members of (4.99) into an inner product with an appropriate arbitrary test function. The *appropriate* test-function space will here be the $\mathscr{C}^\infty$-functions which have convergent Taylor expansion, i.e., the space of *analytic* functions on $(-\pi, \pi]$. Note that the Fourier coefficients of (4.99) are $(2\pi)^{-1/2}\exp(iny)$.

Exercise 4.36. Prove in the same sense that the theta function (4.64)–(4.65) admits the formal representation

$$\theta(x,\tau) = \exp(\tau d^2/dx^2)\delta(x), \tag{4.100}$$

showing that the Fourier coefficients of both sides are equal. In Section 5.1 this will be seen to correspond to the time evolution of a localized infinitely hot spot in a conducting ring. Note the analogy with Exercise 1.27.

4.5.7. On Convergence of Function Sequences

The reader who has felt uncomfortable differentiating discontinuous functions in Eq. (4.85) may well ask, on seeing Eqs. (4.99) and (4.100), whether infinite-order differential operators can ever be applied with any rigor to such beings as the Dirac δ. The framework for these developments constitutes the body of functional analysis. We shall draw here only a rough map of this territory, using as reference points the concepts and examples which have appeared thus far. First, we must remark that we have used *three* kinds of convergence of sequences of functions $\{\mathbf{f}_k\}_{k=1}^{\infty}$ to their limits $\mathbf{f}$:

(a) *Uniform pointwise convergence* if $\lim_{k\to\infty}[f_k(x) - f(x)] = 0$ uniformly for all x in the domain of the $\mathbf{f}_k$ and $\mathbf{f}$. This was the kind of convergence assured by the Dirichlet theorem.

(b) *Convergence in the norm* (or *strong* convergence) if $\lim_{k\to\infty}\|\mathbf{f}_k - \mathbf{f}\| = 0$. This is a less stringent condition and requires only that the function within the norm bars be square-integrable (in the sense of Lebesgue). We have anticipated in Section 4.1 that this space, $\mathscr{L}^2(-\pi, \pi)$, is particularly important in much of mathematical physics, and we shall have more to say about it below.

(c) *Componentwise convergence* (or *weak* convergence) if

$$\lim_{k\to\infty} (\mathbf{g}, \mathbf{f}_k - \mathbf{f}) = 0$$

for all *test* functions $\mathbf{g}$ in some suitable space of functions $\mathscr{S}$. "Suitable" spaces have been $\mathscr{C}^{(0)}$, $\mathscr{C}^{(p)}$, $\mathscr{C}^{(\infty)}$, or the space of analytic functions. This is a still less stringent requirement than convergence in the norm, and it is in this sense that sequences of functions converge to the Dirac δ or its pth derivatives. Equality (or equivalence) of functions—ordinary or generalized—can be similarly conditioned. When we showed that the Fourier components of two expressions such as the divergent series for $\delta^{(p)}(x)$ in (4.94) or Eqs. (4.99) or (4.100) were equal, we were only proving *weak* equality in the sense (c).

So that the inner product $(\mathbf{g}, \mathbf{f})$ will be finite when $\mathbf{f}$ is a generalized function in a class $\mathscr{S}'$ with Fourier coefficients f_n which increase with $|n|$, the class of test functions $\mathscr{S}$ to which $\mathbf{g}$ may belong must be such that its g_n decrease even faster so that $\sum_n g_n^* f_n < \infty$. The "larger" $\mathscr{S}'$ is, the "smaller" $\mathscr{S}$ must be. The former is the $\mathscr{L}^2$-*dual* space of the latter. This is illustrated with the successive derivatives of the δ and the nested $\mathscr{C}^{(p)}$-spaces. The space of functions which is *self-dual* in this sense is precisely that of *square-integrable* functions $\mathscr{L}^2(-\pi, \pi)$, since there $\|\mathbf{f}\| = (\mathbf{f}, \mathbf{f})^{1/2} < \infty$. It can be shown that, in fact, $\mathscr{S} \subseteq \mathscr{L}^2(-\pi, \pi) \subseteq \mathscr{S}'$, the relevant convergence being (b) and (c), respectively, for the elements in the last two spaces.

4.5.8. On Cauchy Sequences and Complete Function Spaces

Since sequences of functions in $\mathscr{L}^2(-\pi, \pi)$ may converge (in the appropriate sense) to objects outside this space, as in the case of the Dirichlet, rectangle, and theta functions "converging" to the Dirac δ, it is useful to introduce a convergence criterion in order to characterize spaces which are *complete*, i.e., where the limits of sequences belong to the same space. We thus define a sequence of functions $\{\mathbf{f}_k\}_{k=1}^{\infty}$ to be a *Cauchy* sequence if for every given $\varepsilon > 0$ one can find an N such that for $n, m > N$, $\|\mathbf{f}_n - \mathbf{f}_m\| < \varepsilon$. Now, a vector space endowed with a positive inner product where every such Cauchy sequence converges to a function within the space is said to be a *Hilbert* space. All finite-dimensional spaces are Hilbert spaces. A fundamental theorem by Riesz and Fischer states that $\mathscr{L}^2(\mathscr{I})$ is a Hilbert space. Another Hilbert space one can construct is l^2, the space of all infinite-dimensional vectors $\tilde{\mathbf{f}} := \{f_n\}_{n\in\mathscr{Z}}$ with inner product $(\tilde{\mathbf{f}}, \tilde{\mathbf{g}})_{l^2} := \sum_{n\in\mathscr{Z}} f_n^* g_n$. As Fourier analysis and synthesis suggest, there is a mapping between elements in $\mathscr{L}^2(-\pi, \pi)$, $\mathbf{f}$, $\mathbf{g}$, etc., and elements in l^2, $\tilde{\mathbf{f}}$, $\tilde{\mathbf{g}}$, etc., which preserves the angles between any pair of vectors, as $(\mathbf{f}, \mathbf{g})_{\mathscr{L}^2} = (\tilde{\mathbf{f}}, \tilde{\mathbf{g}})_{l^2}$. Such a mapping is said to be *isometric*. Moreover, this mapping is one-to-one and can be shown to transform the *whole* of $\mathscr{L}^2(\mathscr{I})$ *onto* l^2 and conversely. Such an isometric mapping is said to be *unitary*. The difference between isometric and unitary mappings appears only in infinite-dimensional spaces. The result for the mapping between $\mathscr{L}^2(-\pi, \pi)$ and l^2 actually generalizes to another important theorem which states that any two (infinite-dimensional *separable*) Hilbert spaces can be mapped onto each other through a unitary transformation. Other Hilbert spaces besides $\mathscr{L}^2(-\pi, \pi)$ and l^2 will be discussed in Part IV.

4.5.9. Complete Bases for a Function Space

The last subject to be outlined is the question of what constitutes a basis for $\mathscr{L}^2(-\pi, \pi)$. A denumerable set of nonzero, linearly independent vectors $\{\boldsymbol{\varphi}_n\}_{n\in\mathscr{Z}}$ is said to be a *complete basis* for a Hilbert space if for every one of its elements $\mathbf{f}$, $(\mathbf{f}, \boldsymbol{\varphi}_n) = 0$, $n \in \mathscr{Z}$, implies $\mathbf{f} = \mathbf{0}$. One can then find coefficients f_n such that the sequence

$$\bar{\mathbf{f}}_k = \sum_{|n|\leqslant k} f_n \boldsymbol{\varphi}_n \tag{4.101}$$

converges in the norm to $\mathbf{f}$. The set of vectors given by the imaginary exponential functions (4.9), the *Fourier basis* for $\mathscr{L}^2(-\pi, \pi)$, is an example. Note that $f(x)$ need not satisfy the Dirichlet conditions which refer to pointwise convergence but must only be in $\mathscr{L}^2(-\pi, \pi)$. If the basis is orthonormal [i.e., if $(\boldsymbol{\varphi}_n, \boldsymbol{\varphi}_m) = \delta_{nm}$], the coefficients f_n are simply $(\boldsymbol{\varphi}_n, \mathbf{f})$, and we can write

$$\mathbf{f} = \sum_{n\in\mathscr{Z}} f_n \boldsymbol{\varphi}_n, \qquad f_n = (\boldsymbol{\varphi}_n, \mathbf{f}), \tag{4.102}$$

valid in the norm. Equation (4.102) is actually valid *weakly* for $\mathbf{f} \in \mathscr{S}'$. The basis is said to be *dense* in these spaces.

4.5.10. Dirac's Generalized Basis

When we deal not only with Hilbert spaces but with triplets $\mathscr{S} \subseteq \mathscr{L}^2(-\pi, \pi) \subseteq \mathscr{S}'$, completeness of a basis in the norm appears too stringent. Edging toward abuse of notation, we can speak of *Dirac's generalized basis* $\{\boldsymbol{\delta}_y\}$, $\boldsymbol{\delta}_y := \mathbb{T}_{-y}\boldsymbol{\delta} \in \mathscr{S}'$, where the label y ranges over $(-\pi, \pi]$. Such a basis is to allow for the expansion of any $\mathbf{f}$, weakly, as

$$\mathbf{f} = \int_{-\pi}^{\pi} dy f(y)\boldsymbol{\delta}_y, \qquad f(y) = (\boldsymbol{\delta}_y, \mathbf{f}). \tag{4.103}$$

The vectors of this basis are *orthonormal in Dirac's sense*:

$$(\boldsymbol{\delta}_y, \boldsymbol{\delta}_z) = \delta(y - z). \tag{4.104}$$

[See Eq. (4.93).] Exchanging the vector space "integral" (4.103) with ordinary integration, we can verify, for instance,

$$\begin{aligned}(\boldsymbol{\varphi}_n, \mathbf{f}) &= \left(\boldsymbol{\varphi}_n, \int_{-\pi}^{\pi} dy f(y)\boldsymbol{\delta}_y\right) = \int_{-\pi}^{\pi} dy f(y)(\boldsymbol{\varphi}_n, \mathbb{T}_{-y}\boldsymbol{\delta}) \\ &= \int_{-\pi}^{\pi} dy f(y)(\boldsymbol{\delta}, \mathbb{T}_y\boldsymbol{\varphi}_n)^* \\ &= (2\pi)^{-1/2}\int_{-\pi}^{\pi} dy f(y)\exp(-iny) = f_n \end{aligned} \tag{4.105a}$$

or

$$\begin{aligned}(\boldsymbol{\delta}_x, \mathbf{f}) &= \left(\boldsymbol{\delta}_x, \int_{-\pi}^{\pi} dy f(y)\boldsymbol{\delta}_y\right) = \int_{-\pi}^{\pi} dy f(y)(\boldsymbol{\delta}_x, \boldsymbol{\delta}_y) \\ &= \int_{-\pi}^{\pi} dy f(y)\delta(y - x) = f(x). \end{aligned} \tag{4.105b}$$

The two bases are related by Eqs. (4.102) and (4.103) as

$$\boldsymbol{\delta}_x = \sum_{n\in\mathscr{Z}} (\boldsymbol{\varphi}_n, \boldsymbol{\delta}_x)\boldsymbol{\varphi}_n = (2\pi)^{-1/2}\sum_{n\in\mathscr{Z}} \exp(-inx)\boldsymbol{\varphi}_n, \tag{4.106a}$$

$$\boldsymbol{\varphi}_n = \int_{-\pi}^{\pi} dx(\boldsymbol{\delta}_x, \boldsymbol{\varphi}_n)\boldsymbol{\delta}_x = (2\pi)^{-1/2}\int_{-\pi}^{\pi} dx \exp(inx)\boldsymbol{\delta}_x. \tag{4.106b}$$

The point of view which emerges from the introduction of the Fourier-$\boldsymbol{\varphi}$ and Dirac-$\boldsymbol{\delta}$ bases into generalized function spaces is that a vector $\mathbf{f}$ can be represented in the former as an infinite column vector with elements $\{f_n\}_{n\in\mathscr{Z}}$ and in the latter as a column vector of height 2π whose "rows" are labeled by a continuous index $x \in (-\pi, \pi]$ and whose xth entry is $f(x)$. The transformation from one representation to the other is achieved by

$$f(x) = (\boldsymbol{\delta}_x, \mathbf{f}) = \sum_{n \in \mathscr{Z}} (\boldsymbol{\delta}_x, \boldsymbol{\varphi}_n)(\boldsymbol{\varphi}_n, \mathbf{f}), \tag{4.107a}$$

$$f_n = (\boldsymbol{\varphi}_n, \mathbf{f}) = \int_{-\pi}^{\pi} dx (\boldsymbol{\varphi}_n, \boldsymbol{\delta}_x)(\boldsymbol{\delta}_x, \mathbf{f}), \tag{4.107b}$$

which are nothing more than the Fourier synthesis and analysis, Eqs. (4.32). In terms of vector components, we can visualize Eqs. (4.107) as the transformation through a "rectangular" matrix $\boldsymbol{\Phi} = \|\varphi_n(x)\| = \|(\boldsymbol{\delta}_x, \boldsymbol{\varphi}_n)\|$ with rows labeled by x and columns by n. Fourier synthesis (4.32a) is then the multiplication of $\boldsymbol{\Phi}$ and the discrete-row vector (f_n), giving the continuous-row vector $[f(x)]$, while Fourier analysis (4.32b) is the multiplication of the transposed conjugate $\boldsymbol{\Phi}^\dagger$ and $[f(x)]$, giving back (f_n). In the latter case we integrate rather than sum over the continuous label in the matrix and vector.

Exercise 4.37. Compare the point of view regarding $\boldsymbol{\Phi}$ as a (passive) transformation between coordinates $f(x)$ and f_n with that developed in Section 1.3. Note that in comparison with Eq. (1.28), the $\boldsymbol{\varepsilon}$- and $\boldsymbol{\delta}$-bases play analogous roles, as do the $\bar{\boldsymbol{\varepsilon}}$- and $\boldsymbol{\varphi}$-bases.

Exercise 4.38. Verify that $\boldsymbol{\Phi}$, although "rectangular," is a *unitary* matrix. Show that $\boldsymbol{\Phi}^\dagger\boldsymbol{\Phi}$ is, because of (4.10), an infinite unit matrix with discrete rows and columns, while $\boldsymbol{\Phi}\boldsymbol{\Phi}^\dagger$ is, by virtue of (4.82), a unit matrix with a continuum of rows and columns and a Dirac δ sitting along the diagonal. These are two representations of the unit operator in the $\boldsymbol{\varphi}$- and $\boldsymbol{\delta}$-bases, respectively. This will be elaborated in Section 4.6.

Depending on the reader's inclination toward pure or applied mathematics, he may want to pursue the subject of generalized functions to their complete formulation, or he may be content with the physicist's point of view of accepting a reasonably working and economical structure and ask for the applications to justify its use. The work of Gel'fand *et al.* (1964–1968) (in five volumes) is a detailed rendering of the theory and fortunately not the acme of abstraction. Most texts on quantum mechanics or practical communication theory make extensive use of plane waves, localized states, or unit impulse functions, so there is little to be added in terms of the usefulness of the concepts and their adaptability to the degree of rigor demanded by the circumstances.

4.6. Linear Operators, Infinite Matrices, and Integral Kernels

In Section 4.3 we introduced the translation and inversion operators $\mathbb{T}_a$ and $\mathbb{I}_0$ defined by Eqs. (4.36) and (4.41) as linear mappings in the space of functions $\mathscr{V}^D$ which satisfy the Dirichlet conditions. These can be extended to generalized functions as they stand. Later, in Section 4.4 we dealt with the operation of differentiation which is linear but which can map elements of $\mathscr{V}^D$ out of this space; in particular, in Section 4.5 we saw that discontinuous functions were transformed under differentiation into generalized functions in $\mathscr{S}'$ represented by divergent Fourier series. Repeated integration, on the other hand, can bring functions in $\mathscr{S}'$ back into $\mathscr{V}^D$. We shall ask our operators here to be *linear* mappings in the space of generalized functions, but we cannot in general be too precise about their domain and range. In this section, rigor is explicitly disclaimed. We are presenting here mathematics as applied in quantum mechanics à la Dirac. It has intuitive appeal and represents a real economy in notation.

4.6.1. Operators and Their Matrix Representatives

Let $\mathbb{A}$ be a linear operator whose action on the vectors of the orthonormal $\boldsymbol{\varphi}$-basis is known:

$$\mathbb{A}\boldsymbol{\varphi}_n = \boldsymbol{\varphi}_n{}^A = \sum_{m\in\mathscr{Z}} A_{mn}\boldsymbol{\varphi}_m, \tag{4.108a}$$

where we have used (4.102) for $\boldsymbol{\varphi}_n^A$ so that

$$A_{mn} = (\boldsymbol{\varphi}_m, \boldsymbol{\varphi}_n{}^A) = (\boldsymbol{\varphi}_m, \mathbb{A}\boldsymbol{\varphi}_n). \tag{4.108b}$$

Its action on any infinite linear combination $\mathbf{f}$ of these is then

$$\begin{aligned}\mathbb{A}\mathbf{f} = \mathbb{A}\sum_{n\in\mathscr{Z}} f_n\boldsymbol{\varphi}_n &= \sum_{n\in\mathscr{Z}} f_n\mathbb{A}\boldsymbol{\varphi}_m = \sum_{n,m\in\mathscr{Z}} f_nA_{mn}\boldsymbol{\varphi}_m \\ =: \mathbf{f}^A &= \sum_{m\in\mathscr{Z}} f_m{}^A\boldsymbol{\varphi}_m.\end{aligned} \tag{4.109}$$

Performing the inner product with the vectors of the $\boldsymbol{\varphi}$-basis, or using their linear independence, we find

$$f_m{}^A = \sum_{n\in\mathscr{Z}} A_{mn}f_n. \tag{4.110}$$

The column vector (f_n) is seen to transform into $(f_m{}^A)$ by multiplication by the matrix $\mathbf{A} = \|A_{mn}\|$, which *represents* the operator $\mathbb{A}$ in the $\boldsymbol{\varphi}$-basis. The matrix is infinite, its rows and columns numbered by $m, n \in \mathscr{Z}$, but otherwise our construction proceeds exactly as in Section 1.3. The orthonormal basis we shall use in the remainder of this section is the Fourier $\boldsymbol{\varphi}$-basis.

Exercise 4.39. Find the matrix $\mathbf{T}_a$ representing the translation operator $\mathbb{T}_a$. This can be done by either calculating $(\mathbb{T}_a)_{mn}$ by (4.108b) and (4.36a) or, for

$\mathbf{f}^T = \mathbb{T}_a\mathbf{f}$, comparing (4.110) with the result (4.36b). One finds the matrix to be diagonal:

$$(\mathbf{T}_a)_{mn} = \delta_{mn} \exp(ina). \tag{4.111}$$

In particular, for $\mathbb{T}_0 = \mathbb{1}$, (4.111) is the infinite *unit* matrix.

Exercise 4.40. Find the matrix $\mathbf{I}_0$ representing the inversion operator $\mathbb{I}_0$. Again, this can be done by (4.108b) or (4.110) using (4.41). It is an antidiagonal matrix:

$$(\mathbf{I}_0)_{mn} = \delta_{m,-n} = \delta_{m+n,0}. \tag{4.112}$$

Exercise 4.41. Verify that the products of translations and inversion matrix representatives (4.111) and (4.112) follow Eqs. (4.42).

Exercise 4.42. Consider the operator of differentiation: $\mathbf{f}^{(p)} = \mathbb{V}^p\mathbf{f}$. Find the matrix $\mathbf{\nabla}$ representing it, again, either by (4.108b) or by (4.110) and (4.51). One can show $\mathbf{\nabla}$ to be a diagonal matrix whose elements are

$$\nabla_{mn} = \delta_{mn} in. \tag{4.113}$$

Find its powers as well.

4.6.2. Operators and Integral Kernels

We also have the Dirac generalized basis to describe the function vector space [Eq. (4.103)]. Correspondingly, operators will have their matrix representatives in this basis. These "matrices," however, will have their rows and columns labeled by continuous indices in the range $(-\pi, \pi]$. We follow the argument (4.108)–(4.110), assuming now that the action on Dirac's basis is known:

$$\mathbb{A}\boldsymbol{\delta}_y = \boldsymbol{\delta}_y{}^A = \int_{-\pi}^{\pi} dx A(x, y)\boldsymbol{\delta}_x, \tag{4.114a}$$

having used (4.103) on $\boldsymbol{\delta}_y^A$, where

$$A(x, y) = (\boldsymbol{\delta}_x, \boldsymbol{\delta}_y{}^A) = (\boldsymbol{\delta}_x, \mathbb{A}\boldsymbol{\delta}_y). \tag{4.114b}$$

As before, we can find the action of $\mathbb{A}$ on any $\mathbf{f}$ by (4.103) as

$$\begin{aligned}\mathbb{A}\mathbf{f} &= \mathbb{A}\int_{-\pi}^{\pi} dy f(y)\boldsymbol{\delta}_y = \int_{-\pi}^{\pi} dy f(y)\mathbb{A}\boldsymbol{\delta}_y \\ &= \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy f(y)A(x, y)\boldsymbol{\delta}_x =: \mathbf{f}^A = \int_{-\pi}^{\pi} dx f^A(x)\boldsymbol{\delta}_x. \end{aligned} \tag{4.115}$$

Performing the inner product with the vectors in the $\boldsymbol{\delta}$-basis and using (4.104), or by linear independence alone, we find

$$f^A(x) = \int_{-\pi}^{\pi} dy A(x, y) f(y) \tag{4.116}$$

as the analogue of (4.110) in the Dirac basis. Equation (4.116) shows that the operator $\mathbb{A}$ is represented here by an *integral kernel* $A(x, y)$ which acts as if it were a matrix $\|A(x, y)\|$ with a continuum of rows and columns acting on like column vectors, integration replacing sum over the entries.

Exercise 4.43. Show the integral kernel $T_a(x, y)$ representing the translation operation $\mathbb{T}_a$ to be

$$T_a(x, y) = \delta(x - y + a) \tag{4.117}$$

(where a, x, and y are to be considered modulo 2π), i.e., an off-diagonal "matrix." Verify that (4.117) in (4.116) correctly reproduces the translation (4.36a). In particular, for $\mathbb{T}_0 = \mathbb{1}$ this defines the unit or *reproducing* kernel.

Exercise 4.44. Show the integral kernel $I_0(x, y)$ representing inversions $\mathbb{I}_0$ to be

$$I_0(x, y) = \delta(x + y), \tag{4.118}$$

i.e., an antidiagonal "matrix."

Exercise 4.45. Verify the products (4.42) for the integral kernels (4.117) and (4.118) representing the operators.

Exercise 4.46. Find the integral kernel $\nabla(x, y)$ representing the operator of differentiation $\mathbb{V}$. Using (4.98), show that

$$\nabla(x, y) = \delta^{(1)}(x - y). \tag{4.119}$$

Find also the integral kernel representing $\mathbb{V}^p$.

4.6.3. The Link: Fourier Transformation

The matrices representing the operator $\mathbb{A}$ in two bases can be related, as in Section 1.3, by the transformation linking the two bases. Indeed, between the Fourier and Dirac bases we have

$$\begin{aligned} A(x, y) &= (\boldsymbol{\delta}_x, \mathbb{A}\boldsymbol{\delta}_y) = \sum_{m,n\in\mathscr{Z}} (\boldsymbol{\delta}_x, \boldsymbol{\varphi}_m)(\boldsymbol{\varphi}_m, \mathbb{A}\boldsymbol{\varphi}_n)(\boldsymbol{\varphi}_n, \boldsymbol{\delta}_y) \\ &= (2\pi)^{-1} \sum_{m,n\in\mathscr{Z}} A_{mn} \exp[i(mx - ny)], \end{aligned} \tag{4.120a}$$

$$\begin{aligned} A_{mn} &= (\boldsymbol{\varphi}_m, \mathbb{A}\boldsymbol{\varphi}_n) = \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy (\boldsymbol{\varphi}_m, \boldsymbol{\delta}_x)(\boldsymbol{\delta}_x, \mathbb{A}\boldsymbol{\delta}_y)(\boldsymbol{\delta}_y, \boldsymbol{\varphi}_n) \\ &= (2\pi)^{-1} \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy A(x, y) \exp[-i(mx - ny)]. \end{aligned} \tag{4.120b}$$

Exercise 4.47. Verify the relations (4.120) between the matrices and integral kernels representing the translation, inversion, and differentiation operators found above.

Exercise 4.48. Interpret Eqs. (4.120) as the matrix equations

$$A = \mathbf{\Phi A \Phi^{\dagger}}, \qquad \mathbf{A} = \mathbf{\Phi}^{\dagger} A \mathbf{\Phi}, \qquad \mathbf{\Phi} := \|(\boldsymbol{\delta}_x, \boldsymbol{\varphi}_n)\|, \tag{4.120c}$$

where $\mathbf{\Phi}$ is the "rectangular" matrix suggested in the discussion at the end of Section 4.5.

Exercise 4.49. Prove

$$\mathbb{T}_a \mathbb{V} = \mathbb{V} \mathbb{T}_a, \tag{4.121a}$$

$$\mathbb{I}_0 \mathbb{V} = -\mathbb{V} \mathbb{I}_0 \tag{4.121b}$$

by their action on an arbitrary function $f(x)$, on its Fourier coefficients, or their matrix or integral kernel representatives.

4.6.4. Hermitian and Isometric Operators

Proceeding along the lines of Chapter 1, in classifying and studying the properties of operators, now in function (Hilbert) spaces, we shall define an operator $\mathbb{H}$ to be *hermitian* if

$$(\mathbb{H}\mathbf{f}, \mathbf{g}) = (\mathbf{f}, \mathbb{H}\mathbf{g}) \tag{4.122a}$$

for all $\mathbf{f}$ and $\mathbf{g}$ in the domain of $\mathbb{H}$. It is easy to see that if (4.122a) holds and the $\boldsymbol{\varphi}$- and $\boldsymbol{\delta}$-basis vectors are in the domain of $\mathbb{H}$, then $\mathbb{H}$ is represented by a *hermitian* matrix and kernel, i.e., those which are equal to their transposed conjugates:

$$H_{mn} = H_{nm}^{*}, \tag{4.122b}$$

$$H(x, y) = H(y, x)^{*}. \tag{4.122c}$$

In particular, the inversion operator $\mathbb{I}_0$ and $-i\mathbb{V}$ are represented by manifestly hermitian matrices and kernels [Eqs. (4.112), (4.113), (4.118), and (4.119)].

An operator $\mathbb{U}$ is said to be *isometric* if

$$(\mathbb{U}\mathbf{f}, \mathbb{U}\mathbf{g}) = (\mathbf{f}, \mathbf{g}) \tag{4.123a}$$

for all $\mathbf{f}$ and $\mathbf{g}$ in its domain. Again, for the vectors in the $\boldsymbol{\varphi}$- and $\boldsymbol{\delta}$-bases we can write out the inner product and find the condition on the representatives to be

$$\sum_{m \in \mathscr{Z}} U_{mn}^{*} U_{ml} = \delta_{n,l}, \tag{4.123b}$$

$$\int_{-\pi}^{\pi} dy U(y, x)^{*} U(y, z) = \delta(x - z). \tag{4.123c}$$

The translation operators $\mathbb{T}_a$ are represented by such matrices and kernels [Eqs. (4.111) and (4.117)].

4.6.5. Self-Adjoint and Unitary Operators

Not much has been said here about the *domain* of the operators, although this is in fact the key element which allows one to know when the results of finite-dimensional matrices on complete eigenbases can be translated to the infinite-dimensional case. For this, let us remark that the adjoint $\mathbb{A}^\dagger$ of an operator $\mathbb{A}$ is defined as that linear mapping which, if it exists, satisfies $(\mathbb{A}^\dagger\mathbf{f}, \mathbf{g}) = (\mathbf{f}, \mathbb{A}\mathbf{g})$. A *self-adjoint* operator is a hermitian operator where the domain of $\mathbb{A}$ and $\mathbb{A}^\dagger$ are the same. Similarly, a *unitary* operator is an isometric one where this happens.

It is for self-adjoint and unitary operators that powerful results on eigenbases hold. Fortunately all of the operators which we shall handle and most of the operators the reader is likely to meet in quantum mechanics are either self-adjoint or unitary or have *extensions* which are. However, one does occasionally stumble upon innocuous-looking operators which under closer scrutiny turn out to be only hermitian or isometric, but it would not serve the purpose of this text to insist too much on these.

Exercise 4.50. Show that the translation and differentiation operators are related by

$$\mathbb{T}_a = \exp(a\mathbb{V}). \tag{4.124}$$

This is easy to verify for the matrix representatives (4.111) and (4.113) or for the kernels (4.117) and (4.119) using (4.99). It is true for the operator as well, due to the fact that $-i\mathbb{V}$ has a self-adjoint extension here. From (4.124) it is also clear that $\mathbb{T}_a$ *commutes* with $\mathbb{V}$.

4.6.6. Some Facts Concerning the Spectra and Eigenbases of Self-Adjoint Operations

When a vector $\mathbf{f}$ in the domain of an operator $\mathbb{A}$ satisfies

$$\mathbb{A}\mathbf{f} = \lambda\mathbf{f}, \qquad \lambda \in \mathscr{C}, \tag{4.125}$$

it is said to be an *eigenvector* of $\mathbb{A}$ with *eigenvalue* λ. This definition is the analogue of that given in Section 1.7 for finite-dimensional spaces and has already appeared in (4.46) in the language of functions. The set of all possible eigenvalues λ in (4.125) constitutes the *point spectrum* of $\mathbb{A}$. In addition to the point spectrum (values of λ such that $\mathbb{A} - \lambda\mathbb{1}$ has no inverse), operators may have a *continuous* spectrum (values of λ for which $\mathbb{A} - \lambda\mathbb{1}$ is one-to-one but not onto). This is the main difference from the matrix spectra of Section 1.7, which are only point spectra. For *rigged* Hilbert spaces, i.e., triples of spaces $\mathscr{S} \subset \mathscr{L}^2(\mathscr{J}) \subset \mathscr{S}'$ with an inner product, briefly presented in Section 4.5, one can define *generalized* eigenvectors $\mathbf{f} \in \mathscr{S}'$ of $\mathbb{A}$ by the weaker property $(\mathbb{A}^\dagger\mathbf{g}, \mathbf{f}) = \lambda(\mathbf{g}, \mathbf{f})$ for every $\mathbf{g} \in \mathscr{S}$. The main facts concerning eigenvectors and eigenvalues of self-adjoint and unitary operators follow those given in Section 1.7, namely: (a) The spectra of self-adjoint and unitary operators are subsets of, respectively, the real line and the unit circle. (b) Eigenvectors corresponding to different eigenvalues are orthogonal. The proofs follow (1.106) and (1.112). (c) The set of eigenvectors of a given self-adjoint or unitary operator constitutes a *complete* generalized basis for the Hilbert space. (d) The eigenvalues can be used to label the eigenvectors; if the subspaces corresponding to a given eigenvalue are of dimension higher than 1, however, one or more extra operators commuting with $\mathbb{A}$ and among themselves have to be found in order to resolve the labeling degeneracy.

4.6.7. The Fourier and Dirac Bases

Regarding the operators we have been working with, we have already remarked that the Fourier basis $\{\boldsymbol{\varphi}_n\}_{n\in\mathscr{Z}}$ is the eigenbasis of all $\mathbb{T}_a$. In fact, it is also the eigenbasis of $-i\mathbb{V}$ since

$$-i\mathbb{V}\boldsymbol{\varphi}_n = n\boldsymbol{\varphi}_n, \qquad n \in \mathscr{Z}. \tag{4.126}$$

This can be ascertained easily from (4.50) or (4.113) and links with the previous fact by (4.124). The $\boldsymbol{\varphi}$-basis could have been constructed in searching for the eigenbasis of $-i\mathbb{V}$ in the space of periodic functions of period 2π. The spectrum of $-i\mathbb{V}$ on this space is the set of integers $\mathscr{Z}$. [If this domain were not specified, the eigenfunctions would be $\exp(icx)$ for $c \in \mathscr{C}$. Were we to ask for the domain to be instead that of functions in $[0, \infty)$, $-i\mathbb{V}$ would not be self-adjoint.]

Exercise 4.51. Construct the Fourier basis for $\mathscr{L}^2(-\pi, \pi)$ as an eigenbasis of $\mathbb{V}^2$. This leaves $\boldsymbol{\varphi}_n$ and $\boldsymbol{\varphi}_{-n}$ belonging to the same eigenvalue $-n^2$ and hence not uniquely labeled. As detailed in Section 1.7, one has to search for other operators to resolve the labeling degeneracy. Try $\mathbb{I}_0$ which satisfies (4.121b) and show that it leads to the sine and cosine Fourier series functions $2^{-1/2}(\boldsymbol{\varphi}_n \pm \boldsymbol{\varphi}_{-n})$.

Turning to the Dirac $\boldsymbol{\delta}$-basis, assume we have an operator $\mathbb{K}$ which is represented by a *diagonal* kernel $K(x, y) = \delta(x - y)k(x)$, where $k(x)$ is some continuous function of $x \in (-\pi, \pi]$. From (4.114) we can then see that the elements of the $\boldsymbol{\delta}$-basis are eigenvectors of $\mathbb{K}$, as

$$\mathbb{K}\boldsymbol{\delta}_y = k(y)\boldsymbol{\delta}_y, \qquad y \in (-\pi, \pi], \tag{4.127}$$

and can thus be used to *define* Dirac's basis as an eigenbasis of such operators.

Exercise 4.52. Show that the action of *function operators* such as (4.127) on the vectors of function space is

$$\mathbb{K}\mathbf{f} = \mathbf{k}(\boldsymbol{\delta})\,\mathbf{f}, \quad \text{i.e.,} \quad (\mathbb{K}\mathbf{f})(x) = k(x)f(x). \tag{4.128}$$

Exercise 4.53. Construct a general operator represented by a diagonal matrix as $G_{mn} = \delta_{mn} g_n$. Show that the action of these *convolution operators* on a general vector is

$$\mathbb{G}\mathbf{f} = \mathbf{g}(\boldsymbol{\varphi})\,\mathbf{f}, \quad \text{i.e.,} \quad (\mathbb{G}\mathbf{f})(x) = (\mathbf{g} * \mathbf{f})(x). \tag{4.129}$$

The concepts outlined in the last two sections will be used in Chapter 5 and in Part III on Fourier integral transforms, where the domain of all functions will be the full real line. For the reader interested in pursuing the subject of operator spectral theory, we may suggest one of the volumes by Gel'fand *et al.* (1964, Vol. 4, Chapter 1). The general subject of operators in Hilbert spaces is a broad subject indeed. Classics in this field are the works of Dunford and Schwartz (1960), Courant and Hilbert (1962), Yoshida (1965), and L. Schwartz (1966). The book by Kato (1966) presents results on spectra and perturbations for finite- as well as infinite-dimensional spaces.

Closer to our approach and in the specific field of Fourier series, the volume by Whittaker and Watson (1903, Chapter IX) gives a reasonable survey of the field as it stood at the turn of the century. Selected modern treatments—in the vein of functional analysis—are those of Lanczos (1966), Edwards (1967), Dym and McKean (1972), and Oberhettinger (1973). Most texts on mathematical methods in physics will have at least one chapter devoted to Fourier series, although those dealing with quantum mechanics will tend to present the vector space approach of this section. We recall the books by Messiah (1964) and Fano (1971).

Infinite-order differential operators such as (4.124) and others which will appear in the following chapters are one of the bases for Lie groups and algebras [see Miller (1972)]. On hyperdifferential operators of "higher" types such as (4.100), i.e., exponentials of *second*-order differential operators, there are the mathematical treatments by Trèves (1969), Steinberg and Trèves (1970), and Miller and Steinberg (1971).

4.7. Fourier Series for Any Period and the Infinite-Period Limit

In this section we shall provide the Fourier series expression for the expansion of periodic functions of period $2L$. This will serve to prepare the way for describing the vibrating string in Section 5.2 and, in letting $L \to \infty$, finding the Fourier integral transform, which is the subject of Part III.

4.7.1. Fourier Series for Arbitrary Period

Periodic functions of period 2π can be expanded in their Fourier series,

$$f(x) = (2\pi)^{-1/2} \sum_{n \in \mathscr{Z}} f_n \exp(inx) \tag{4.130a}$$

$$f_n = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) \exp(-inx), \tag{4.130b}$$

and the Parseval identity is

$$(\mathbf{f}, \mathbf{g}) = \int_{-\pi}^{\pi} dx f(x)^* g(x) = \sum_{n \in \mathscr{Z}} f_n^* g_n. \tag{4.130c}$$

It is often convenient to have explicit formulas giving a similar expansion for functions of arbitrary period $2L$. We thus define the following quantities:

$$q := xL/\pi \qquad \text{so} \quad x \in (-\pi, \pi] \Rightarrow q \in (-L, L], \tag{4.131a}$$

$$f_n^L := (L/\pi)^{1/2} f_n, \qquad f^L(q) := (L/\pi)^{-1/2} f(x). \tag{4.131b}$$

Substituting (4.131) into (4.130) and dropping the L on $f^L(q)$, we find the period $2L$ Fourier series,

$$f(q) = (2\pi)^{-1/2}(\pi/L) \sum_{n \in \mathscr{Z}} f_n^L \exp(\pi i n q/L), \tag{4.132a}$$

$$f_n^L = (2\pi)^{-1/2} \int_{-L}^{L} dq f(q) \exp(-\pi i n q/L), \tag{4.132b}$$

and the Parseval identity reads

$$(\mathbf{f}, \mathbf{g})_L := \int_{-L}^{L} dq f(q)^* g(q) = (\pi/L) \sum_{n \in \mathscr{Z}} f_n^{L*} g_n^L. \tag{4.132c}$$

For $L = \pi$ we regain (4.130). Of course, all the results on Fourier series in the form (4.130) hold for (4.132) with the appropriate changes of scale (4.131).

4.7.2. Odd Functions on $(-L, L)$

In Section 5.2 we shall be interested in Fourier expansions of functions which are *odd* under reflection through the origin. Since $f(-q) = -f(q)$ and $f(0) = 0 = f(L)$, the values in the interval $(0, L)$ are sufficient to determine the values of the Fourier coefficients (4.132b), which will display the symmetry of odd functions: $f_{-n}^L = -f_n^L$ (Table 4.2). The most economical description can thus be seen to be in terms of the Fourier *sine* series and its partial-wave coefficients $f_n^{L-} = 2^{1/2} i f_n^L$. Using the oddness of $f(q)$ and defining for convenience

$$f_n^{\circ} := (\pi/2L)^{1/2} f_n^{L-} = i(\pi/L)^{1/2} f_n^L, \qquad n = 1, 2, 3, \ldots, \tag{4.133}$$

Eqs. (4.132) can be written again as

$$f(q) = (2/L)^{1/2} \sum_{n \in \mathscr{Z}^+} f_n^{\circ} \sin(n\pi q/L), \tag{4.134a}$$

$$f_n^{\circ} = (2/L)^{1/2} \int_0^L dq f(q) \sin(n\pi q/L), \tag{4.134b}$$

$$(\mathbf{f}, \mathbf{g})_L^{\circ} := \int_0^L dq f(q)^* g(q) = \sum_{n \in \mathscr{Z}^+} f_n^{\circ *} g_n^{\circ}. \tag{4.134c}$$

We see thus that a function $f(q) \in \mathscr{V}^D$ for $q \in (0, L)$ can be expanded in a series of sine functions with all the properties of the Fourier series. Outside this interval, however, $f(q)$ will be odd under inversions and with period $2L$.

Exercise 4.54. Consider a rectangle function of width ε and height η centered at $q = q_0$, i.e., $R^{(\varepsilon,\eta)}(q - q_0)$. Find its sine Fourier coefficients

$$(\mathbb{T}_{-q_0}\mathbf{R}^{(\varepsilon,\eta)})_n{}^o = 2(2L)^{1/2}\eta(\pi n)^{-1}\sin(n\pi\varepsilon/2L)\sin(n\pi q_0/L). \tag{4.135}$$

In particular, note that the series coefficients imply $R^{(L+\varepsilon,\eta)}(q - L/2) = R^{(L-\varepsilon,\eta)}(q - L/2)$. How do you interpret this fact in view of the antisymmetry of the periodic functions under inversion? Note that the rectangle function in $(0, L)$ has a corresponding negative "phantom" rectangle in $(-L, 0)$. This will turn out to be the Green's function for elastic media with fixed boundaries in Section 5.2.

Exercise 4.55. Under the assumption that $f(q)$ is *even* under inversion through the origin, find from (4.132) the analogue of (4.134), expanding $f(q)$ in cosine functions. This is simply

$$f(q) = (2/L)^{1/2} \sum_{n\in 0,\mathscr{Z}^+} f_n{}^e \cos(n\pi x/L), \tag{4.136a}$$

$$f_n{}^e = (2/L)^{1/2} \int_0^L dq f(q)\cos(n\pi x/L), \tag{4.136b}$$

$$(\mathbf{f}, \mathbf{g})_L{}^e := \int_0^L dq f(q)^* g(q) = \sum_{n\in 0,\mathscr{Z}^+} f_n^{e*} g_n{}^e. \tag{4.136c}$$

Note that if $f(q)$ is assumed differentiable, $\lim_{q\to 0,L} df(q)/dq = 0$.

4.7.3. The Limit $L \to \infty$ and Fourier Integral Transforms

We now turn back to (4.132) and examine what happens when we let $L \to \infty$. It is convenient to introduce the further new variables

$$p := \pi n/L \in \{0, \pm\Delta p, \pm 2\Delta p, \ldots\} =: \pi\mathscr{Z}/L, \qquad \Delta p := \pi/L, \tag{4.137a}$$

$$\tilde{f}(p) := f_n{}^L = (L/\pi)^{1/2} f_n. \tag{4.137b}$$

Equations (4.132) can then be written in the form

$$f(q) = (2\pi)^{-1/2} \sum_{p\in\pi\mathscr{Z}/L} \Delta p \tilde{f}(p)\exp(ipq), \tag{4.138a}$$

$$\tilde{f}(p) = (2\pi)^{-1/2} \int_{-L}^{L} dq f(q)\exp(-ipq), \tag{4.138b}$$

$$(\mathbf{f}, \mathbf{g})_L = \int_{-L}^{L} dq f(q)^* g(q) = \sum_{p\in\pi\mathscr{Z}/L} \Delta p \tilde{f}(p)^* \tilde{g}(p). \tag{4.138c}$$

As in Section 3.4, the limit $L \to \infty$ is seen to lead to Riemann integration over

$p \in \mathscr{R}$ in (4.138a) and (4.138c) as $\Delta p \to 0$. Provided the limits exist, we can write

$$f(q) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp \tilde{f}(p) \exp(ipq), \tag{4.139a}$$

$$\tilde{f}(p) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f(q) \exp(-ipq), \tag{4.139b}$$

$$(\mathbf{f}, \mathbf{g}) := \int_{-\infty}^{\infty} dq f(q)^* g(q) = \int_{-\infty}^{\infty} dp \tilde{f}(p) \tilde{g}(p), \tag{4.139c}$$

where $\tilde{f}(p)$ now stands for the function of $p \in \pi\mathscr{Z}/L$ extended to the full real line by a step function which takes the value $\tilde{f}(p)$ for all p in the intervals centered at the original points. In Section 7.1 we shall prove the *Fourier integral theorem* [Eqs. (4.139)] independently and shall comment on its range of validity. In Section 3.4 and here we have shown that (4.139) arises formally from Fourier finite transforms and series.