Integral Transforms in Science and Engineering

Kurt Bernardo Wolf

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Integral Transforms in Science and Engineering

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Kurt Bernardo Wolf

Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas
Universidad Nacional Autónoma de México
México D.F., México

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To Ayalá
and little Gunnar

Preface

Integral transforms are among the main mathematical methods for the solution of equations describing physical systems, because, quite generally, the coupling between the elements which constitute such a system—these can be the mass points in a finite spring lattice or the continuum of a diffusive or elastic medium—prevents a straightforward "single-particle" solution. By describing the same system in an appropriate reference frame, one can often bring about a mathematical *uncoupling* of the equations in such a way that the solution becomes that of noninteracting constituents. The "tilt" in the reference frame is a finite or integral transform, according to whether the system has a finite or infinite number of elements. The types of coupling which yield to the integral transform method include diffusive and elastic interactions in "classical" systems as well as the more common quantum-mechanical potentials.

The purpose of this volume is to present an orderly exposition of the theory and some of the applications of the finite and integral transforms associated with the names of Fourier, Bessel, Laplace, Hankel, Gauss, Bargmann, and several others in the same vein.

The volume is divided into four parts dealing, respectively, with finite, series, integral, and canonical transforms. They are intended to serve as independent units. The reader is assumed to have greater mathematical sophistication in the later parts, though.

Part I, which deals with finite transforms, covers the field of complex vector analysis with emphasis on particular linear operators, their eigenvectors, and their eigenvalues. Finite transforms apply naturally to lattice structures such as (finite) crystals, electric networks, and finite signal sets.

Fourier and Bessel series are treated in Part II. The basic theorems are proven here in the customary classical analysis framework, but when

introducing the Dirac δ, we do not hesitate in translating the vector space concepts from their finite-dimensional counterparts, aiming for the rigor of most mathematical physics developments. The appropriate warning signs are placed where one is bound, nevertheless, to be led astray by finite-dimensional analogues. Applications include diffusive and elastic media of finite extent and infinite lattices.

Fourier transforms occupy the major portion of Part III. After their introduction and the study of their main properties, we turn to the treatment of certain special functions which have close connection with Fourier transforms and which are, moreover, of considerable physical interest: the attractive and repulsive quantum oscillator wave functions and coherent states. Other integral transforms (Laplace, Mellin, Hankel, etc.) related to the Fourier transform and applications occupy the rest of this part.

"Canonical transforms" is the name of a parametrized continuum of transforms which include, as particular cases, most of the integral transforms of Part III. They also include Bargmann transforms, a rather modern tool used for the description of shell-model nuclear physics and second-quantized boson field theories. In the presentation given in Part IV, we are adapting recent research material such as canonical transformations in quantum mechanics, hyperdifferential operator realizations for the transforms, and similarity groups for a class of differential equations. We do not explicitly use Lie group theory, although the applications we present in the study of the diffusion and related Schrödinger equations should cater to the taste of the connoisseur.

On the whole, the pace and tone of the text have been set by the balance of intuition and rigor as practiced in applied mathematics with the aim that the contents should be useful for senior undergraduate and graduate students in the scientific and technical fields. Each part contains a flux diagram showing the logical concatenation of the sections so as to facilitate their use in a variety of courses. The graduate student or research worker may be interested in some particular sections such as the fast Fourier transform computer algorithm, the Gibbs phenomenon, causality, or oscillator wave functions. These are subjects which have not been commonly included under the same cover. Part IV, moreover, may spur his or her interest in new directions. We have tried to give an adequate bibliography whenever our account of an area had to stop for reasons of specialization or space. References are cited by author's name and year of publication, and they are listed alphabetically at the end of the book. A generous number of figures and some tables should enable the reader to browse easily. New literals are defined by "≔"; thus $f \coloneqq A$ means f is defined as the expression A. Vectors and unargumented functions are denoted by lowercase boldface type and matrices by uppercase boldface. Operators appear in "double" type, e.g., $\mathbb{Q}, \mathbb{P}$, and sets in script, e.g., $\mathscr{R}, \mathscr{C}$. A symbol list is included at the end.

Exercises are used mainly to suggest alternative proofs, extensions to the text material, or cross references, usually providing the answers as well as further comments. They are meant to be read at least cursorily as part of the text. Equations are numbered by chapter.

I would like to express my gratitude to Professor Tomás Garza for his encouragement and support of this project; to my colleagues Drs. Charles P. Boyer, Jorge Ize, and Antonmaría Minzoni among many others at IIMAS, Instituto de Física, and Facultad de Ciencias, for their critical comments on the manuscript; and to my students for bearing with the first versions of the material in this volume. The graphics were programmed by the author on the facilities of the Centro de Servicios y Cómputo and plotted at the Instituto de Ingeniería, UNAM. Special acknowledgment is due to Miss Alicia Vázquez for her fine secretarial work despite many difficulties.

Ciudad Universitaria, México D.F. Kurt Bernardo Wolf

Contents

PART I. FINITE-DIMENSIONAL VECTOR SPACES AND THE FOURIER TRANSFORM

PART II. FOURIER AND BESSEL SERIES

PART III. FOURIER AND RELATED INTEGRAL TRANSFORMS

PART IV. CANONICAL TRANSFORMS

Part I

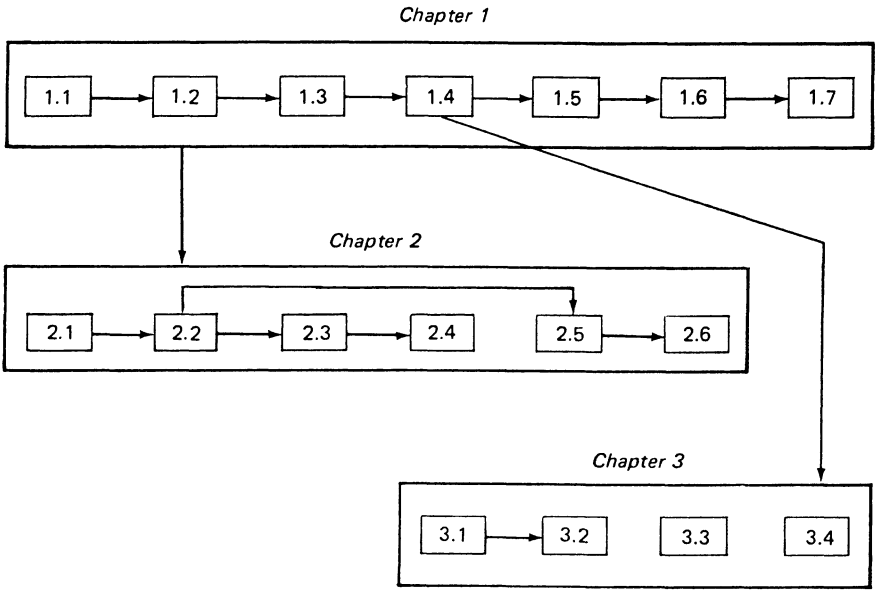
Finite-Dimensional Vector Spaces and the Fourier Transform

In this part we develop the mathematical framework of finite-dimensional Fourier transforms and give the basics of two fields where it has found fruitful application: in the analysis of coupled systems and in communication theory and technology.

Chapter 1 deals with complex vector analysis in N dimensions and leads rather quickly to the tools of Fourier analysis: unitary transformations and self-adjoint operators. The uncoupling of lattices representing one-dimensional crystals and electric *RLC* networks is undertaken in Chapter 2. We examine in detail the fundamental solutions, normal modes, and traveling waves for first-neighbor interactions in simple crystal lattices and extend these to farther-neighbor, molecular, and diatomic crystals. The Fourier formalism is also used to describe the analytical mechanics of these systems: phase space, energy, evolution operators, and other conservation laws. Chapter 3 introduces convolution and correlation, sketching their use in filtering, windowing, and modulation of signals and their detection in the presence of background noise. The workings of the fast Fourier transform (FFT) computation algorithm are given in Section 3.3. Finally, in Section 3.4, some properties of Fourier series and integral transforms (Parts II and III) are put in the form of corresponding properties of the finite Fourier transform on vector spaces whose dimension grows without bound.

Chapters 2 and 3 are independent of each other and can be chosen according to the reader's interest. With the first choice, Sections 1.6 and 1.7 will be particularly needed. The understanding of Chapter 3, on the other hand, does not require basically more than Sections 1.1–1.4. Before going

to the following parts in this text, the reader may find Section 3.4 useful. Table 1.1, which gives the main properties of the finite Fourier transform, is placed at the end of Chapter 1.



I

Concepts from Complex Vector Analysis and the Fourier Transform

In this chapter we present the basic properties of complex vector spaces and the Fourier transform. Sections 1.1 and 1.2 prepare the subject through the standard definitions of linear independence, bases, coordinates, inner product, and norm. In Section 1.3 we introduce linear transformations in vector spaces, emphasizing the conceptual difference between passive and active ones: the former refer to changes in reference coordinates, while the latter imply a "physical" process actually transforming the points of the space. Permutations of reference axes and the Fourier transformation are prime examples of coordinate changes (Section 1.4), while the second-difference operator in particular and self-adjoint operators in general (Section 1.5) will be important in applications. We give, in Section 1.6, the elements of invariance group considerations for a finite N-point lattice. Finally, in Section 1.7 we examine the axes of a transformation and develop the properties of self-adjoint and unitary operators.

If the reader so wishes, he can proceed from Section 1.4 directly to Chapter 3 for applications in communication and the fast Fourier transform algorithm. The rest of the sections are needed, however, for the treatment of coupled systems in Chapter 2.

1.1. N-Dimensional Complex Vector Spaces

The elements of real vector analysis are surely familiar to the reader, so the material in this section will serve mainly to fix notation and to enlarge slightly the concepts of this analysis to the field $\mathscr{C}$ of complex numbers.

1.1.1. Axioms

Let $c_1, c_2, \ldots$ be complex numbers, elements of $\mathscr{C}$, and let $\mathbf{f}_1, \mathbf{f}_2, \ldots$ be the elements of a set $\mathscr{V}$ called *vectors* and denoted by boldface letters. We shall allow for two operations within $\mathscr{V}$:

(a) To every pair $\mathbf{f}_1$ and $\mathbf{f}_2$ in $\mathscr{V}$, there is an associated element $\mathbf{f}_3$ in $\mathscr{V}$, called the *sum* of the pair: $\mathbf{f}_3 = \mathbf{f}_1 + \mathbf{f}_2$.
(b) To every $\mathbf{f} \in \mathscr{V}$ ("$\mathbf{f}$ element of $\mathscr{V}$") and every $c \in \mathscr{C}$, there is an associated element $c\mathbf{f}$ in $\mathscr{V}$, referred to as the product of $\mathbf{f}$ by c.

With respect to the sum, $\mathscr{V}$ must satisfy the following:

(a1) *Commutativity:* $\mathbf{f}_1 + \mathbf{f}_2 = \mathbf{f}_2 + \mathbf{f}_1$,
(a2) *Associativity:* $(\mathbf{f}_1 + \mathbf{f}_2) + \mathbf{f}_3 = \mathbf{f}_1 + (\mathbf{f}_2 + \mathbf{f}_3)$,
(a3) $\mathscr{V}$ must contain a *zero* vector $\mathbf{0}$ such that $\mathbf{f} + \mathbf{0} = \mathbf{f}$ for all $\mathbf{f} \in \mathscr{V}$,
(a4) For every $\mathbf{f} \in \mathscr{V}$, there exists a $(-\mathbf{f}) \in \mathscr{V}$ such that $\mathbf{f} + (-\mathbf{f}) = \mathbf{0}$.

With respect to the product it is required that $\mathscr{V}$ satisfy

(b1) $1 \cdot \mathbf{f} = \mathbf{f}$,
(b2) $c_1(c_2\mathbf{f}) = (c_1c_2)\mathbf{f}$.

Finally, the two operations are to intertwine *distributively*, i.e.,

(c1) $c(\mathbf{f}_1 + \mathbf{f}_2) = c\mathbf{f}_1 + c\mathbf{f}_2$,
(c2) $(c_1 + c_2)\mathbf{f} = c_1\mathbf{f} + c_2\mathbf{f}$.

The last requirement relates the sum in $\mathscr{C}$ with the sum in $\mathscr{V}$. We use the same symbol "+" for both. Immediate consequences of these axioms are $0\mathbf{f} = \mathbf{0}$ and $(-1)\mathbf{f} = -\mathbf{f}$.

1.1.2. Linear Independence

Except for allowing the numbers $c_1, c_2, \ldots$ to be complex, the main concepts from ordinary vector analysis remain unchanged: A set of (nonzero) vectors $\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_N$ is said to be *linearly independent* when

$$\sum_{n=1}^{N} c_n\mathbf{f}_n = \mathbf{0} \Leftrightarrow c_n = 0, \qquad n = 1, 2, \ldots, N. \tag{1.1}$$

If the implication to the right does not hold, the set of vectors is said to be linearly *dependent*. A complex vector space $\mathscr{V}$ is said to be *N-dimensional* when it is possible to find at most N linearly independent vectors. We affix N to $\mathscr{V}$ as a superscript: $\mathscr{V}^N$. Let $\{\boldsymbol{\varepsilon}_n\}_{n=1}^N := \{\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2, \ldots, \boldsymbol{\varepsilon}_N\}$ be a maximal

set of linearly independent vectors, called a *basis* for $\mathscr{V}^N$. We can then express any $\mathbf{f} \in \mathscr{V}^N$ as a linear combination of the basis vectors as

$$\mathbf{f} = \sum_{n=1}^{N} f_n \boldsymbol{\varepsilon}_n, \tag{1.2}$$

where $f_n \in \mathscr{C}$ is the *nth coordinate* of $\mathbf{f}$ with respect to the basis $\{\boldsymbol{\varepsilon}_n\}_{n=1}^N$. If $\mathbf{f}$ has coordinates $\{f_n\}_{n=1}^N$ and $\mathbf{g}$ coordinates $\{g_n\}_{n=1}^N$, then the coordinates of a vector $\mathbf{h} = a\mathbf{f} + b\mathbf{g}$ will be $h_n = af_n + bg_n$ for $n = 1, 2, \ldots, N$, as implied by (1.1) and the linear independence of the basis vectors. The vector $\mathbf{0}$ has all its coordinates zero.

1.1.3. Canonical Representation

Any two N-dimensional vector spaces are isomorphic, as we need only establish a one-to-one correspondence between the basis vectors. A most convenient realization of $\{\boldsymbol{\varepsilon}_n\}_{n=1}^N$ is given through the *canonical* column-vector representation

$$\boldsymbol{\varepsilon}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\varepsilon}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \ldots, \boldsymbol{\varepsilon}_N = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad \text{i.e., } \mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{N-1} \\ f_N \end{pmatrix}. \tag{1.3}$$

Throughout Part I, we shall consider finite-dimensional complex vector spaces.

Exercise 1.1. Map the complex vector space $\mathscr{V}^N$ onto a $2N$-dimensional *real* vector space (i.e., only real numbers allowed). You can number the basis vectors in the latter as $\boldsymbol{\varepsilon}_n{}^R := \boldsymbol{\varepsilon}_n$ and $\boldsymbol{\varepsilon}_{N+n}^I := i\boldsymbol{\varepsilon}_n$, $n = 1, 2, \ldots, N$. (Any other choice?) How do the coordinates of a vector $\mathbf{f} \in \mathscr{V}^N$ relate to the coordinates of the corresponding vector in the real space?

For economy of notation we shall henceforth indicate summations as in (1.2) by $\sum_n$, the range of the index being implied by the context. Double sums will appear as $\sum_{n,m}$, etc. If any ambiguities should arise, we shall revert to the full summation symbol.

1.2. Inner Product and Norm in $\mathscr{V}^N$

In this section we shall generalize the inner (or "scalar") product and norm of ordinary vector analysis to corresponding concepts in complex vector spaces.

1.2.1. Inner Product

To every ordered pair of vectors $\mathbf{f}, \mathbf{g}$ in $\mathscr{V}^N$, we associate a complex number $(\mathbf{f}, \mathbf{g})$, their *inner product*. It has the properties of being *linear* in the second argument, i.e.,

$$(\mathbf{f}, c_1\mathbf{g}_1 + c_2\mathbf{g}_2) = c_1(\mathbf{f}, \mathbf{g}_1) + c_2(\mathbf{f}, \mathbf{g}_2), \tag{1.4}$$

and *antilinear* in the first,

$$(c_1\mathbf{f}_1 + c_2\mathbf{f}_2, \mathbf{g}) = c_1^*(\mathbf{f}_1, \mathbf{g}) + c_2^*(\mathbf{f}_2, \mathbf{g}), \tag{1.5}$$

where the asterisk denotes complex conjugation. Such an inner product is thus a *sesquilinear* ("1½ linear") operation: $\mathscr{V}^N \times \mathscr{V}^N \to \mathscr{C}$. We shall assume that the inner product is *positive*; that is, $(\mathbf{f}, \mathbf{f}) > 0$ for every $\mathbf{f} \neq \mathbf{0}$.

1.2.2. Orthonormal Bases

Two vectors whose inner product is zero are said to be *orthogonal*. A basis such that its vectors satisfy

$$(\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}_m) = \delta_{n,m} \coloneqq \begin{cases} 1 & \text{if } n = m, \\ 0 & \text{if } n \neq m \end{cases} \tag{1.6}$$

is said to be an *orthonormal basis*. It can easily be shown as in real vector analysis, by the Schmidt construction, that one can always find an orthonormal basis for $\mathscr{V}^N$. Conversely, we can define the inner product by demanding (1.6) for a given basis and then extend the definition through (1.4) and (1.5) to the whole space $\mathscr{V}^N$. For two arbitrary vectors $\mathbf{f}$ and $\mathbf{g}$ written in terms of the basis, we have

$$\begin{aligned} (\mathbf{f}, \mathbf{g}) &= \Big(\sum_n f_n\boldsymbol{\varepsilon}_n, \sum_m f_m\boldsymbol{\varepsilon}_m\Big) && \text{[from (1.2)]} \\ &= \sum_m g_m\Big(\sum_n f_n\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}_m\Big) && \text{[from (1.4)]} \\ &= \sum_{n,m} f_n^* g_m(\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}_m) && \text{[from (1.5)]} \\ &= \sum_n f_n^* g_n. && \text{[from (1.6)]} \end{aligned} \tag{1.7}$$

It is now easy to verify that

$$(\mathbf{f}, \mathbf{f}) \geqslant 0, \qquad (\mathbf{f}, \mathbf{f}) = 0 \Leftrightarrow \mathbf{f} = \mathbf{0}, \tag{1.8}$$

$$(\mathbf{f}, \mathbf{g}) = (\mathbf{g}, \mathbf{f})^*. \tag{1.9}$$

[In fact, Eqs. (1.4), (1.8), and (1.9) are sometimes used to *define* the inner product in a vector space: the two sets of axioms are equivalent whenever

an orthonormal basis exists. This is the case for finite N-dimensional spaces but not always when N is infinite. In the latter, the definition (1.4)–(1.8)–(1.9) is used.]

1.2.3. Coordinates

The nth coordinate of a vector $\mathbf{f}$ in the orthonormal basis $\{\boldsymbol{\varepsilon}_n\}_{n=1}^N$ is easily recovered from $\mathbf{f}$ itself through the inner product: Performing the inner product of a fixed $\boldsymbol{\varepsilon}_m$ with Eq. (1.2), we find

$$(\boldsymbol{\varepsilon}_m, \mathbf{f}) = \left(\boldsymbol{\varepsilon}_m, \sum_n f_n \boldsymbol{\varepsilon}_n\right) = \sum_n f_n(\boldsymbol{\varepsilon}_m, \boldsymbol{\varepsilon}_n) = f_m. \tag{1.10}$$

Hence, we can write

$$\mathbf{f} = \sum_n \boldsymbol{\varepsilon}_n(\boldsymbol{\varepsilon}_n, \mathbf{f}). \tag{1.11}$$

1.2.4. Schwartz Inequality

Two vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ were said to be orthogonal if $(\mathbf{f}_1, \mathbf{f}_2) = 0$. On the other hand, two vectors $\mathbf{g}_1$ and $\mathbf{g}_2$ are *parallel* if $\mathbf{g}_1 = c\mathbf{g}_2$, $c \in \mathscr{C}$, in which case

$$(\mathbf{g}_1, \mathbf{g}_2) = c^*(\mathbf{g}_2, \mathbf{g}_2) = c^{-1}(\mathbf{g}_1, \mathbf{g}_1) = [c^* c^{-1}(\mathbf{g}_1, \mathbf{g}_1)(\mathbf{g}_2, \mathbf{g}_2)]^{1/2}, \tag{1.12}$$

where, note, $|c^* c^{-1}| = 1$. For $|(\mathbf{f}, \mathbf{g})|$, zero is a lower bound, while, in the event $\mathbf{f}$ and $\mathbf{g}$ are parallel, $|(\mathbf{f}, \mathbf{g})| = [(\mathbf{f}, \mathbf{f})(\mathbf{g}, \mathbf{g})]^{1/2}$. These are the extreme values, as stated in the well-known *Schwartz inequality*:

$$|(\mathbf{f}, \mathbf{g})|^2 \leqslant (\mathbf{f}, \mathbf{f})(\mathbf{g}, \mathbf{g}). \tag{1.13}$$

We can prove (1.13) as follows. Consider the vector $\mathbf{f} - c\mathbf{g}$. Then, because of (1.8),

$$0 \leqslant (\mathbf{f} - c\mathbf{g}, \mathbf{f} - c\mathbf{g}) = (\mathbf{f}, \mathbf{f}) - c(\mathbf{f}, \mathbf{g}) - c^*(\mathbf{g}, \mathbf{f}) + |c|^2(\mathbf{g}, \mathbf{g}). \tag{1.14}$$

Now choose (for $\mathbf{g} \neq \mathbf{0}$)

$$c = (\mathbf{f}, \mathbf{g})^*/(\mathbf{g}, \mathbf{g}). \tag{1.15}$$

Replacement in (1.14) and a rearrangement of terms yield (1.13).

1.2.5. Norm

The *norm* (or *length*) of a vector $\mathbf{f} \in \mathscr{V}^N$ is defined as

$$\|\mathbf{f}\| := (\mathbf{f}, \mathbf{f})^{1/2}. \tag{1.16}$$

It is a mapping from $\mathscr{V}^N$ onto $\mathscr{R}^+$ (the nonnegative halfline), having the properties

$$\|\mathbf{f}\| \geqslant 0, \qquad \|\mathbf{f}\| = 0 \Leftrightarrow \mathbf{f} = \mathbf{0}, \tag{1.17}$$

$$\|c\mathbf{f}\| = |c|\,\|\mathbf{f}\|, \tag{1.18}$$

$$\|\mathbf{f} + \mathbf{g}\| \leqslant \|\mathbf{f}\| + \|\mathbf{g}\|. \tag{1.19}$$

Equations (1.17) and (1.18) are easily proven from (1.8) and (1.4)–(1.5), while Eq. (1.19) is the *triangle inequality*, which states, quite geometrically, that the length of the sum of two vectors cannot exceed the sum of the lengths of the vectors. It can be proven from (1.14), setting $c = -1$, that

$$\begin{aligned} 0 \leqslant \|\mathbf{f} + \mathbf{g}\|^2 &= \|\mathbf{f}\|^2 + 2\,\mathrm{Re}(\mathbf{f}, \mathbf{g}) + \|\mathbf{g}\|^2 \\ &\leqslant \|\mathbf{f}\|^2 + 2|(\mathbf{f}, \mathbf{g})| + \|\mathbf{g}\|^2 \qquad (\text{from } \mathrm{Re}\, z \leqslant |z|) \\ &\leqslant \|\mathbf{f}\|^2 + 2\|\mathbf{f}\| \cdot \|\mathbf{g}\| + \|\mathbf{g}\|^2 \qquad [\text{from (1.13)}]. \end{aligned} \tag{1.20}$$

The square root of the second and last terms yields Eq. (1.19).

Exercise 1.2. From (1.14) show that

$$\|\mathbf{f} - \mathbf{g}\| \geqslant |\,\|\mathbf{f}\| - \|\mathbf{g}\|\,|. \tag{1.21}$$

This is another form of the triangle inequality.

We have obtained the properties of the norm, Eqs. (1.17)–(1.19), as consequences of the definition and properties of the inner product. The abstract definition of a *norm*, however, is that of a mapping from $\mathscr{V}^N$ onto $\mathscr{R}^+$, with properties (1.17)–(1.19). It is a weaker requirement than that of an inner product and quite independent of it. The definition (1.16) only represents a particular kind of norm. Again, in infinite-dimensional spaces one may define a norm but have no inner product.

Exercise 1.3. Prove the *polarization* identity

$$(\mathbf{f}, \mathbf{g}) = \tfrac{1}{4}(\|\mathbf{f} + \mathbf{g}\|^2 - \|\mathbf{f} - \mathbf{g}\|^2) + i\tfrac{1}{4}(\|\mathbf{f} - i\mathbf{g}\|^2 - \|\mathbf{f} + i\mathbf{g}\|^2). \tag{1.22}$$

Note that this identity hinges on the validity of (1.16). It *cannot* be used to define an inner product from a norm.

Exercise 1.4. Define the complex angle between two vectors by

$$\cos\Theta := (\mathbf{f}, \mathbf{g})/\|\mathbf{f}\| \cdot \|\mathbf{g}\|, \qquad \Theta = \theta_R + i\theta_I. \tag{1.23}$$

Show that this restricts Θ to a region $|\sinh\theta_I| \leqslant |\sin\theta_R| \leqslant 1$.

1.3. Passive and Active Transformations

In this section we shall introduce two kinds of transformations on the coordinates of vectors in $\mathscr{V}^N$, those which arise from a change in the basis used for the description of the space, referred to as *passive* transformations, and *active* transformations produced by operators which bodily move the vectors in $\mathscr{V}^N$. Although the resulting expressions for the two kinds of transformations are quite similar, the difference in their interpretation is important.

1.3.1. Transformation of the Basis Vectors

Consider the complex vector space $\mathscr{V}^N$ and the orthonormal basis $\{\boldsymbol{\varepsilon}_n\}_{n=1}^N$ (henceforth called the $\boldsymbol{\varepsilon}$-basis, for short). Out of the $\boldsymbol{\varepsilon}$-basis we can construct the set of vectors

$$\bar{\boldsymbol{\varepsilon}}_m = \sum_n V_{nm}\boldsymbol{\varepsilon}_n, \qquad n = 1, 2, \ldots, N, \tag{1.24}$$

where $V_{nm} \in \mathscr{C}$. The question of the linear independence of the vector set (1.24) can be posed as follows. Let $\bar{c}_1, \bar{c}_2, \ldots, \bar{c}_N$ be a set of constants such that

$$\mathbf{0} = \sum_m \bar{c}_m\bar{\boldsymbol{\varepsilon}}_m = \sum_{m,n} \bar{c}_m V_{nm}\boldsymbol{\varepsilon}_n = \sum c_n\boldsymbol{\varepsilon}_n, \tag{1.25}$$

where $c_n = \sum_m \bar{c}_m V_{nm}$. Now, the vectors of the $\boldsymbol{\varepsilon}$-basis are linearly independent, so $c_n = 0$ for $n = 1, 2, \ldots, N$. For this to imply that all the $\bar{c}_m = 0$, $m = 1, 2, \ldots, N$, it is necessary that the matrix $\mathbf{V} = \|V_{nm}\|$ have a non-vanishing determinant. Thus, if $\det \mathbf{V} \neq 0$, the linear independence of the $\boldsymbol{\varepsilon}$-basis implies the linear independence of the N vectors in (1.24). The latter are then a basis as well. Henceforth it will be called the $\bar{\boldsymbol{\varepsilon}}$-basis. The $\bar{\boldsymbol{\varepsilon}}$-basis will not in general consist of mutually orthogonal vectors, but

$$\begin{aligned}(\bar{\boldsymbol{\varepsilon}}_n, \bar{\boldsymbol{\varepsilon}}_m) &= \sum_{j,k} (V_{jn}\boldsymbol{\varepsilon}_j, V_{km}\boldsymbol{\varepsilon}_k) \\ &= \sum_k V_{kn}^* V_{km} = (\mathbf{V}^\dagger\mathbf{V})_{nm},\end{aligned} \tag{1.26}$$

where $\mathbf{V}^\dagger = \mathbf{V}^{T*}$ is the transposed conjugate or *adjoint* of the matrix $\mathbf{V}$ and $(\mathbf{V}^\dagger)_{nm} = V_{mn}^*$.

1.3.2. Passive Transformations

We can regard the matrix $\mathbf{V} = \|V_{nm}\|$ as effecting a *change of basis* for $\mathscr{V}^N$: a *passive transformation* whereby the description of the vectors of $\mathscr{V}^N$ in terms of the $\boldsymbol{\varepsilon}$-basis is replaced by their description in terms of the $\bar{\boldsymbol{\varepsilon}}$-basis.

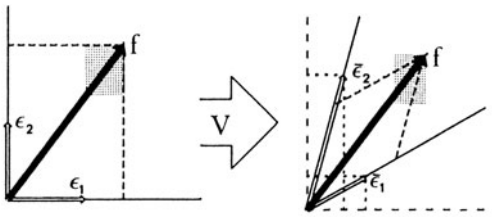


Fig. 1.1. Passive transformation V of a (two-dimensional) vector space. Its description in terms of a basis $\{\boldsymbol{\varepsilon}_i\}$ is replaced by its description in terms of a transformed basis $\{\bar{\boldsymbol{\varepsilon}}_i\}$. The vectors $\mathbf{f}$ in the space are unchanged.

Let $\mathbf{f} \in \mathscr{V}^N$ be a (fixed) vector with coordinates f_n, $n = 1, 2, \ldots, N$, relative to the $\boldsymbol{\varepsilon}$-basis and coordinates $\bar{f}_m$, $m = 1, 2, \ldots, N$, relative to the $\bar{\boldsymbol{\varepsilon}}$-basis. Then (see Fig. 1.1)

$$\sum_n f_n \boldsymbol{\varepsilon}_n = \mathbf{f} = \sum_m \bar{f}_m \bar{\boldsymbol{\varepsilon}}_m = \sum_{n,m} \bar{f}_m V_{nm} \boldsymbol{\varepsilon}_n \qquad \text{(passive)}. \tag{1.27}$$

The first and last members of this equation, due to the linear independence of the basis vectors, yield

$$f_n = \sum_m V_{nm} \bar{f}_m, \qquad \bar{f}_m = \sum_n (\mathbf{V}^{-1})_{mn} f_n. \tag{1.28}$$

The matrix $\mathbf{V}^{-1}$ exists as $\mathbf{V}$ is assumed to be nonsingular (det $\mathbf{V} \neq 0$).

Exercise 1.5. Let the coordinates of $\mathbf{f}$ relative to the $\bar{\boldsymbol{\varepsilon}}$-basis be $\bar{f}_m$ [i.e., second and third members of Eq. (1.27)]. Performing the inner product with $\bar{\boldsymbol{\varepsilon}}_n$ and using (1.26), find $\bar{f}_m$ in terms of $(\bar{\boldsymbol{\varepsilon}}_n, \mathbf{f})$.

Exercise 1.6. Using the result of Exercise 1.5, define the set of vectors $\bar{\boldsymbol{\varepsilon}}_n{}^D$ $(n = 1, 2, \ldots, N)$ so that $\bar{f}_n = (\bar{\boldsymbol{\varepsilon}}_n{}^D, \mathbf{f})$. Show that this defines a basis for $\mathscr{V}^N$. It is called the basis *dual* to the $\bar{\boldsymbol{\varepsilon}}$-basis, since (prove!) $(\bar{\varepsilon}_n, \bar{\varepsilon}_m{}^D) = \delta_{n,m}$. If the $\bar{\boldsymbol{\varepsilon}}$-basis is orthonormal, then $\bar{\boldsymbol{\varepsilon}}_n{}^D = \bar{\boldsymbol{\varepsilon}}_n$ $(n = 1, 2, \ldots, N)$.

Exercise 1.7. Express $(\mathbf{f}, \mathbf{g})$ in terms of the coordinates of $\mathbf{f}$ and $\mathbf{g}$ in the $\bar{\boldsymbol{\varepsilon}}$-basis.

1.3.3. Active Transformations

Active transformations are produced by operators $\mathbb{A}$ mapping $\mathscr{V}^N$ onto $\mathscr{V}^N$, which transform the vectors of the space as $\mathbf{f} \mapsto \mathbf{f}' = \mathbb{A}\mathbf{f}$. We shall assume these operators to be *linear*, i.e.,

$$\mathbb{A}(a\mathbf{f} + b\mathbf{g}) = a\mathbb{A}\mathbf{f} + b\mathbb{A}\mathbf{g}. \tag{1.29}$$

The linearity requirement allows us to find the transformation undergone by every vector in the space when we know the way the vectors in a given basis (say, the $\boldsymbol{\varepsilon}$-basis) are transformed. Let

$$\boldsymbol{\varepsilon}'_m = \mathbb{A}\boldsymbol{\varepsilon}_m, \qquad m = 1, 2, \ldots, N, \tag{1.30}$$

and define the N^2 constants

$$A_{nm} := (\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}'_m) = (\boldsymbol{\varepsilon}_n, \mathbb{A}\boldsymbol{\varepsilon}_m). \tag{1.31}$$

Using Eq. (1.11) with $\boldsymbol{\varepsilon}'_m$ in place of $\mathbf{f}$, we find

$$\boldsymbol{\varepsilon}'_m = \sum_n A_{nm}\boldsymbol{\varepsilon}_n, \tag{1.32}$$

which is formally identical to (1.24) with A_{nm} in place of V_{nm}. The interpretation of (1.32) as a linear active transformation, however, requires that the vectors $\mathbf{f} \in \mathscr{V}^N$ and the basis $\boldsymbol{\varepsilon}$ undergo the same transformation; that is, the coordinates of $\mathbf{f}'$ in the new basis $\boldsymbol{\varepsilon}'$ *continue to be* f_n, $n = 1, 2, \ldots, N$. Now, denoting by f'_n $(n = 1, 2, \ldots, N)$ the coordinates of $\mathbf{f}'$ with respect to the *original* $\boldsymbol{\varepsilon}$-basis, we have

$$\sum_n f'_n\boldsymbol{\varepsilon}_n = \mathbf{f}' = \sum_m f_m\boldsymbol{\varepsilon}'_m = \sum_{m,n} f_m A_{nm}\boldsymbol{\varepsilon}_n \qquad \text{(active)}, \tag{1.33}$$

and this implies

$$f'_n = \sum_m A_{nm}f_m, \tag{1.34}$$

so the coordinates of $\mathbf{f}$ transform as a column vector under the matrix $\mathbf{A} = \|A_{nm}\|$.

1.3.4. Operators and Their Matrix Representatives

As a consequence of the construction (1.31), we see that any linear *operator* $\mathbb{A}$ can be *represented* by a matrix $\mathbf{A}$, acting on the column-vector canonical realization (1.3). The matrix $\mathbf{A}$ was determined uniquely from the linear operator $\mathbb{A}$. Conversely, $\mathbb{A}$ is uniquely determined by $\mathbf{A}$ since the transformation of the basis vectors (1.32) specifies the transformation of any vector in the space. See Fig. 1.2.

We shall now see that this one-to-one correspondence between linear operators and $N \times N$ matrices holds under sum and product of the corresponding quantities. We define the linear combination of two operators

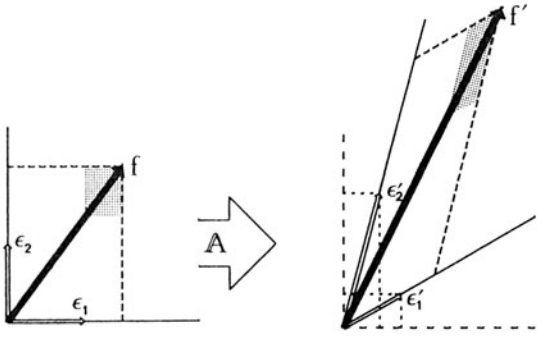


Fig. 1.2. Active transformation $\mathbb{A}$ of a (two-dimensional) vector space. All vectors—basis vectors included—are changed. As the transformation is linear, however, the coordinates of $\mathbf{f}' = \mathbb{A}\mathbf{f}$ in the transformed basis $\{\boldsymbol{\varepsilon}'_i\} = \{\mathbb{A}\boldsymbol{\varepsilon}_i\}$ are the same as those of $\mathbf{f}$ in the original basis.

$\mathbb{C} = a\mathbb{A} + b\mathbb{B}$, quite naturally, as

$$(a\mathbb{A} + b\mathbb{B})\mathbf{f} \coloneqq a\mathbb{A}\mathbf{f} + b\mathbb{B}\mathbf{f}. \tag{1.35}$$

Now let **A**, **B**, and **C** be the representing matrices. Then, using (1.31),

$$\begin{aligned} C_{nm} &= (\boldsymbol{\varepsilon}_n, (a\mathbb{A} + b\mathbb{B})\boldsymbol{\varepsilon}_m) = a(\boldsymbol{\varepsilon}_n, \mathbb{A}\boldsymbol{\varepsilon}_m) + b(\boldsymbol{\varepsilon}_n, \mathbb{B}\boldsymbol{\varepsilon}_m) \\ &= aA_{nm} + bB_{nm}, \end{aligned} \tag{1.36}$$

so that $\mathbf{C} = a\mathbf{A} + b\mathbf{B}$. Similarly, for the product $\mathbb{D} = \mathbb{A}\mathbb{B}$,

$$(\mathbb{A}\mathbb{B})\mathbf{f} \coloneqq \mathbb{A}(\mathbb{B}\mathbf{f}). \tag{1.37}$$

The correspondence with the representing matrices **D**, **A**, and **B** can be established using (1.31), (1.11) for $\mathbb{B}\boldsymbol{\varepsilon}_m$, and the linearity of the operators involved,

$$\begin{aligned} D_{nm} &= (\boldsymbol{\varepsilon}_n, \mathbb{A}\mathbb{B}\boldsymbol{\varepsilon}_m) = \Big(\boldsymbol{\varepsilon}_n, \mathbb{A}\sum_k \boldsymbol{\varepsilon}_k(\boldsymbol{\varepsilon}_k, \mathbb{B}\boldsymbol{\varepsilon}_m)\Big) \\ &= \sum_k (\boldsymbol{\varepsilon}_n, \mathbb{A}\boldsymbol{\varepsilon}_k)(\boldsymbol{\varepsilon}_k, \mathbb{B}\boldsymbol{\varepsilon}_m) = \sum_k A_{nk}B_{km}, \end{aligned} \tag{1.38}$$

so that $\mathbf{D} = \mathbf{AB}$.

1.3.5. Representations in Different Bases

We shall use passive transformations when a given system lends itself to a more convenient description in terms of a new set of coordinates. Active transformations, on the other hand, will describe, for instance, the time evolution of the *state vector* of a system. Note that active transformations of $\mathscr{V}^N$ should not depend on the basis used for the description of the space. Indeed, the representation of $\mathbb{A}$ by a matrix $\mathbf{A} = \|A_{nm}\|$ in (1.31) was made relative to the $\boldsymbol{\varepsilon}$-basis, but under any (passive) change of basis to, say, the $\bar{\boldsymbol{\varepsilon}}$-basis, the same operator $\mathbb{A}$ would be described by a different matrix $\bar{\mathbf{A}} = \|\bar{A}_{nm}\|$ whose elements are

$$\begin{aligned} \bar{A}_{nm} &= (\bar{\boldsymbol{\varepsilon}}_n, \mathbb{A}\bar{\boldsymbol{\varepsilon}}_m) = \sum_{j,k} (V_{jn}\boldsymbol{\varepsilon}_j, \mathbb{A}V_{km}\boldsymbol{\varepsilon}_k) \\ &= \sum_{j,k} V^*_{jn}A_{jk}V_{km} = (\mathbf{V}^\dagger\mathbf{A}\mathbf{V})_{nm}. \end{aligned} \tag{1.39}$$

Exercise 1.8. Show that

$$(\mathbb{A}\mathbf{f}, \mathbb{A}\mathbf{g}) = \sum_{m,n} f^*_m(\mathbf{A}^\dagger\mathbf{A})_{mn}g_n. \tag{1.40}$$

Do the same in terms of coordinates in a nonorthonormal basis.

Exercise 1.9. Define the operator $\mathbb{A}^\dagger$ as that having a matrix representation $\mathbf{A}^\dagger$ in some (orthonormal) basis. We call $\mathbb{A}^\dagger$ the adjoint of $\mathbb{A}$. Show that

$$(\mathbf{f}, \mathbb{A}^\dagger\mathbf{g}) = (\mathbb{A}\mathbf{f}, \mathbf{g}). \tag{1.41}$$

Show that this definition of $\mathbb{A}^\dagger$ does not depend on the matrix representation and that, for any other basis, $\overline{\mathbf{A}^\dagger} = (\bar{\mathbf{A}})^\dagger$.

Exercise 1.10. Let $\mathbb{A}$ and $\mathbb{B}$ be linear operators, $\mathbb{C} = a\mathbb{A} + b\mathbb{B}$ and $\mathbb{D} = \mathbb{A}\mathbb{B}$. Find the representing matrices $\overline{\mathbf{C}}$ and $\overline{\mathbf{D}}$ in the (in general nonorthogonal) $\bar{\boldsymbol{\varepsilon}}$-basis.

Exercise 1.10 should convince the reader that by far the simplest description of vector space operations is in terms of orthonormal bases. In fact, from now on we shall deal exclusively with these bases. This imposes severe restrictions on the allowed $\mathbf{V}$ in (1.24), which will be examined below. If the reader wants to deepen this necessarily brief account of vector spaces, inner products, and linear transformations, he may find useful the excellent text by Bowen and Wang (1976, Chapters 0–5).

1.4. Unitary Transformations: Permutations and the Fourier Transform

1.4.1. Definition of Unitarity

A transformation $\mathbf{V}$ which maps an orthonormal basis of the space $\mathscr{V}^N$, $\boldsymbol{\varepsilon}$, to another orthonormal basis $\bar{\boldsymbol{\varepsilon}}$ is called a *unitary* transformation. The necessary and sufficient condition for this to happen can be seen from (1.26) to be

$$\sum_k V_{kn}^* V_{km} = \delta_{n,m}, \quad \text{i.e.,} \quad \mathbf{V}^\dagger \mathbf{V} = \mathbf{1}, \tag{1.42}$$

where $\mathbf{1}$ is the $N \times N$ unit matrix. Such a matrix $\mathbf{V}$ is also called *unitary*, and clearly satisfies $\mathbf{V}^{-1} = \mathbf{V}^\dagger$: Its inverse equals its adjoint. As now both the $\boldsymbol{\varepsilon}$- and $\bar{\boldsymbol{\varepsilon}}$-bases are orthonormal, it follows that

$$(\mathbf{f}, \mathbf{g}) = \sum_n f_n^* g_n = \sum_n \bar{f}_n^* \bar{g}_n. \tag{1.43}$$

This is the *Parseval identity* between the coordinates of two vectors $\mathbf{f}$ and $\mathbf{g}$ in two bases related by a unitary transformation. (Compare with the result of Exercise 1.7.)

1.4.2. Groups of Unitary Matrices

Geometrically, a unitary transformation can be seen as a *rigid rotation* and/or *reflection* in a complex N-dimensional space: the angle Θ between any two vectors [Eq. (1.23)] is unchanged. Note that, as $\det \mathbf{V}^\dagger = (\det \mathbf{V})^*$, it follows from (1.42) that

$$|\det \mathbf{V}| = 1 \qquad (\mathbf{V} \text{ unitary}). \tag{1.44}$$

One general property of unitary transformations is that they constitute a

group. This will be defined now. Consider the set $\mathscr{U}$ of unitary matrices. Then, as will be verified below,

(a) $\mathbf{V}_1, \mathbf{V}_2 \in \mathscr{U} \Rightarrow \mathbf{V}_1 \cdot \mathbf{V}_2 \in \mathscr{U}$.
(b) $\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3 \in \mathscr{U} \Rightarrow (\mathbf{V}_1 \cdot \mathbf{V}_2) \cdot \mathbf{V}_3 = \mathbf{V}_1 \cdot (\mathbf{V}_2 \cdot \mathbf{V}_3)$.
(c) There exists a *unit* element $\mathbf{E} \in \mathscr{U}$ such that $\mathbf{E} \cdot \mathbf{V} = \mathbf{V}$ for all $\mathbf{V} \in \mathscr{U}$.
(d) For every $\mathbf{V} \in \mathscr{U}$, there exists a $\mathbf{V}^{-1} \in \mathscr{U}$ such that $\mathbf{V}\mathbf{V}^{-1} = \mathbf{E}$.

Abstractly, if the set $\mathscr{U}$ satisfies (a)–(d), it is said to constitute a *group* under the product operation "$\cdot$". In our case, "$\cdot$" is matrix multiplication, and we can verify (a): Let $\mathbf{V}_1^\dagger = \mathbf{V}_1^{-1}$ and $\mathbf{V}_2^\dagger = \mathbf{V}_2^{-1}$; then $(\mathbf{V}_1\mathbf{V}_2)^\dagger = \mathbf{V}_2^\dagger \mathbf{V}_1^\dagger = \mathbf{V}_2^{-1}\mathbf{V}_1^{-1} = (\mathbf{V}_1\mathbf{V}_2)^{-1}$. (b) Complex matrix multiplication is always associative. (c) The unit matrix $\mathbf{1}$ satisfies $\mathbf{1}^\dagger = \mathbf{1} = \mathbf{1}^{-1}$ and thus belongs to $\mathscr{U}$; it has the property $\mathbf{1} \cdot \mathbf{V} = \mathbf{V}$, so we identify $\mathbf{E} = \mathbf{1}$. (d) $(\mathbf{V}^{-1})^\dagger = \mathbf{V}^{\dagger\dagger} = \mathbf{V} = (\mathbf{V}^{-1})^{-1}$.

We conclude that *the set of unitary matrices constitutes a group under multiplication*. Although we shall use the notions of groups sparingly in this text, showing on occasion that sets of operations or objects have the group property under the appropriate product and drawing some immediate consequences, we should emphasize that group theory has been one of the fastest growing branches in applied mathematics. For the reader interested in further study on this field, we can suggest the books by Hamermesh (1962) and Miller (1972).

Exercise 1.11. Show that a vector space has the structure of a group under the "+" operation. The unit element is the zero vector.

We shall now examine two particularly important unitary transformations: permutations and the Fourier transformation.

1.4.3. Permutations

A *permutation* p of the basis vectors $\{\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2, \ldots, \boldsymbol{\varepsilon}_N\}$ (or of any set of numbered objects) is a transformation to a new basis $\{\bar{\boldsymbol{\varepsilon}}_1, \bar{\boldsymbol{\varepsilon}}_2, \ldots, \bar{\boldsymbol{\varepsilon}}_N\} = \{\boldsymbol{\varepsilon}_{p(1)}, \boldsymbol{\varepsilon}_{p(2)}, \ldots, \boldsymbol{\varepsilon}_{p(N)}\}$, where only the order of the elements in the set is changed. The string of numbers $p(1), p(2), \ldots, p(N)$ is a permutation p of $1, 2, \ldots, N$, and $p(m) = p(n) \Leftrightarrow m = n$.

1.4.4. Representing Permutations by Matrices

We can display p by the symbol

$$\begin{pmatrix} 1 & 2 & \cdots & N \\ p(1) & p(2) & \cdots & p(N) \end{pmatrix} =: \begin{pmatrix} m \\ p(m) \end{pmatrix},$$

which on any numbered set replaces the mth element by the $p(m)$th one. The order of the columns in this symbol is irrelevant. Such a permutation is achieved in (1.24) by a matrix $\mathbf{P} = \|P_{nm}\|$ whose mth column has a single nonzero element—of value 1—in the $p(m)$th row, i.e.,

$$\left[\mathbf{P}\begin{pmatrix} p \\ p(1) \end{pmatrix}\begin{pmatrix} 2 & \cdots & N \\ p(2) & \cdots & p(N) \end{pmatrix}\right]_{nm} = \delta_{n,p(m)}, \tag{1.45}$$

so that $\bar{\boldsymbol{\varepsilon}}_m = \boldsymbol{\varepsilon}_{p(m)}$. The inverse p^{-1} of the permutation p permutes the set $p(1), p(2), \ldots, p(N)$ back to $1, 2, \ldots, N$. This is achieved by

$$\left[\mathbf{P}\begin{pmatrix} 1 & 2 & \cdots & N \\ p(1) & p(2) & \cdots & p(N) \end{pmatrix}^{-1}\right]_{nm} = \left[\mathbf{P}\begin{pmatrix} p(1) & p(2) & \cdots & p(N) \\ 1 & 2 & \cdots & N \end{pmatrix}\right]_{nm}$$

$$= \delta_{m,p(n)} = \left[\mathbf{P}\begin{pmatrix} 1 & 2 & \cdots & N \\ p(1) & p(2) & \cdots & p(N) \end{pmatrix}^{\dagger}\right]_{nm}, \tag{1.46}$$

so that $\bar{\boldsymbol{\varepsilon}}_{p(m)} = \boldsymbol{\varepsilon}_m$. As the elements of $\mathbf{P}$ and $\mathbf{P}^{-1}$ are real, it was concluded in (1.46) that $\mathbf{P}^{-1} = \mathbf{P}^{\dagger}$. It follows that the permutation matrix (1.45) is unitary and that *the permutation of basis vectors is a unitary transformation in* $\mathscr{V}^N$.

The product of two permutations p_1, p_2 is a permutation p_3 since, applied to any numbered set on the right of the symbols,

$$\begin{pmatrix} m \\ p_2(m) \end{pmatrix}\begin{pmatrix} m \\ p_1(m) \end{pmatrix} = \begin{pmatrix} m \\ p_2(p_1(m)) \end{pmatrix} = \begin{pmatrix} m \\ p_3(m) \end{pmatrix}. \tag{1.47}$$

Note that the product of two permutations is not commutative in general. The identity permutation $e = \binom{m}{m}$ which leaves every element in a numbered set in its position is obviously a permutation represented in (1.45) by the unit matrix. Finally, as the inverse p^{-1} of a given permutation p is also a permutation represented in (1.46) by $\mathbf{P}^{-1} = \mathbf{P}^{\dagger}$, *the set of all permutations is a group*. We shall denote it by π_N. It has $N!$ elements. As permutations are a subset of the group of unitary transformations, they are said to be a *subgroup* of the latter.

Exercise 1.12. Note that, since the matrices involved are real, $\det \mathbf{P} = \pm 1$. Show that the matrices representing *transpositions* of two elements [i.e., $\left(\begin{smallmatrix} 1 & 2 & \cdots & k & \cdots & l & \cdots & N \\ 1 & 2 & \cdots & l & \cdots & k & \cdots & N \end{smallmatrix}\right)$, where only k and l are exchanged] have a determinant equal to -1.

Exercise 1.13. Show that the product of two transpositions which have one element in common has the form of a *three-cycle* [i.e., $\left(\begin{smallmatrix} 1 & 2 & \cdots & k & \cdots & l & \cdots & m & \cdots & N \\ 1 & 2 & \cdots & l & \cdots & m & \cdots & k & \cdots & N \end{smallmatrix}\right)$, where only k, l, and m are exchanged]. Show that the matrix representing a three-cycle has determinant $+1$.

Exercise 1.14. Consider the real space $\mathscr{V}^3$ for definiteness. Show that permutations with determinant $+1$ are rotations of the coordinate axes, while permutations with determinant -1 involve reflections across planes.

Exercise 1.15. For $N > 3$, one can produce four-cycles, etc. (up to N-cycles), from the product of a three-cycle, etc. [up to $(N-1)$-cycle], and a transposition with one element in common. Show that n-cycles are represented by matrices with determinant $(-1)^{n+1}$. When this is $+1$ they can be realized as rotations of the coordinate axes in N-space.

Exercise 1.16. Show that all permutations represented by matrices (1.45) with determinant $+1$ form a *subgroup* of the permutation group. Show that those with determinant -1 do not.

1.4.5. The Fourier Transformation

The unitary transformation which is the prime subject of this part is the *Fourier transformation*, defined in $\mathscr{V}^N$ by the matrix $\mathbf{F} = \|F_{mn}\|$ with elements

$$F_{mn} \coloneqq N^{-1/2} \exp(-2\pi imn/N) = F_{nm}. \tag{1.48}$$

We can verify directly that (1.48) is a unitary transformation, i.e.,

$$(\mathbf{F}^\dagger\mathbf{F})_{mn} = \sum_k F^*_{mk}F_{nk} = N^{-1} \sum_k \exp[-2\pi ik(n-m)/N] = \delta_{m,n}. \tag{1.49}$$

Using the geometric progression formula with $b+1$ terms

$$x^a + x^{a+1} + \cdots + x^{a+b} = \begin{cases} (1-x)^{-1}x^a(1-x^{b+1}), & x \neq 1, \\ b+1, & x = 1, \end{cases} \tag{1.50}$$

and letting $x = \exp[-2\pi i(n-m)/N]$, $a = 1$, and $b = N-1$, we see that for $m \neq n$, $x \neq 1$, and the sum in (1.49) adds to zero, while for $m = n$, $x = 1$, and it adds to N.

1.4.6. Coordinates in the ε- and φ-Bases

From the above it follows that the coordinates of a vector $\mathbf{f}$ in two bases related by the Fourier transformation are given by (1.28), with $\mathbf{F}^{-1} = \mathbf{F}^\dagger$ by

$$\tilde{f}_n = N^{-1/2} \sum_m f_m \exp(2\pi imn/N), \tag{1.51a}$$

$$f_n = N^{-1/2} \sum_m \tilde{f}_m \exp(-2\pi imn/N). \tag{1.51b}$$

The set $\{\tilde{f}_n\}_{n=1}^N$ is said to be the (finite) *Fourier transform* of the set $\{f_n\}_{n=1}^N$ and the latter, the *inverse* Fourier transform of the former. In our approach,

we want to emphasize, they are the coordinates of the same vector $\mathbf{f}$ in two bases.

The reasons for regarding the Fourier transformation as a particularly important unitary transformation should become clear in the applications of Chapters 2 and 3. Meanwhile, we reserve the tildes in Eqs. (1.51a) and (1.51b) for Fourier transforms, and we shall call the corresponding basis (called the $\bar{\boldsymbol{\varepsilon}}$-basis in Section 1.3) the $\boldsymbol{\varphi}$-basis. Explicitly,

$$\boldsymbol{\varphi}_n = N^{-1/2} \sum_m \boldsymbol{\varepsilon}_m \exp(-2\pi imn/N), \tag{1.52a}$$

$$\boldsymbol{\varepsilon}_n = N^{-1/2} \sum_m \boldsymbol{\varphi}_m \exp(2\pi imn/N), \tag{1.52b}$$

$$\sum_n f_n \boldsymbol{\varepsilon}_n = \mathbf{f} = \sum_n \tilde{f}_n \boldsymbol{\varphi}_n. \tag{1.52c}$$

Clearly, the mth coordinate of $\boldsymbol{\varphi}_n$ in the $\boldsymbol{\varepsilon}$-basis is F_{mn}. In Fig. 1.3 we show the real and imaginary parts of these coordinates for $N = 7$. We have let m take on continuous values and have drawn them as dotted lines in the figure.

1.4.7. Powers of the Fourier Transformation

One of the properties of the Fourier transformation matrix (1.48) is that it is *a fourth root of the unit matrix*. Indeed,

$$(\mathbf{F}^2)_{mn} = \sum_k F_{mk} F_{kn} = N^{-1} \sum_k \exp[-2\pi ik(m + n)/N]. \tag{1.53}$$

Using (1.50), we see that (1.53) equals 1 whenever $m + n = N$ or $2N$, as then all the N summands are N^{-1}. Hence, $\mathbf{F}^2$ is a matrix with 1's above the main antidiagonal and in the N–N position, with zeros elsewhere. In fact, it is a permutation

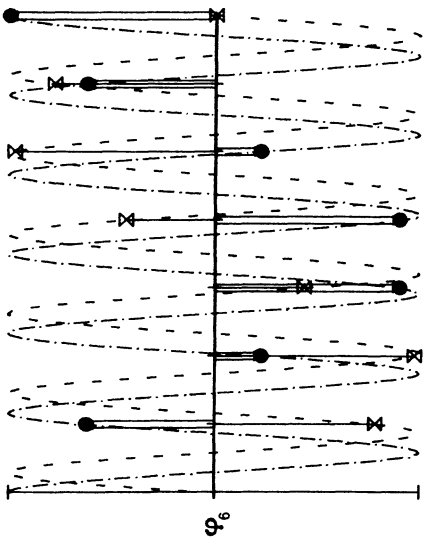
$$\mathbf{F}^2 = \mathbf{P}\begin{pmatrix} 1 & 2 & \cdots & N-2 & N-1 & N \\ N-1 & N-2 & \cdots & 2 & 1 & N \end{pmatrix} =: \mathbf{I}_0. \tag{1.54}$$

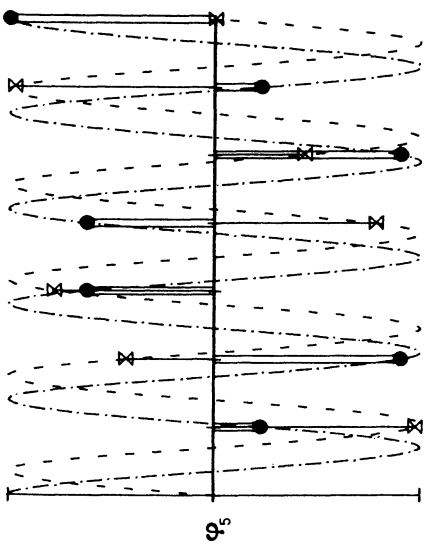
We shall call this the *inversion* matrix. Squaring (1.54), we find

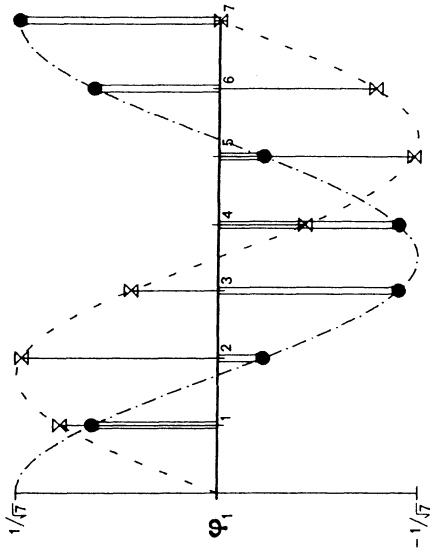
$$\mathbf{F}^4 = \mathbf{1}. \tag{1.55}$$

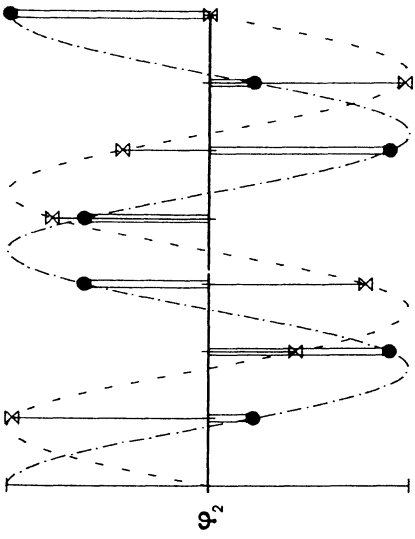
Exercise 1.17. Decompose the coordinates of a vector $\mathbf{f}$ in $\mathscr{V}^N$ into their real and imaginary parts as $f_n = f_n^R + if_n^I$ and $\tilde{f}_n = \tilde{f}_n^R + i\tilde{f}_n^I$. Relate these by (1.51a) and (1.51b).

Exercise 1.18. Associate to every vector $\mathbf{f}$ in $\mathscr{V}^N$ another vector $\mathbf{f}^*$ whose coordinates in the $\boldsymbol{\varepsilon}$-basis are $(\mathbf{f}^*)_n = (f_n)^*$, the complex conjugates of the original









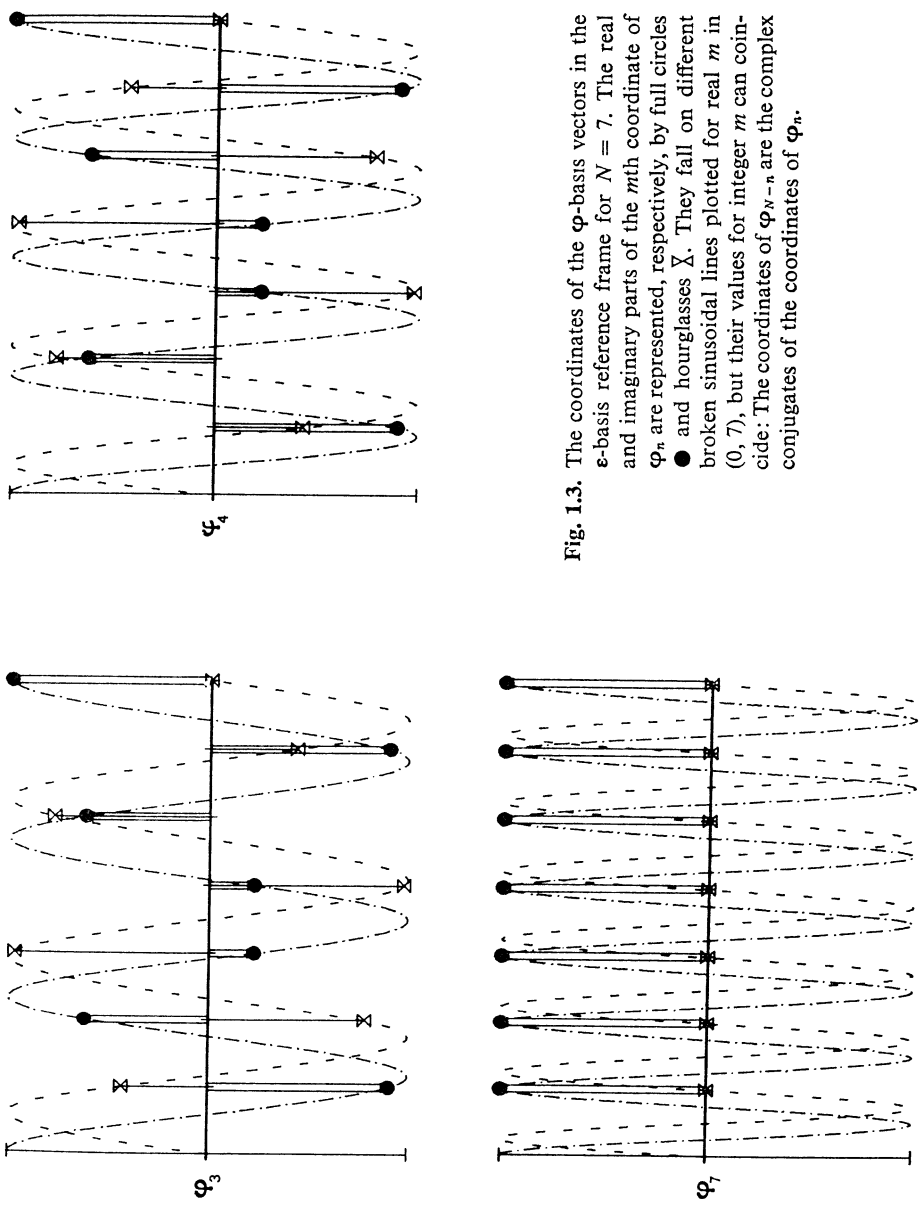


Fig. 1.3. The coordinates of the φ-basis vectors in the ε-basis reference frame for $N = 7$. The real and imaginary parts of the mth coordinate of φ_n are represented, respectively, by full circles ● and hourglasses ⧖. They fall on different broken sinusoidal lines plotted for real m in $(0, 7)$, but their values for integer m can coincide: The coordinates of φ_{N-n} are the complex conjugates of the coordinates of φ_n.

vector. Note that this *cannot* be produced by a linear operator. Show that, in the φ-basis, the coordinates of $\mathbf{f}^*$ are $\widetilde{(\mathbf{f}^*)}_n = (\tilde{f}_{N-n})^*$.

Exercise 1.19. Prove that the components of a vector $\mathbf{f}$ are *positive* if and only if their Fourier transforms are *positive definite*, i.e.,

$$f_n > 0 \Leftrightarrow \sum_{m,m'} \tilde{f}_{m-m'} \tilde{g}_m^* \tilde{g}_{m'} > 0 \tag{1.56}$$

for an arbitrary vector $\mathbf{g}$ with components $\tilde{g}_m$ in the φ-basis. This is easy when you show that the second expression in (1.56) is $N^{1/2} \sum_n f_n |g_n|^2$. The coordinates f_n are numbered modulo N ($n \equiv n \bmod N$).

1.5. Self-Adjoint Operators

1.5.1. Definition of Adjunction

We have seen that linear operators $\mathbb{A}$ producing active transformations in $\mathscr{V}^N$ could be represented by matrices $\mathbf{A}$. We define the *adjoint* of $\mathbb{A}$, $\mathbb{A}^\dagger$, as that operator fulfilling

$$(\mathbf{f}, \mathbb{A}^\dagger \mathbf{g}) = (\mathbb{A}\mathbf{f}, \mathbf{g}) \tag{1.57}$$

for every pair of $\mathbf{f}, \mathbf{g} \in \mathscr{V}^N$. Equation (1.57) defines $\mathbb{A}^\dagger$ uniquely if it defines its matrix representative in a unique way. That this is so can be seen letting $\mathbf{f}$ and $\mathbf{g}$ be $\boldsymbol{\varepsilon}_n$ and $\boldsymbol{\varepsilon}_m$ (for $n, m = 1, 2, \ldots, N$) and setting a matrix $\mathbf{A}^\dagger$ to represent $\mathbb{A}^\dagger$. Equation (1.57) then tells us that

$$(\mathbf{A}^\dagger)_{nm} = (\boldsymbol{\varepsilon}_n, \mathbb{A}^\dagger \boldsymbol{\varepsilon}_m) = (\mathbb{A}\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}_m) = (\boldsymbol{\varepsilon}_m, \mathbb{A}\boldsymbol{\varepsilon}_n)^* = A_{mn}^*, \tag{1.58}$$

so that $\mathbf{A}^\dagger$ is indeed, as the notation suggested, the adjoint (transposed conjugate) of the matrix $\mathbf{A}$. Now, Eq. (1.57) is independent of the basis used to describe the space, so this property is independent of the matrix realization of the operator (see Exercise 1.9).

1.5.2. Self-Adjointness and Hermiticity

One particularly important class of operators is comprised of those which are equal to their adjoints, i.e.,

$$\mathbb{H}^\dagger = \mathbb{H}. \tag{1.59}$$

Such operators are called *self-adjoint*. They are represented by *hermitian* matrices $\mathbf{H}^\dagger = \mathbf{H}$. (The distinction between hermiticity and self-adjointness may be a matter of semantics for finite-dimensional spaces $\mathscr{V}^N$; it becomes important, though, for infinite-dimensional ones.)

1.5.3. The Second-Difference Operator $\mathbb{\Delta}$

The operator which will occupy us through most of Chapter 2 is the *second-difference* operator $\mathbb{\Delta}$ whose representing matrix in the $\boldsymbol{\varepsilon}$-basis is

$$\boldsymbol{\Delta} := \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -2 & 1 & & & \\ 0 & 0 & 1 & -2 & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & & & \ddots & -2 & 1 \\ 1 & 0 & \cdots & & 0 & 1 & -2 \end{pmatrix}. \tag{1.60}$$

Again, as the notation suggests, $\mathbb{\Delta}$ is the finite-dimensional analogue of the Laplacian. As $\boldsymbol{\Delta}$ is manifestly hermitian (as well as real), $\mathbb{\Delta}$ is self-adjoint.

1.5.4. The $\mathbb{\Delta}$ Operator Represented in the $\boldsymbol{\varphi}$-Basis

The matrix $\tilde{\boldsymbol{\Delta}}$ representing $\mathbb{\Delta}$ in the $\boldsymbol{\varphi}$-basis can be found from (1.39), (1.48), and (1.60) as

$$\begin{aligned} \tilde{\Delta}_{mn} &= (\mathbf{F}^{\dagger}\boldsymbol{\Delta}\mathbf{F})_{mn} = N^{-1} \sum_{j,k} \Delta_{jk} \exp[2\pi i(kn - jm)/N] \\ &= N^{-1} \sum_{k} \big(-2 \exp[2\pi ik(n - m)/N] + \exp\{2\pi i[kn - (k + 1)m]/N\} \\ &\qquad + \exp\{2\pi i[kn - (k - 1)m]/N\}\big). \end{aligned} \tag{1.61a}$$

The last step uses (1.60) explicitly. From the second and third summands we can extract factors $\exp(\mp 2\pi im/N)$, respectively, so that

$$\begin{aligned} \tilde{\Delta}_{mn} &= N^{-1}[-2 + \exp(-2\pi im/N) + \exp(2\pi im/N)] \sum_{k} \exp[2\pi ik(n - m)/N] \\ &= [-2 + 2\cos(2\pi m/N)]\delta_{m,n} \end{aligned} \tag{1.61b}$$

[see Eq. (1.49)]; hence $\tilde{\boldsymbol{\Delta}}$ is seen to be a *diagonal matrix*:

$$\tilde{\Delta}_{mn} = \delta_{m,n}\lambda_m \tag{1.62a}$$

$$\lambda_m := -4 \sin^2(\pi m/N). \tag{1.62b}$$

In fact, the usefulness of the $\boldsymbol{\varphi}$-basis is the property that $\mathbb{\Delta}$ is represented in it by a diagonal matrix. This will be seen time and again in the following

sections. At the end of Section 1.7 we indicate how **F** is found by asking for the property (1.62a).

Exercise 1.20. If the linear operator $\mathbb{A}$ is represented in the $\boldsymbol{\varepsilon}$- and $\boldsymbol{\varphi}$-bases by matrices **A** and $\tilde{\mathbf{A}}$, and similarly for $\mathbb{B}$, show that

$$\tilde{\mathbf{A}} + \tilde{\mathbf{B}} = \widetilde{(\mathbf{A} + \mathbf{B})}, \tag{1.63a}$$

$$\tilde{\mathbf{A}}\tilde{\mathbf{B}} = \widetilde{\mathbf{AB}}. \tag{1.63b}$$

Exercise 1.21. Show that the product of two hermitian matrices is not necessarily hermitian. The set of these matrices therefore does *not* form a group.

Exercise 1.22. Show that the matrix $\boldsymbol{\Delta}$ in (1.60) has zero determinant and hence $\boldsymbol{\Delta}^{-1}$ does not exist (nor does $\mathbb{\Delta}^{-1}$). This can be done using the fact that, in (1.62b), $\lambda_N = 0$. Which subspace of $\mathscr{V}^N$ is mapped on **0**?

Exercise 1.23. Show that the matrix representing $\mathbb{\Delta}^2$ in the $\boldsymbol{\varepsilon}$-basis is

$$\boldsymbol{\Delta}^2 = \begin{pmatrix} 6 & -4 & 1 & 0 & \cdots & 0 & 1 & -4 \\ -4 & 6 & -4 & 1 & \cdots & 0 & 0 & 1 \\ 1 & -4 & 6 & -4 & \cdot & & & 0 \\ 0 & 1 & -4 & 6 & \cdot & \cdot & & \vdots \\ \vdots & \vdots & \cdot & \cdot & \cdot & \cdot & 1 & 0 \\ 0 & 0 & & \cdot & \cdot & 6 & -4 & 1 \\ 1 & 0 & & & 1 & -4 & 6 & -4 \\ -4 & 1 & 0 & \cdots & 0 & 1 & -4 & 6 \end{pmatrix}. \tag{1.64}$$

Which matrix represents $\mathbb{\Delta}^2$ in the $\boldsymbol{\varphi}$-basis?

Exercise 1.24. Show that, for $2p + 1 \leqslant N$, $\mathbb{\Delta}^p$ is represented in the $\boldsymbol{\varepsilon}$-basis by the matrix $\boldsymbol{\Delta}^p$ with elements

$$(\boldsymbol{\Delta}^p)_{mn} = (-1)^{m-n+p}\binom{2p}{p+m-n} = (\boldsymbol{\Delta}^p)_{m,N-n} = (\boldsymbol{\Delta}^p)_{N-m,n}, \tag{1.65}$$

where $\binom{r}{s}$ is the binomial coefficient. Verify the cases $p = 0$, $p = 1$ [Eq. (1.60)], and $p = 2$ [Eq. (1.64)]. Show that $\widetilde{\boldsymbol{\Delta}^p} = (\tilde{\boldsymbol{\Delta}})^n$ represents $\mathbb{\Delta}^p$ in the $\boldsymbol{\varphi}$-basis, and find its elements.

Exercise 1.25. Consider the *projection* operator $\mathbb{P}_k$ which maps every vector in $\mathscr{V}^N$ to its projection along $\boldsymbol{\varepsilon}_k$. Show that this is represented in the $\boldsymbol{\varepsilon}$- and $\boldsymbol{\varphi}$-bases by matrices with elements

$$(\mathbf{P}_k)_{mn} = \delta_{mn}\delta_{kn}, \tag{1.66a}$$

$$(\tilde{\mathbf{P}}_k)_{mn} = N^{-1}\exp[2\pi ik(m-n)/N]. \tag{1.66b}$$

These operators are self-adjoint.

Exercise 1.26. From the projection operators of Exercise 1.25, build (for N even) $\mathbb{E}_1 := \sum_{k=1}^{N/2} \mathbb{P}_{2k-1}$ and $\mathbb{E}_2 := \sum_{k=1}^{N/2} \mathbb{P}_{2k}$. Show that these are represented in the ε- and φ-bases by

$$\mathbf{E}_1 = \begin{pmatrix} 1 & & & & & & 0 \\ & 0 & & & & & \\ & & 1 & & & & \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & 1 & \\ 0 & & & & & & 0 \end{pmatrix}, \qquad \tilde{\mathbf{E}}_1 = \begin{pmatrix} \tfrac{1}{2}\mathbf{1} & -\tfrac{1}{2}\mathbf{1} \\ -\tfrac{1}{2}\mathbf{1} & \tfrac{1}{2}\mathbf{1} \end{pmatrix}, \tag{1.67a}$$

$$\mathbf{E}_2 = \begin{pmatrix} 0 & & & & & & 0 \\ & 1 & & & & & \\ & & 0 & & & & \\ & & & 1 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \\ 0 & & & & & & 1 \end{pmatrix}, \qquad \tilde{\mathbf{E}}_2 = \begin{pmatrix} \tfrac{1}{2}\mathbf{1} & \tfrac{1}{2}\mathbf{1} \\ \tfrac{1}{2}\mathbf{1} & \tfrac{1}{2}\mathbf{1} \end{pmatrix}. \tag{1.67b}$$

These operators will be used in Chapter 2.

1.5.5. Functions of Matrices and Operators

The results (1.35) to (1.38) linking linear combination and product of operators with the corresponding operations between the representing matrices show that if $P_n(x)$ is a polynomial of degree n in x, then the operator $\mathbb{B} = P_n(\mathbb{A})$ is well defined and represented by the matrices $\mathbf{B} = P_n(\mathbf{A})$ and $\tilde{\mathbf{B}} = P_n(\tilde{\mathbf{A}}) = P_n(\mathbf{A})$, which are also well defined. [The last equality is a direct consequence of (1.63).] Now, if we allow n to grow without bound into an *analytic function* $P(x)$ expressible as a Taylor series convergent in some region $|x| < \rho$, what happens with $P(\mathbf{A})$? If the result is a well-defined matrix, this will give us a working definition for the operator $P(\mathbb{A})$. The functions $P(x)$ we shall use later are of the type $\exp(ax)$, $\cosh bx$, $(\sinh x)/x$, while others such as $(1 - x)^{-1}$ are quite commonly used [see, for example, the book by Goertzel and Tralli (1960).] Thus assume that

$$P(x) = \sum_{n=0}^{\infty} p_n x^n \tag{1.68}$$

converges for $|x| < \rho$. Consider now the same series, replace x by the matrix $\mathbf{A}$, and let α be the maximum of the absolute values of its matrix elements: $|A_{nm}| \leqslant \alpha$. Then a bound for the matrix elements of $\mathbf{A}^2$ will be $N\alpha^2$ (the

equality will happen when a row of maximal elements α of $\mathbf{A}$ meets a column of similar elements). Inductively, we see that a bound for the elements of $\mathbf{A}^n$ is $N^{-1}(N\alpha)^n$, and hence *a bound for the elements of* $P(\mathbf{A})$ *is* $N^{-1}P(N\alpha)$ *so that for* $\alpha < \rho/N$, $P(\mathbf{A})$ *exists*. For the exponential and hyperbolic functions, ρ is infinite, so $P(\mathbf{A})$ exists for any $\mathbf{A}$. Correspondingly, the operator $P(\mathbb{A})$ is defined. Note that if the constants p_n in (1.68) are real, as $(\mathbb{A}^\dagger)^n = (\mathbb{A}^n)^\dagger$, it follows that $P(\mathbb{A}^\dagger) = P(\mathbb{A})^\dagger$. Hence, if $\mathbb{H}$ is self-adjoint, $P(\mathbb{H})$ will be also.

1.5.6. Multiplication and Commutation

Although we can comfortably work with functions of matrices and operators, we have to be careful about their *composition*, since the rules of ordinary algebra may not apply when several matrices or operators are involved. Consider the well-known relation $\exp(a + b) = \exp a \cdot \exp b$ for numbers a and b. The direct proof proceeds as follows:

$$\exp(a+b) = \sum_{n=0}^{\infty} \frac{1}{n!}(a+b)^n = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} \binom{n}{k} a^k b^{n-k}$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!} a^m \sum_{l=0}^{\infty} \frac{1}{l!} b^l = \exp a \cdot \exp b, \tag{1.69}$$

where in the third step we used a double-sum exchange relation. See Appendix C. The *second* step [expanding the binomial $(a + b)^n$] is only true, however, if a and b commute, i.e., $ab = ba$, so that all powers of a can be put to the left and those of b to the right. This is *not* true for matrices $\mathbf{A}$ and $\mathbf{B}$, which do not commute. [For a thorough treatment of such problems, called Baker–Campbell–Hausdorff relations, see the article by Mielnik and Plebañski (1970).] The most we can say here is that Eq. (1.69) is valid for matrices $\mathbf{A}$ and $\mathbf{B}$ when these commute, as is the case when they are *both diagonal matrices* or when $\mathbf{B}$ is a *multiple* of $\mathbf{A}$, i.e.,

$$\exp(a\mathbf{A}) \cdot \exp(b\mathbf{A}) = \exp[(a+b)\mathbf{A}]. \tag{1.70}$$

This relation will be used often.

1.5.7. Diagonalization and Exponentiation of Various Matrices

The problem of actually exponentiating or obtaining any function of a matrix $\mathbf{A}$ is another matter. If $\mathbf{A}$ represents an operator $\mathbb{A}$, it may be that in some basis $\mathbb{A}$ is represented by a diagonal matrix $\bar{\mathbf{A}}$. This is the case for $\mathbb{A}$, represented by $\boldsymbol{\Delta}$ in the $\boldsymbol{\varepsilon}$-basis [Eq. (1.60)] and by a diagonal matrix $\tilde{\boldsymbol{\Delta}}$ in the $\boldsymbol{\varphi}$-basis [Eq. (1.62)]. For self-adjoint and unitary operators this is developed in Section 1.7 in some detail. Since any sum or power of diagonal

matrices is a diagonal matrix, its elements are given by the sum or powers of the original diagonal elements. If $\mathbf{V}$ is a transformation relating the representing matrices $\mathbf{A}$ and the diagonal $\bar{\mathbf{A}}$ of $\mathbb{A}$ [see Eq. (1.37)], then $P(\mathbf{A})$ can be explicitly calculated by

$$P(\mathbf{A}) = \mathbf{V}\mathbf{V}^{-1}P(\mathbf{A})\mathbf{V}\mathbf{V}^{-1} = \mathbf{V}\left(\sum_{n=0}^{\infty} p_n \mathbf{V}^{-1}\mathbf{A}^n\mathbf{V}\right)\mathbf{V}^{-1}$$

$$= \mathbf{V}\left[\sum_{n=0}^{\infty} p_n(\mathbf{V}^{-1}\mathbf{A}\mathbf{V})^n\right]\mathbf{V}^{-1} = \mathbf{V}P(\bar{\mathbf{A}})\mathbf{V}^{-1}. \tag{1.71}$$

Exercise 1.27. Using Eq. (1.71) as well as (1.60) and (1.62), show that

$$\mathbb{G}^{1,0,1}(\tau) := \exp(\tau\mathbb{\Delta}) \tag{1.72a}$$

is represented in the φ- and ε-bases by

$$\tilde{G}^{1,0,1}_{m,n}(\tau) = [\exp(\tau\tilde{\mathbf{\Delta}})]_{mn} = \delta_{m,n}\exp(\tau\lambda_m), \tag{1.72b}$$

$$G^{1,0,1}_{m,n}(\tau) = [\exp(\tau\mathbf{\Delta})]_{mn} = N^{-1}\sum_k \exp(\tau\lambda_k)\exp[2\pi ik(n-m)/N], \tag{1.72c}$$

$$\lambda_m = -4\sin^2(\pi m/N). \tag{1.72d}$$

The operator $\mathbb{G}^{1,0,1}(\tau)$ will appear in Exercise 2.17 as the time-evolution operator for the finite-difference analogue of the heat equation.

Exercise 1.28. From (1.60) it is obvious that $\sum_n \Delta_{nm} = 0$ for $m = 1, 2, \ldots, N$. Prove that $\sum_n (\mathbf{\Delta}^p)_{nm} = 0$ and

$$\sum_n [\exp(\tau\mathbf{\Delta})]_{mn} = 1, \qquad m = 1, 2, \ldots, N. \tag{1.73}$$

Note that this property holds only for the ε-basis, where $\mathbb{\Delta}$ is represented by $\mathbf{\Delta}$. Innocuous as it seems, Eq. (1.73) will lead to the (discrete analogue of) total heat conservation (Exercise 2.18).

Exercise 1.29. Noting that $(\sinh x)/x$ contains only even powers of x in its Taylor expansion, define

$$\mathbb{G}^{0,1,1}(\tau) = \mathbb{\Delta}^{-1/2}\sinh\tau\mathbb{\Delta}^{1/2}. \tag{1.73a}$$

Show that this is represented in the φ- and ε-bases by

$$\tilde{G}^{0,1,1}_{m,n}(\tau) = \delta_{mn}\frac{1}{\omega_m}\sin\omega_m\tau \tag{1.73b}$$

$$G^{0,1,1}_{m,n}(\tau) = N^{-1}\sum_k \omega_k^{-1}\sin\omega_k\tau\exp[2\pi ik(n-m)/N] \tag{1.73c}$$

$$\omega_m = (-\lambda_m)^{1/2} = 2\sin(\pi m/N). \tag{1.73d}$$

This operator will appear in Section 2.2. It is the time-evolution operator for the finite difference analogue of the wave equation.

Exercise 1.30. Prove that if $\mathbf{H}$ is a hermitian matrix, it *generates* a set of unitary matrices

$$\mathbf{U}(\tau) = \exp(i\tau\mathbf{H}) \tag{1.74}$$

with τ real. Define thus *unitary operators*. They have the property

$$(\mathbb{U}\mathbf{f}, \mathbb{U}\mathbf{g}) = (\mathbf{f}, \mathbf{g}) \tag{1.75}$$

for all $\mathbf{f}, \mathbf{g} \in \mathscr{V}^N$.

Exercise 1.31. Let $\mathbf{A}(\tau)$ be a matrix whose elements are differentiable functions of τ. Define the derivative of $\mathbf{A}(\tau)$ with respect to τ as

$$\frac{d}{d\tau}\mathbf{A}(\tau) = \lim_{\varepsilon \to 0} \varepsilon^{-1}[\mathbf{A}(\tau + \varepsilon) - \mathbf{A}(\tau)] = \mathbf{A}'(\tau). \tag{1.76}$$

From this see that matrix differential calculus is similar to ordinary calculus. In particular, the Leibnitz rule

$$\frac{d}{d\tau}(\mathbf{AB}) = \mathbf{A}'\mathbf{B} + \mathbf{AB}', \qquad \mathbf{A} = \mathbf{A}(\tau), \qquad \mathbf{B} = \mathbf{B}(\tau) \tag{1.77}$$

holds. As commutativity does not hold, we must keep straight the order of the factors.

Exercise 1.32. Let $\mathbf{A}^{-1}(\tau)$ be the matrix inverse to $\mathbf{A}(\tau)$. Show that

$$\frac{d}{d\tau}\mathbf{A}^{-1} = -\mathbf{A}^{-1}\mathbf{A}'\mathbf{A}^{-1}. \tag{1.78}$$

Exercise 1.33. Regarding (1.74), show that

$$\mathbf{H} = -i\frac{d}{d\tau}\mathbf{U}(\tau)|_{\tau=0}. \tag{1.79}$$

If $\mathbf{U}(\tau)$ is a unitary matrix, show that $\mathbf{H}$ is hermitian. You will be using Eq. (1.78).

Exercise 1.34. Show that *every linear operator* $\mathbb{A}$ *can be written as*

$$\mathbb{A} = \mathbb{H}_1 + i\mathbb{H}_2, \tag{1.80}$$

where $\mathbb{H}_1$ *and* $\mathbb{H}_2$ *are self-adjoint.* Equation (1.80) recalls the decomposition of an arbitrary complex number into a real and an imaginary part.

1.6. The Dihedral Group

In Section 1.4 we introduced the permutation group π_N and saw some of its properties. Here we shall study a subset of π_N which constitutes a group by itself, called the dihedral group D_N, which will be seen to mesh in interesting ways with the Fourier transform and the $\mathbb{\Delta}$ operator, and will be used extensively later on.

1.6.1. Rotations and Inversions of a Finite, Closed Lattice

Consider the two permutations $\mathbb{R}$ and $\mathbb{I}_0$, represented by the matrices [Eq. (1.45)]

$$\mathbb{R}: \quad \mathbf{R} \coloneqq \mathbf{P}\begin{pmatrix} 1 & 2 & \cdots & N-1 & N \\ 2 & 3 & \cdots & N & 1 \end{pmatrix} = \begin{pmatrix} 0 & & & & 1 \\ 1 & 0 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ 0 & & & 1 & 0 \end{pmatrix}, \tag{1.81}$$

$$\mathbb{I}_0: \quad \mathbf{I}_0 \coloneqq \mathbf{P}\begin{pmatrix} 1 & 2 & \cdots & N-1 & N \\ N-1 & N-2 & \cdots & 1 & N \end{pmatrix} = \begin{pmatrix} 0 & & & 1 & 0 \\ & & \iddots & & \\ & \iddots & & & \\ 1 & & & & \\ 0 & & & & 1 \end{pmatrix}. \tag{1.82}$$

[Note that $\mathbf{I}_0$ has already appeared in (1.54).] The concepts we shall present here can be illustrated as applied to a finite lattice of N masses joined by pairs through springs, as shown in Fig. 1.4(a). Assume the lattice is vibrating. Although the precise description of the time development of the system will be undertaken in Chapter 2, this system will serve to apply the ideas involved.

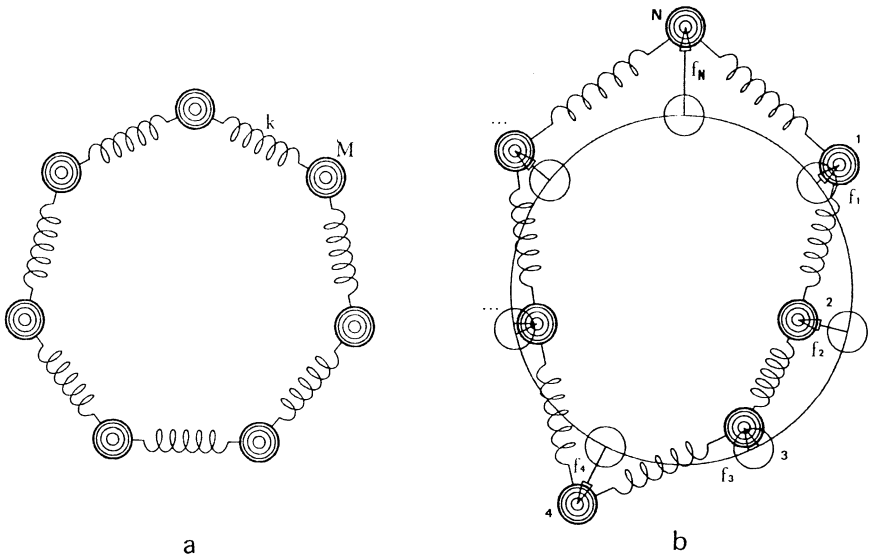


Fig. 1.4. (a) A linear, closed *lattice* constituted by masses M and springs k. (b) The same lattice undergoing vibrational motion. The time-dependent coordinates $f_n(t)$, $n = 1, 2, \ldots, N$, of the masses define the coordinates of the state vector $\mathbf{f}(t)$ of the system.

Let $f_n(t)$ be the elongation of the nth mass at time t, and construct the time-dependent N-dimensional vector $\mathbf{f}(t) = \sum_n f_n(t)\boldsymbol{\varepsilon}_n$, which will be referred to as the *state* vector describing the system. The components of the state vector $\mathbf{f}$ are shown as the arrows indicating the elongations of the vibrating lattice, for some fixed time t, in Fig. 1.4(b). We can express $\mathbf{f}(t)$ in a new basis $\{\bar{\boldsymbol{\varepsilon}}_n\}_{n=1}^N$ by the use of a (passive) transformation which for (1.81) is $\bar{\boldsymbol{\varepsilon}}_n = \boldsymbol{\varepsilon}_{n+1}$. Here and in what follows it will serve us to consider, as Fig. 1.4 suggests, that mass number $N + 1$ is the same as mass number 1, $N + 2$ the same as 2, etc., thus letting the component label n be numbered, as before, modulo N, so that the statement $\bar{\boldsymbol{\varepsilon}}_n = \boldsymbol{\varepsilon}_{n+1}$ implies, in particular, $\bar{\boldsymbol{\varepsilon}}_N = \boldsymbol{\varepsilon}_1$. In the $\bar{\boldsymbol{\varepsilon}}$-basis, $\mathbf{f}(t)$ has its coordinates given by $\bar{f}_n(t) = f_{n-1}(t)$, $n \equiv n \bmod N$. Insofar as Fig. 1.4 is concerned, the same shape $\mathbf{f}(t)$ of the lattice is described by a relabeling of the masses which shifts the old labels clockwise by one unit, while the elongations $\bar{f}_n(t)$ are correspondingly shifted counterclockwise by one unit.

1.6.2. Producing New Solutions from Old Ones

Now consider (1.81) and (1.82) as matrices representing in the $\boldsymbol{\varepsilon}$-basis *active* transformations in $\mathscr{V}^N$, $\mathbb{R}$, and $\mathbb{I}_0$. In this case, under (1.81), again $\boldsymbol{\varepsilon}'_n = \boldsymbol{\varepsilon}_{n+1}$, but the lattice is now bodily moved clockwise by one unit, and the new state vector $\mathbf{f}'(t) = \sum_n f_n(t)\boldsymbol{\varepsilon}'_n = \mathbb{R}\mathbf{f}(t)$ will describe its time evolution. It is quite obvious, however, that in applying $\mathbb{R}$ to the system in Fig. 1.4 we have preserved the neighbor relation between the masses and that the original and the rotated lattices are indistinguishable except for our labeling of the masses. The physical lattices are the same and thus should be described by the same equations of motion. What we have done then is *to produce out of the state vector* $\mathbf{f}(t)$ *a new state vector* $\mathbf{f}'(t) = \mathbb{R}\mathbf{f}(t)$ *which also describes a possible vibration state for Fig. 1.4*, which is the old solution rotated clockwise by one unit.

1.6.3. Invariance of the Equations of Motion

Any transformation which maps the undeformed lattice in Fig. 1.4(a) onto itself (*invariance* transformations of the figure) will correspondingly *produce a new solution vector* $\mathbf{f}'(t)$ *out of any given solution* $\mathbf{f}(t)$ *and should leave the equations of motion invariant*, changing only the initial conditions which determine their subsequent time development.

The *dihedral transformations are the largest set* D_N *of permutations leaving Fig. 1.4(a) invariant* as described and will *constitute a group* since, again quite clearly, the successive application of two invariance transformations is a transformation which also leaves the figure invariant, and the

identity transformation $E = P(\binom{n}{n})$ is an element in this set. These two observations state that the set of invariance transformations of a system satisfies the group axioms (a) and (c) (Section 1.4.2). Now axiom (b) (associativity) is satisfied since every element of D_N is within π_N, where this property holds. Last, since π_N has only a finite number of elements, for any $\mathbb{T} \in D_N$ we can construct the successive powers $\mathbb{T}, \mathbb{T}^2, \mathbb{T}^3, \ldots \in D_N$ and eventually reach $\mathbb{T}^p = \mathbb{1}$, the identity transformation, so $\mathbb{T}^{p-1} = \mathbb{T}^{-1} \in D_N$ and axiom (d) is also satisfied. Hence $D_N \subset \pi_N$ is a group by itself and a subgroup of π_N.

Exercise 1.35. Show that the successive powers $\mathbb{T}, \mathbb{T}^2, \mathbb{T}^3, \ldots$ cannot enter into a "loop" without involving the identity element.

1.6.4. Multiplying Rotations and Inversions for N Odd

Let N be an odd number and consider the two permutations $\mathbb{R}$ and $\mathbb{I}_0$ represented by (1.81) and (1.82). We saw that $\mathbb{R}$ effects a clockwise rotation by $2\pi/N$. See Fig. 1.5a. Similarly, $\mathbb{I}_0$ reflects the figure across a line which passes through the Nth mass and the midpoint of the spring joining the $[\frac{1}{2}(N-1)]$th and the $[\frac{1}{2}(N+1)]$th masses. They are invariance transformations of the figure. Applying $\mathbb{R}$ k times in succession, we see that $\mathbb{R}^k$ performs a rotation by $2\pi k/N$ and that $\mathbb{R}^N = \mathbb{1}$. Under $\mathbb{R}^k$, the mth mass is brought onto the $(m+k)$th mass. We can use the shorthand

$$\mathbb{R}^k[m] = [m + k]. \tag{1.83}$$

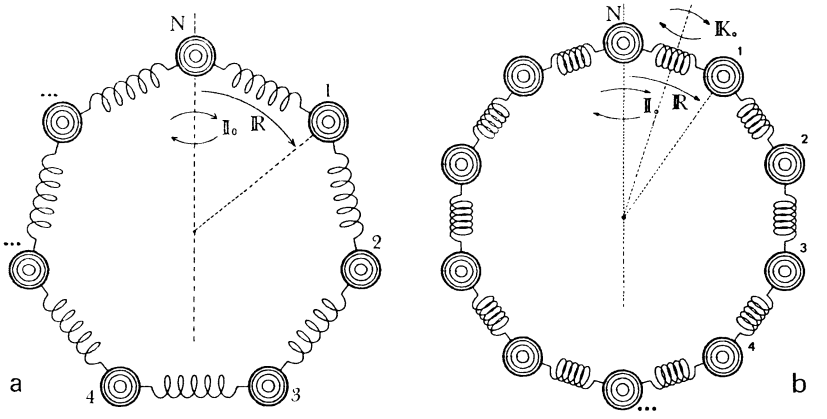


Fig. 1.5. (a) Dihedral group symmetries for an N-mass lattice when N is odd: rotations $\mathbb{R}$ and inversions $\mathbb{I}_0$ through a mass center. (b) Dihedral group symmetries for an N-mass lattice when N is even: In addition to rotations $\mathbb{R}$ and inversions $\mathbb{I}_0$ through a mass center, we have the possibility of inversions $\mathbb{K}_0$ through a spring midpoint.

Next consider $\mathbb{I}_0$, leaving mass N in its place; i.e.,

$$\mathbb{I}_0[m] = [N - m] \tag{1.84}$$

and $[N] \equiv [0] \bmod N$. It is not difficult to conclude that

$$\mathbb{I}_k \coloneqq \mathbb{R}^k \mathbb{I}_0 \mathbb{R}^{-k}, \tag{1.85}$$

where $\mathbb{R}^{-k} \coloneqq (\mathbb{R}^{-1})^k$ is a reflection of the figure which leaves mass k invariant, since $\mathbb{R}^{-k}$ maps mass k into the position N left invariant by $\mathbb{I}_0$ and $\mathbb{R}^k$ maps this back to its original place. This can be verified using the shorthand (1.83)–(1.84):

$$\begin{aligned} \mathbb{I}_k[m] &= \mathbb{R}^k \mathbb{I}_0 \mathbb{R}^{-k}[m] = \mathbb{R}^k \mathbb{I}_0[m - k] = \mathbb{R}^k[N - m + k] \\ &= [N + 2k - m]. \end{aligned} \tag{1.86}$$

The products of an $\mathbb{R}$ and an $\mathbb{I}$ or of two $\mathbb{I}$'s can be easily calculated in the same way.

Exercise 1.36. For N odd, prove that the $2N$ elements of D_N satisfy the "multiplication" table:

$$\mathbb{R}^k \mathbb{R}^l = \mathbb{R}^{k+l}, \tag{1.87a}$$

$$\mathbb{R}^k \mathbb{I}_l = \begin{cases} \mathbb{I}_{l+1/2(k)}, & k \text{ even}, \\ \mathbb{I}_{l+1/2(N+k)}, & k \text{ odd}, \end{cases} \tag{1.87b}$$

$$\mathbb{I}_l \mathbb{R}^k = \begin{cases} \mathbb{I}_{l-1/2(k)}, & k \text{ even}, \\ \mathbb{I}_{l-1/2(N+k)}, & k \text{ odd}, \end{cases} \tag{1.87c}$$

$$\mathbb{I}_k \mathbb{I}_l = \mathbb{R}^{2(k-l)}. \tag{1.87d}$$

Exercise 1.37. Show that the set $C_N \coloneqq \{\mathbb{1}, \mathbb{R}, \mathbb{R}^2, \ldots, \mathbb{R}^{N-1}\}$ is a subgroup of D_N. It is called the *cyclic* group of N elements.

Exercise 1.38. Show that the operators $\mathbb{R}^k$ and $\mathbb{I}_l$ are represented, in the $\boldsymbol{\varepsilon}$-basis, by the matrices

$$\mathbb{R}^k = \begin{pmatrix} \mathbf{0} & \mathbf{1}_k \\ \mathbf{1}_{N-k} & \mathbf{0} \end{pmatrix}, \tag{1.88a}$$

$$\mathbb{I}_l = \begin{pmatrix} \mathbf{1}^A_{N-l-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1}^A_{l+1} \end{pmatrix}, \tag{1.88b}$$

where $\mathbf{1}_p$ is the unit $p \times p$ matrix, $\mathbf{1}_q{}^A$ is the unit antidiagonal $q \times q$ matrix, and the $\mathbf{0}$'s are adequate rectangular null matrices. Compare with (1.81), its powers, and (1.82).

Exercise 1.39. Verify that the elements of (1.88) can be written as

$$(\mathbf{R}^k)_{mn} = \delta_{m,n+k}, \tag{1.89a}$$

$$(\mathbf{I}_l)_{mn} = \delta_{m,N+2l-n}, \tag{1.89b}$$

recalling that row (and column) labels are to be considered modulo N. In particular, matrices (1.88)–(1.89) acting on row vectors should transform the entries according to (1.83) and (1.86).

1.6.5. Representative Matrices in the Fourier Basis

Since the elements of D_N are now operators, we can ask for their representing matrices in the φ-basis. Indeed, using (1.39), the Fourier transform (1.48), and (1.89), we find

$$\begin{aligned}(\tilde{\mathbf{R}})_{mn} &= (\mathbf{F}^\dagger \mathbf{R} \mathbf{F})_{mn} \\ &= N^{-1} \sum_{j,l} \delta_{j,l+1} \exp[2\pi i(jm - ln)/N] \\ &= N^{-1} \exp(2\pi i m/N) \sum_{l} \exp[2\pi i l(m - n)/N]. \end{aligned} \tag{1.90}$$

Hence, $\widetilde{\mathbf{R}^k} = \tilde{\mathbf{R}}^k$ is a diagonal matrix,

$$(\tilde{\mathbf{R}}^k)_{mn} = \delta_{m,n} \exp(2\pi i k m/N). \tag{1.91}$$

Similarly, we can show that $\tilde{\mathbf{I}}_l$ is antidiagonal:

$$(\tilde{\mathbf{I}}_l)_{mn} = \delta_{m,N-n} \exp(4\pi i l m/N), \tag{1.92}$$

and in particular

$$\tilde{\mathbf{I}}_0 = \mathbf{I}_0, \tag{1.93}$$

which is obvious from (1.54). All the operators in D_N are unitary since the matrices of π_N-transformations are. In addition, all $\mathbb{I}_l$ are self-adjoint.

In performing the calculations leading to (1.91) and (1.92) we can see a real advantage in treating the row and column indices modulo N, since we can automatically keep track of $n \equiv n + mN \bmod N$ and $-n \equiv N - n \bmod N$. We are dealing with matrices $M_{mn} = f(m, n)$ which are periodic functions of m and n of period N in both variables. This property holds not only for the matrices representing operators in D_N but for the matrix $\mathbf{F}$ representing the Fourier transform (1.48) as well as $\boldsymbol{\Delta}$ and $\tilde{\boldsymbol{\Delta}}$ [Eqs. (1.60) and (1.62)] representing $\mathbb{\Delta}$. Since we are identifying the $(N + k)$th row with the kth one and similarly for columns, we are actually bending any such matrix into a torus. The linear combination and product of any two such matrices have the same property.

Exercise 1.40. Show that if $\mathbf{g} = \mathbb{R}^k \mathbf{f}$, then their coordinates relate as

$$g_n = f_{n-k}, \qquad \tilde{g}_n = \exp(2\pi i k n/N) \tilde{f}_n, \tag{1.94}$$

while if $\mathbf{h} = \mathbb{I}_0 \mathbf{f}$,

$$h_n = f_{N-n}, \qquad \tilde{h}_n = \tilde{f}_{N-n}. \tag{1.95}$$

Out of (1.94) and (1.95) you can find the coordinates of $\mathbb{I}_l \mathbf{f}$.

1.6.6. Invariance of $\mathbb{\Delta}$ under the Dihedral Group

One last property we want to point out for the operators in D_N is that they all commute with the operator $\mathbb{\Delta}$ introduced in Section 1.5.3, i.e.,

$$\mathbb{\Delta}\mathbb{R}^k = \mathbb{R}^k\mathbb{\Delta}, \tag{1.96a}$$

$$\mathbb{\Delta}\mathbb{I}_l = \mathbb{I}_l\mathbb{\Delta}. \tag{1.96b}$$

Equation (1.96a) can easily be proven using the representatives of $\mathbb{\Delta}$ and $\mathbb{R}^k$ in the φ-basis, which are diagonal matrices [Eqs. (1.62) and (1.91)], since all diagonal matrices commute among themselves. Equation (1.96b) can be proven for $l = 0$, noting that for any matrix $\mathbf{A}$, $(\mathbf{I}_0\mathbf{A}\mathbf{I}_0)_{mn} = A_{N-m,N-n}$. For arbitrary l, $\mathbf{I}_l$ can be written in terms of $\mathbf{R}^l$ and $\mathbf{I}_0$ by (1.85) and the equation can be proven thence.

Exercise 1.41. Show that any operator *function* of $\mathbb{\Delta}$ will also commute with operators in the dihedral group.

1.6.7. N Even

When the number N of masses in a lattice is even, then, in addition to the $\mathbb{I}_l$-transformations which leave masses l and $\frac{1}{2}N + l$ in their places, we can perform transformations which invert the lattice with respect to the centers of two opposite springs so that no mass is left in its place (see Fig. 1.5b). We thus define the operator $\mathbb{K}_0$ by its action on the lattice masses:

$$\mathbb{K}_0[m] = [N - m + 1]. \tag{1.97}$$

Note that $\mathbb{K}_0[1] = [N]$, $\mathbb{K}_0[\frac{1}{2}N] = [\frac{1}{2}N + 1]$, and $(\mathbb{K}_0)^2 = \mathbb{1}$. In analogy with (1.85) we can define $\mathbb{K}_l = \mathbb{R}^l\mathbb{K}_0\mathbb{R}^{-l}$, which reflects through the midpoints of the springs joining masses $[l]$ and $[l + 1]$ and masses $[\frac{1}{2}N + l]$ and $[\frac{1}{2}N + l + 1]$.

Exercise 1.42. Construct the multiplication table of $\mathbb{K}$'s, $\mathbb{R}$'s, and $\mathbb{I}$'s. Among others, show the relations

$$\mathbb{K}_k\mathbb{K}_l = \mathbb{R}^{2(k-l)}, \qquad \mathbb{K}_k\mathbb{I}_l = \mathbb{R}^{2(k-l)+1}, \qquad \mathbb{I}_l\mathbb{K}_k = \mathbb{R}^{2(l-k)-1}. \tag{1.98}$$

In particular, if N is a multiple of 2 but *not* a multiple of 4, note that $\mathbb{K}_0$ and $\mathbb{I}_{(N+2)/4}$ commute. Why?

Exercise 1.43. Show that the matrices representing $\mathbb{K}_0$ in the ε- and φ-bases are hermitian and unitary:

$$(\mathbf{K}_0)_{mn} = \delta_{m,N-n+1}, \qquad (\tilde{\mathbf{K}}_0)_{mn} = \delta_{m,N-n}\exp(2\pi im/N). \tag{1.99}$$

Show that for N even, $\mathbf{K}_0$ is an antidiagonal matrix all of whose diagonal elements are zero, while $\tilde{\mathbf{K}}_0$ has the same shape as $\tilde{\mathbf{I}}_0$ but different elements. Also show that, as in (1.96),

$$\mathbb{\Delta}\mathbb{K}_l = \mathbb{K}_l\mathbb{\Delta}. \tag{1.100}$$

Exercise 1.44. Show that D_N has $2N$ distinct elements: N rotations (including the identity element) and N inversions. Verify this for N odd as well as even.

1.6.8. Polar Decomposition of Operators

We make one last remark about the role of self-adjoint and unitary operators with respect to the set of all operators in $\mathscr{V}^N$: *every non-singular operator* $\mathbb{A}$ (i.e., such that $\det \mathbf{A} \neq 0$) *can be represented in the form*

$$\mathbb{A} = \mathbb{H}\mathbb{U}, \tag{1.101}$$

where $\mathbb{H}$ *is self-adjoint and* $\mathbb{U}$ *unitary.* For the proof we refer to Gel'fand (1961, Section II-15). Recalling Eq. (1.80), we are reminded by (1.101) of the decomposition of an arbitrary complex number into the product of its modulus (a positive real number) and its phase. The phase itself is the imaginary exponential of a real number. Here, see Eq. (1.74).

1.7. The Axes of a Transformation: Eigenvalues and Eigenvectors

When applying an operator $\mathbb{A}$ to the vectors of $\mathscr{V}^N$, a good insight into the nature of $\mathbb{A}$ is given by the directions in $\mathscr{V}^N$ left invariant by the operator. As we are particularly interested in self-adjoint and unitary operators, we shall develop here the results for these cases. In fact, the knowledge of these transformation axes (and the eigenvalues) specify the operator uniquely.

1.7.1. Invariant Directions

Assume a vector $\mathbf{x} \in \mathscr{V}^N$ is mapped by the action of $\mathbb{A}$ into a multiple of itself:

$$\mathbb{A}\mathbf{x} = \mu\mathbf{x}, \qquad \mu \in \mathscr{C}. \tag{1.102}$$

This only means that the *direction* defined by $\mathbf{x}$ is invariant under the action of $\mathbb{A}$. When an equation such as (1.102) holds, $\mathbf{x}$ is said to be an *eigenvector* of $\mathbb{A}$ with *eigenvalue* μ. This is the problem, for instance, of determining which directions in the $\mathscr{V}^2$-plane in Fig. 1.2 are left invariant by the action of the operator. In a basis where $\mathbb{A}$ is represented by a matrix $\mathbf{A}$, Eq. (1.102) can be written as

$$(\mathbf{A} - \mu\mathbf{1})\mathbf{x} = \mathbf{0}. \tag{1.103}$$

1.7.2. Characteristic Equation

If there exists a nonzero vector $\mathbf{x}$ satisfying (1.102), then (1.103), being a set of N homogeneous equations, requires

$$p_N(\mu) := \det(\mathbf{A} - \mu\mathbf{1}) = 0. \tag{1.104}$$

This is called the *characteristic equation* for $\mathbb{A}$, and $p_N(\mu)$ is its *characteristic polynomial.* As this is an Nth-degree polynomial in μ, we are assured by the fundamental theorem of algebra that there exist exactly N roots μ_i, $i = 1, 2, \ldots, N$, of p_N such that (1.104) holds. Of course some of these can be multiple roots of p_N, but not all of them can be zero, as $p_N(\mu) = \mu^N = 0$ would imply that $\mathbf{A} = \mathbf{0}$ and $\mathbb{A}$ would map all of $\mathscr{V}^N$ into $\mathbf{0}$. The set of eigenvalues is said to be the *spectrum* of the operator. This is a property of the operator, not of the particular matrix representation. This is true as long as the defining bases are all nondegenerate, for suppose we subject the basis in which $\mathbb{A}$ is represented by $\mathbf{A}$ to an invertible transformation $\mathbf{V}$ as given by (1.39). Then, from (1.103) it follows that

$$\mathbf{0} = \mathbf{V}^{-1}(\mathbf{A} - \mu_i\mathbf{1})\mathbf{x}_i = (\mathbf{V}^{-1}\mathbf{A}\mathbf{V} - \mu_i\mathbf{1})\mathbf{V}^{-1}\mathbf{x}_i = (\bar{\mathbf{A}} - \mu_i\mathbf{1})\mathbf{V}^{-1}\mathbf{x}_i = \mathbf{0}, \quad (1.105)$$

i.e., the vectors $\mathbf{V}^{-1}\mathbf{x}_i$ are eigenvectors of $\bar{\mathbf{A}}$ (representing $\mathbb{A}$ in the $\bar{\boldsymbol{\varepsilon}}$-basis) with the *same* eigenvalues μ_i.

1.7.3. Spectrum and Eigenbasis of a Self-adjoint Operator

We consider now the case when $\mathbb{A}$ is a self-adjoint operator $\mathbb{H}^\dagger = \mathbb{H}$. When this happens, we shall prove that (a) *the spectrum of* $\mathbb{H}$ *is real* and (b) *eigenvectors corresponding to different eigenvalues are orthogonal.* Indeed, consider eigenvectors $\mathbf{x}_1$ and $\mathbf{x}_2$ corresponding to eigenvalues μ_1 and μ_2, which are not necessarily distinct. Then, Eq. (1.102) for $\mathbf{x}_1$ in inner product with $\mathbf{x}_2$ yields

$$\mu_1(\mathbf{x}_2, \mathbf{x}_1) = (\mathbf{x}_2, \mathbb{H}\mathbf{x}_1) = (\mathbb{H}\mathbf{x}_2, \mathbf{x}_1) = \mu_2^*(\mathbf{x}_2, \mathbf{x}_1), \quad (1.106a)$$

i.e.,

$$(\mu_1 - \mu_2^*)(\mathbf{x}_2, \mathbf{x}_1) = 0. \quad (1.106b)$$

Equation (1.106b) for $\mathbf{x}_1 = \mathbf{x}_2$ implies that the eigenvalue μ_1 is real. This then holds for all eigenvalues. Next, if $\mathbf{x}_2 \neq \mathbf{x}_1$ and $\mu_2 \neq \mu_1$, Eq. (1.106b) tells us that $\mathbf{x}_2$ is orthogonal to $\mathbf{x}_1$.

1.7.4. Invariant Subspaces of Multiple Roots

Last, we shall now show that for self-adjoint operators (c) the *m-fold roots* μ_i *of the characteristic polynomial are associated with mutually orthogonal m-dimensional subspaces of* $\mathscr{V}^N$, *each invariant under* $\mathbb{H}$. When all roots are distinct ($m = 1$), we have shown above that $(\mathbf{x}_i, \mathbf{x}_j) = 0$ for $\mu_i \neq \mu_j$, $i, j = 1, 2, \ldots, N$, and the set of eigenvectors of $\mathbb{A}$ is a basis for $\mathscr{V}^N$. When multiplicity occurs in some of the roots μ_i, we can proceed as follows: Consider a first eigenvalue $\mu_1 \neq 0$, a corresponding eigenvector $\mathbf{x}_1$, and the $(N - 1)$-dimensional subspace $\mathscr{V}_{\perp 1}^{N-1}$ orthogonal to $\mathbf{x}_1$. Then, as $\mathbb{H}$ leaves

the direction of $\mathbf{x}_1$ invariant, it will also transform $\mathscr{V}_{\perp 1}^{N-1}$ only onto itself: let $\mathbf{y} \in \mathscr{V}_{\perp 1}^{N-1}$ so $(\mathbf{y}, \mathbf{x}_1) = 0$; then, since $\mathbb{H}$ is self-adjoint,

$$0 = \mu_1(\mathbf{y}, \mathbf{x}_1) = (\mathbf{y}, \mathbb{H}\mathbf{x}_1) = (\mathbb{H}\mathbf{y}, \mathbf{x}_1), \tag{1.107a}$$

so that $\mathbb{H}\mathbf{y}$ is still orthogonal to $\mathbf{x}_1$ and thus in $\mathscr{V}_{\perp 1}^{N-1}$. Now, choosing an orthonormal basis in $\mathscr{V}_{\perp 1}^{N-1}$, $\{\boldsymbol{\varepsilon}_1^{(N-1)}, \boldsymbol{\varepsilon}_2^{(N-1)}, \ldots, \boldsymbol{\varepsilon}_{N-1}^{(N-1)}\}$, and scaling $\mathbf{x}_1$ if necessary so that $\|\mathbf{x}_1\| = 1$, we can build a matrix $\mathbf{X}_1$ with columns given by the vectors

$$\mathbf{X}_1 := \|\mathbf{x}_1, \boldsymbol{\varepsilon}_1^{(N-1)}, \boldsymbol{\varepsilon}_2^{(N-1)}, \ldots, \boldsymbol{\varepsilon}_{N-1}^{(N-1)}\|. \tag{1.107b}$$

Now, since any two columns n, m of $\mathbf{X}_1$ are orthogonal,

$$\sum_k (\mathbf{X}_1)_{kn}^* (\mathbf{X}_1)_{km} = \delta_{n,m}, \qquad \mathbf{X}_1^\dagger \mathbf{X}_1 = \mathbf{1}, \tag{1.107c}$$

so that $\mathbf{X}_1$ is a *unitary* matrix. If we multiply the hermitian matrix $\mathbf{H}$ by $\mathbf{X}_1$, the first column of $\mathbf{H}\mathbf{X}_1$ will be $\mu_1 \mathbf{x}_1$, while the other columns will be

$$\mathbf{H}\boldsymbol{\varepsilon}_k^{(N-1)} = \sum_{l=1}^{N-1} H_{lk}^1 \boldsymbol{\varepsilon}_l^{(N-1)} \in \mathscr{V}_{\perp 1}^{N-1}. \tag{1.107d}$$

Hence

$$\mathbf{H}\mathbf{X}_1 = \mathbf{X}_1 \begin{pmatrix} \mu_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}^1 \end{pmatrix}, \tag{1.108a}$$

or

$$\mathbf{X}_1^\dagger \mathbf{H} \mathbf{X}_1 = \begin{pmatrix} \mu_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}^1 \end{pmatrix}, \tag{1.108b}$$

and adjoining (1.108b), we can see that $\mathbf{H}^1$ is an $(N-1) \times (N-1)$ hermitian matrix. Thus far we have used one eigenvector corresponding to a nonzero eigenvalue to perform a *unitary* transformation on $\mathbf{H}$ and reduce it to a block-diagonal form. Moreover, the characteristic polynomial (1.104) can be written as

$$\begin{aligned} p_N(\mu) &= \det(\mathbf{H} - \mu\mathbf{1}) = \det(\mathbf{X}_1^\dagger(\mathbf{H} - \mu\mathbf{1})\mathbf{X}_1) = \det(\mathbf{X}_1^\dagger \mathbf{H}\mathbf{X}_1 - \mu\mathbf{1}) \\ &= (\mu_1 - \mu)\det(\mathbf{H}^1 - \mu\mathbf{1}) = (\mu_1 - \mu)p_{N-1}(\mu), \end{aligned} \tag{1.109}$$

where in the term before last $\mathbf{1}$ is the $(N-1) \times (N-1)$ unit matrix. In this way we see that the characteristic polynomial $p_{N-1}(\mu)$ of $\mathbf{H}^1$ has all the roots of $p_N(\mu)$ but μ_1.

The process for $\mathbf{H}$ can now be repeated for $\mathbf{H}^1$ using some other nonzero root μ_2 (which may be equal to μ_1 if this root turns out to be multiple) to successively "extract" root by root. If eigenvectors $\mathbf{x}_j^{(1)} \cdots \mathbf{x}_j^{(m)}$ belong to the

same m-fold root μ_j, then any linear combination will also belong to the same eigenvalue, as

$$\mathbf{H}\sum_{r=1}^{m} c_r \mathbf{x}_j^{(r)} = \sum_{r=1}^{m} c_r \mathbf{H}\mathbf{x}_j^{(r)} = \mu_j \sum_{r=1}^{m} c_r \mathbf{x}_j^{(r)}, \tag{1.110}$$

and thus the set $\{\mathbf{x}_j^{(r)}\}_{r=1}^{m}$ spans an m-dimensional space $\mathscr{V}_j^m$, invariant under $\mathbb{H}$ and orthogonal to all other invariant subspaces or axes. If at the end of the recursive process we find m_0 zero roots, these will correspond to the m_0-dimensional subspace $\mathscr{V}_0^{m_0}$ of $\mathscr{V}^N$ orthogonal to all other extracted eigenvectors, and (1.110) holds for $\mathscr{V}_0^{m_0}$ as well. By the Schmidt procedure we can build an orthonormal basis for this subspace.

1.7.5. Diagonalization by Unitary Transformations

In conclusion, we have proven that *if* $\mathbf{H}$ *is a hermitian matrix we can build a unitary matrix* $\mathbf{X} = \mathbf{X}_1\mathbf{X}_2\cdots\mathbf{X}_k$ (the factor $\mathbf{X}_j$ extracting the jth eigenvector and containing $j-1$ ones along the diagonal) *such that*

$$\mathbf{X}^\dagger\mathbf{H}\mathbf{X} = \mathbf{H}^D, \tag{1.111}$$

where $\mathbf{H}^D$ *is a diagonal matrix containing along the diagonal the eigenvalues of* $\mathbf{H}$ *and* $\mathbf{X}$ *containing the eigenvectors of* $\mathbf{H}$ *as columns.*

1.7.6. The Second-Difference Operator and Fourier Transformation

As a concrete example, the operator $\mathbb{\Delta}$ of Section 1.5 was shown to be diagonalized by the Fourier transform, i.e., $\mathbf{F}^\dagger\mathbf{\Delta}\mathbf{F} = \tilde{\mathbf{\Delta}}$ in Eq. (1.61). The eigenvalues of $\mathbb{\Delta}$ are thus the λ_m of Eq. (1.62). Note that $\lambda_m = \lambda_{N-m}$ and $\lambda_N = 0$, so that for odd N, all roots of the characteristic polynomial but one are double, while for even N, $\lambda_{N/2}$ is also simple. Since the eigenvectors of a self-adjoint operator can be made into an orthonormal basis, the matrix representing the operator will be diagonal in that basis. For the $\mathbb{\Delta}$ operator this is precisely the $\boldsymbol{\varphi}$-basis.

1.7.7. Eigenvalues of Functions of Operators

The eigenvalues and eigenvectors of a hermitian operator $\mathbb{H}$ can be used to find those of any function $P(\mathbb{H})$. Indeed, let $\mathbb{H}\mathbf{x} = \mu\mathbf{x}$; then

$$P(\mathbb{H})\mathbf{x} = \sum_{n=0}^{\infty} p_n \mathbb{H}^n\mathbf{x} = \sum_{n=0}^{\infty} p_n \mu^n\mathbf{x} = P(\mu)\mathbf{x}. \tag{1.112}$$

It follows that *if* $\mathbf{x}$ *is an eigenvector of* $\mathbb{H}$ *with eigenvalue* μ *then it will also be an eigenvector of* $P(\mathbb{H})$ *with eigenvalue* $P(\mu)$.

Exercise 1.45. Consider the operators $\mathbb{I}_k$ of the dihedral group represented by the hermitian matrices $\mathbf{I}_k$ in (1.88b). As $\mathbb{I}_k^2 = \mathbb{1}$ and $\mathbb{1}$ has 1 for its sole eigenvalue, show that $\mathbb{I}_k$ can only have eigenvalues ± 1. Find a set of eigenvectors for $\mathbb{I}_k$. For this note that $\mathbb{I}_0 \boldsymbol{\varepsilon}_n = \boldsymbol{\varepsilon}_{N-n}$ and $\mathbb{I}_0 \boldsymbol{\varphi}_m = \boldsymbol{\varphi}_{N-m}$.

1.7.8. Unitary Operators and Their Spectra

The case when $\mathbb{A}$ is a unitary operator $\mathbb{U}$, $\mathbb{U}\mathbb{U}^\dagger = \mathbb{1}$, will now be examined. Of the three main results we proved for self-adjoint operators (on the spectrum, orthogonality, and completeness of eigenvectors) only the first differs for unitary operators. The other two hold *verbatim*. First, note that if $\mathbb{U}\mathbf{x} = \mu\mathbf{x}$ holds, then, multiplying by $\mu^{-1}\mathbb{U}^\dagger$, we find $\mathbb{U}^\dagger\mathbf{x} = \mu^{-1}\mathbf{x}$, so that if $\mathbf{x}$ is an eigenvector of $\mathbb{U}$ with eigenvalue μ, it will also be an eigenvector of $\mathbb{U}^\dagger$ with eigenvalue μ^{-1}. Now consider the analogue of Eq. (1.106) for unitary operators for any two eigenvectors of $\mathbb{U}$ and $\mathbb{U}^\dagger$:

$$\mu_1(\mathbf{x}_2, \mathbf{x}_1) = (\mathbf{x}_2, \mathbb{U}\mathbf{x}_1) = (\mathbb{U}^\dagger\mathbf{x}_2, \mathbf{x}_1) = \mu_2^{-1*}(\mathbf{x}_2, \mathbf{x}_1), \tag{1.112a}$$

i.e.,

$$(\mu_1 - \mu_2^{-1*})(\mathbf{x}_2, \mathbf{x}_1) = 0. \tag{1.112b}$$

For $\mathbf{x}_2 = \mathbf{x}_1$ we thus conclude that the allowed eigenvalues μ must satisfy $\mu^* = \mu^{-1}$, i.e., they can only be complex numbers of unit modulus. Thus *the spectrum of a unitary operator is restricted to lie on the unit circle.* Next, as was the case for hermitian operators from (1.112b), *if* $\mu_1 \neq \mu_2 = \mu_2^{-1*}$, *then the corresponding eigenvectors are orthogonal.* Last, the constructive proof of the statement of Section 1.7.5 can be followed as before with some minor changes. Since $(\mathbb{U}\mathbf{y}, \mathbb{U}\mathbf{x}) = (\mathbf{y}, \mathbf{x}) = (\mathbb{U}^\dagger\mathbf{y}, \mathbb{U}^\dagger\mathbf{x})$, it follows that if $\mathbb{U}$ leaves a subspace of $\mathscr{V}^N$ invariant, so does $\mathbb{U}^\dagger$. The statement stemming from (1.107a) thus also applies for unitary operators. The construction (1.107)–(1.108) can now be followed, replacing hermitian by unitary matrices, and the proof is complete. We do not have to worry about null eigenvalues here.

Exercise 1.46. Consider in $\mathscr{V}^3$ the unitary rotation around the z-axis given by the matrix

$$\mathbf{R}_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.113a}$$

Verify that its normalized eigenvectors are

$$\mathbf{x}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \mathbf{x}_2 = \begin{pmatrix} 1/(2)^{1/2} \\ -i/(2)^{1/2} \\ 0 \end{pmatrix}, \qquad \mathbf{x}_3 = \begin{pmatrix} 1/(2)^{1/2} \\ i/(2)^{1/2} \\ 0 \end{pmatrix} \tag{1.113b}$$

and that they constitute a unitary matrix $\mathbf{X} = \|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\|$. The first of the eigenvectors is the ordinary axis; the second two are *polarization vectors.* Find the

corresponding eigenvalues from (1.113a) by the characteristic equation and check the assignments. Notice that the eigenvalue problem has no complete solution in a purely real space.

Exercise 1.47. The rotation matrices (1.113a) are unitary. Find the hermitian operator which generates the set as (1.74). You can use Eq. (1.79). Verify that the eigenvectors (1.113b) are also eigenvectors of the generating operators. Find the corresponding eigenvalues.

Exercise 1.48. The rotations of the dihedral group D_N in $\mathscr{V}^N$ are unitary. They are represented in the $\boldsymbol{\varepsilon}$-basis by (1.88a), while in the $\boldsymbol{\varphi}$-basis they are represented by (1.91). What are the eigenvalues and eigenvectors?

Exercise 1.49. Consider the *Fourier* transform matrix. Show that its eigenvalues are among the set $\{\pm 1, \pm i\}$. Find eigenvectors for $\mathbf{F}$, noting that $\mathbf{F}$ transforms $\boldsymbol{\varepsilon}_n$ to $\boldsymbol{\varphi}_n$ and $\boldsymbol{\varphi}_n$ to $\boldsymbol{\varepsilon}_{N-n}$.

The reader may ask if any larger class of operators has the property common to self-adjoint and unitary ones: orthogonality and completeness of their eigenvectors. In fact, this is a property of all and only *normal operators*, i.e., those operators $\mathbb{N}$ which commute with their adjoints $\mathbb{N}^\dagger\mathbb{N} = \mathbb{N}\mathbb{N}^\dagger$. The proof of this statement can be seen, for instance, in the book by Fano (1971, Section 2.3). As to the question of whether all operators have eigenvectors which diagonalize their representing matrices, the answer is in the negative. The most one can do in the general case is to achieve a reduction into the *Jacobi canonical form*: a block-diagonal form, one block for each distinct eigenvalue and each block being a matrix with a shifted diagonal of 1's beside the main diagonal. A discussion of this can be found in the book by Gel'fand (1961, Section III).

1.7.9. Eigenbases of Operators with Degenerate Eigenvalues

As we have seen, the eigenvectors of a self-adjoint or unitary operator in $\mathscr{V}^N$ constitute an orthonormal basis for the space called the *spectral basis* or *eigenbasis* of the operator. If this operator describes the time evolution of a system (to be seen in Chapter 2), it is very convenient to use this basis since the coordinate directions defined by the eigenvectors will remain invariant in time and will change only in scale. Moreover, the eigenvectors are conveniently labeled by the eigenvalues of the operator, except, that is, for the ambiguities which may arise when two or more eigenvalues coincide in a multiple root of the characteristic polynomial. Such eigenvalues are said to be *degenerate*. The term is borrowed from quantum mechanics. Our nearest example of degeneracy appears in the eigenvalues of $\mathbb{A}$ which are equal by pairs: $\lambda_n = \lambda_{N-n}$. To resolve the degeneracy and use eigenvalues to label the basis vectors uniquely we may hope to find one (or more) extra operators

whose eigenvalues will specify the eigenvector labels completely within each of the invariant subspaces of the first operator.

1.7.10. Removal of Degeneracy

Specifically, we have $\mathbb{A}\mathbf{x}_i = \mu_i \mathbf{x}_i$ for the first operator, and we need $\mathbb{B}\mathbf{x}_j = \nu_j \mathbf{x}_j$ for the second, so that although some of the μ's and some of the ν's may be degenerate, we hope that the assignment of the *pairs* (μ_i, ν_j) to $\mathbf{x}_{ij}$ will be one to one. We shall prove that *two operators* $\mathbb{A}$ *and* $\mathbb{B}$ *can have simultaneously the same set* $\{\mathbf{x}_i\}_{i=1}^N$ *of eigenvectors if and only if they commute.* If they have the same eigenvector set, they will both be represented in the common spectral basis by diagonal matrices, which commute. If they commute, then once we have found the spectral basis for $\mathbb{A}$ (so that the representing matrix $\bar{\mathbf{A}}$ of $\mathbb{A}$ is diagonal with possibly repeated eigenvalues), the representing matrix $\bar{\mathbf{B}}$ for $\mathbb{B}$ in the same basis can only be block diagonal, each block with the size and position of the sets of degenerate eigenvalues of $\bar{\mathbf{A}}$. Each block in $\bar{\mathbf{B}}$ can be diagonalized as (1.111) without affecting $\bar{\mathbf{A}}$; the result is a final eigenvector basis $\{\bar{\bar{\mathbf{x}}}_i\}_{i=1}^N$ where both $\bar{\mathbf{A}}$ and $\bar{\bar{\mathbf{B}}}$ are fully diagonal.

1.7.11. The Case of the $\mathbb{\Delta}$ Operator

The $\mathbb{\Delta}$ operator, we noted, has doubly degenerate eigenvalues. We can use any of the dihedral operators commuting with $\mathbb{\Delta}$ [Eqs. (1.96)] to complete the labeling. The operator $\mathbb{R}$ seems the wisest choice: in the $\boldsymbol{\varphi}$-basis it is already diagonal [Eq. (1.91) for $k = 1$], and all of its eigenvalues are distinct:

$$\mathbb{R}\boldsymbol{\varphi}_n = \exp(2\pi i n/N)\boldsymbol{\varphi}_n, \qquad n = 1, 2, \ldots, N. \tag{1.114}$$

Indeed, $\mathbb{R}$ could be used alternatively to *define* the $\boldsymbol{\varphi}$-basis vectors uniquely, with no labeling degeneracy. As another choice, the $\mathbb{I}_0$ operator [Eq. (1.92) for $l = 0$] can be used. (The matrix $\tilde{\mathbf{I}}_0$ does not *appear* to be block diagonal since the pairs of degenerate eigenvalue vectors are not placed sequentially in the basis.) If we define

$$\left.\begin{aligned} \boldsymbol{\varphi}_m{}^+ &= 2^{-1/2}(\boldsymbol{\varphi}_m + \boldsymbol{\varphi}_{N-m}), \qquad (1.115a)\\ \boldsymbol{\varphi}_m{}^- &= i2^{-1/2}(\boldsymbol{\varphi}_m - \boldsymbol{\varphi}_{N-m}), \qquad (1.115b) \end{aligned}\right\} m = 1, 2, \ldots, \begin{cases} \tfrac{1}{2}(N-1), & N \text{ odd}, \\ \tfrac{1}{2}N - 1, & N \text{ even}, \end{cases}$$

$$\boldsymbol{\varphi}_0^+ = \boldsymbol{\varphi}_N, \qquad \text{and} \qquad \boldsymbol{\varphi}_{N/2}^+ = \boldsymbol{\varphi}_{N/2} \qquad \text{for } N \text{ even}, \tag{1.115c}$$

we can see that

$$\mathbb{\Delta}\boldsymbol{\varphi}_m{}^\pm = \lambda_m \boldsymbol{\varphi}_m{}^\pm, \tag{1.116a}$$

$$\mathbb{I}_0\boldsymbol{\varphi}_m{}^\pm = \pm\boldsymbol{\varphi}_m{}^\pm, \tag{1.116b}$$

so that (1.115) is the common eigenbasis of $\mathbb{\Delta}$ and $\mathbb{I}_0$.

Exercise 1.50. Verify that the basis (1.115) indeed has N orthonormal vectors.

Exercise 1.51. Find the matrix transforming the φ-basis to the $\varphi^{\pm}$-basis (1.115).

Exercise 1.52. Write out explicitly the matrices representing $\mathbb{A}$, $\mathbb{I}_0$, and $\mathbb{R}$ in the $\varphi^{\pm}$-basis (1.115). You can do this by using the results of Exercise 1.51 or, for the first two operators, directly from (1.116).

Exercise 1.53. Generalize the choices of basis given by (1.114) and (1.115)–(1.116a): Show that $\mathbb{R}^k$ defines a basis equally well as long as k is not a divisor of N. Regarding $\mathbb{I}_l$, construct eigenbases of $\mathbb{A}$ and $\mathbb{I}_l$ with

$$\varphi_m^{(l)\pm} := \alpha_m{}^{\pm}\varphi_m + \beta_m{}^{\pm}\varphi_{N-m}, \qquad |\alpha_m{}^{\pm}|^2 + |\beta_m{}^{\pm}|^2 = 1, \tag{1.117a}$$

$$\mathbb{I}_l\varphi_m^{(l)\pm} = \pm\varphi_m^{(l)\pm}, \tag{1.117b}$$

where the range of m is the same as in Eqs. (1.115). Show that a good choice is

$$\alpha_m{}^{\pm} = 2^{-1/2}\exp(2\pi ilm/N), \qquad \beta_m{}^{\pm} = \pm 2^{-1/2}\exp(-2\pi ilm/N). \tag{1.117c}$$

Show that this indeed generalizes the $\varphi^{\pm}$-basis in Eqs. (1.115)–(1.116).

Exercise 1.54. Recall that for N even the transformations $\mathbb{K}_l$ [(1.97) and below] also come into play. One can define, in analogy to (1.115),

$$\varphi_m^{1+} := 2^{-1/2}[\exp(i\pi m/N)\varphi_m + \exp(-i\pi m/N)\varphi_{N-m}], \tag{1.118a}$$

$$\varphi_m^{1-} := i2^{-1/2}[\exp(i\pi m/N)\varphi_m - \exp(-i\pi m/N)\varphi_{N-m}], \tag{1.118b}$$

for $m = 1, 2, \ldots, \frac{1}{2}N - 1$, and

$$\varphi_{N/2}^{1+} = \varphi_{N/2}, \qquad \varphi_0^{1+} = \varphi_N. \tag{1.118c}$$

Show that these are eigenfunctions of $\mathbb{K}_0$, i.e.,

$$\mathbb{K}_0\varphi_m^{1\pm} = \pm\varphi_m^{1\pm}. \tag{1.118d}$$

Show that the vectors defined above have *real* components in the ε-basis. One can do the same for the other $\mathbb{K}_l$'s.

Exercise 1.55. Consider in all detail, since it can be done algebraically, the eigenvalues and vectors of 2×2 complex matrices, i.e.,

$$\mathbf{M}\mathbf{v}^{\pm} := \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} x^{\pm} \\ y^{\pm} \end{pmatrix} = \lambda^{\pm}\begin{pmatrix} x^{\pm} \\ y^{\pm} \end{pmatrix} = \lambda^{\pm}\mathbf{v}^{\pm}. \tag{1.119}$$

Show that the eigenvalues are

$$\lambda^{\pm} = \tfrac{1}{2}(a + d) \pm \{[\tfrac{1}{2}(a - d)]^2 + bc\}^{1/2}, \tag{1.120}$$

which are real for $\mathbf{M}$ hermitian (a, d real and $b = c^*$). They are also real for $\mathbf{M}$ real and $[\frac{1}{2}(a - d)]^2 + bc \geqslant 0$. Note that $\sum_i \lambda_i = \text{trace } \mathbf{M}$ and $\Pi_i\lambda_i = \det \mathbf{M}$: These are general properties for any dimension.

Exercise 1.56. Examine now the eigenvectors in (1.119). Show that

$$\frac{y^{\pm}}{x^{\pm}} = \frac{\lambda^{\pm} - a}{b} = \frac{c}{\lambda^{\pm} - d}. \tag{1.121}$$

Note that two proper eigenvectors need not exist for arbitrary **M** (for example, when $b = 0$). Show that when $\lambda^{\pm}$ and a are real, the angle between $\mathbf{v}^{+}$ and $\mathbf{v}^{-}$ is (without assuming their normalization)

$$(\mathbf{v}^{+}, \mathbf{v}^{-}) = x^{+*}x^{-}\left[1 - \frac{c}{b^{*}}\frac{(\lambda^{+} - a)^{*}}{\lambda^{+} - a}\right]. \tag{1.122}$$

They are thus orthogonal if **M** is hermitian or unitary. The results of the last exercises will be handy later on.

Exercise 1.57. Show that if **x** is an arbitrary normalized vector in $\mathscr{V}^{N}$, then

$$\mathbf{x}^{I_k\pm} := \tfrac{1}{2}(\mathbb{1} \pm \mathbb{I}_k)\mathbf{x}, \qquad \mathbf{x}^{K_l\pm} := \tfrac{1}{2}(\mathbb{1} \pm \mathbb{K}_l)\mathbf{x} \tag{1.123}$$

are eigenvectors of $\mathbb{I}_k$ and $\mathbb{K}_l$, respectively, with eigenvalues ± 1. The operators $\frac{1}{2}(\mathbb{1} \pm \mathbb{I}_k)$ and $\frac{1}{2}(\mathbb{1} \pm \mathbb{K}_l)$ are *projection* operators onto orthogonal subspaces.

1.7.12. Finding the Fourier Transformation

Exercises 1.58–1.60 show how we can *find* the Fourier transformation **F** as that which diagonalizes the second-difference matrix representative **Δ** given by (1.60).

Exercise 1.58. Consider diagonalizing **Δ** through an (unknown) unitary matrix **F** as $\mathbf{\Delta F} = \mathbf{F\Lambda}$, where **Λ** is diagonal with elements λ_n. Show that the $m - n$ element of this equality leads to the recursion relation

$$F_{m+1,n} = (2 + \lambda_n)F_{mn} - F_{m-1,n}. \tag{1.124}$$

The indices in (1.124) are to be considered modulo N. This allows us to write any F_{mn} in terms of F_{1n} and $F_{0n} \equiv F_{Nn}$ as

$$F_{m+1,n} = U_m(x_n)F_{1n} - U_{m-1}(x_n)F_{0n}, \qquad x_n := 1 + \lambda_n/2, \tag{1.125}$$

where the U_m are polynomials in x_n. Combining the two preceding equations shows that they satisfy the recurrence relation

$$U_m(x_n) = 2x_nU_{m-1}(x_n) - U_{m-2}(x_n), \tag{1.126a}$$

$$U_0(x_n) = 1, \qquad U_1(x_n) = 2x_n. \tag{1.126b}$$

Exercise 1.59. Show that the solution to the recurrence relation (1.126) is given by

$$U_m(x) = \sin[(m + 1)\arccos x]/\sin(\arccos x). \tag{1.127}$$

These are the *Chebyshev polynomials of the second kind* of degree m, and (1.126a) is their Christoffel–Darboux formula. [See the mathematical handbook by Abramowitz and Stegun (1964, Chapter 22).] The recurrence relation for the elements of **F** "closes" for $m = N \equiv 0$. From (1.124) for $m = N$ and from (1.125) for $m = N - 2$ and $N - 1$, show that this leads to a pair of homogeneous

simultaneous equations in F_{0n} and F_{1n}, the vanishing of whose determinant requires

$$U_{N-1}(x)[U_{N-3}(x) + 2x] - [U_{N-2}(x) + 1]^2 = 0. \tag{1.128}$$

The roots of this polynomial equation will determine the allowed values of λ_n. By the use of trigonometric identities, (1.128) can be reduced to

$$\sin\theta(1 - \cos N\theta) = 0, \qquad \cos\theta \coloneqq x = 1 + \lambda/2 \Rightarrow \theta = 2\pi k/N,$$
$$k = 0, \pm 1, \pm 2, \ldots, \tag{1.129}$$

whose roots yield precisely the values of λ_n given by (1.62b), so the index n can serve to number columns—any other one would just permute the λ_n's in $\mathbf{\Lambda}$. Note, though, that all eigenvalues but λ_N (and $\lambda_{N/2}$ if N is even) are twofold degenerate. See Weinstock (1971).

Exercise 1.60. Substituting the eigenvalues λ_n into (1.125) and letting $F_{1n} = \gamma_n F_{0n}$, find F_{mn}. The requirement of unitarity $\sum_m |F_{mn}|^2 = 1$ will fix $|F_{0n}|$ but leaves a three-dimensional freedom in choosing each complex γ_n and the phase of F_{0n}. The choice $\arg F_{0n} = 0$ and $\gamma_n = \exp(-2\pi in/N)$ produces *the* Fourier transform matrix (1.48). Examine first the columns F_{mN} and $F_{m,N/2}$ if N is even. There, $U(x_N) = m + 1$ and $U_m(x_{N/2}) = (-1)^m(m + 1)$. Proceed then to the other columns, noting the twofold eigenvalue degeneracy.

Table 1.1. Coordinates in the ε- and φ-Bases of Vectors Subject to Various Operations or Acted upon by Operators[a]

Operation	$\mathbf{f}$	f_n	$\tilde{f}_m$
Linear combination	$a\mathbf{f} + b\mathbf{g}$	$af_n + bg_n$	$a\tilde{f}_m + b\tilde{g}_m$
Inner product	$(\mathbf{f}, \mathbf{g})$	$\sum_n f_n^* g_n$	$\sum_m \tilde{f}_m^* \tilde{g}_m$
Translation (rotation)	$\mathbb{R}^k\mathbf{f}$	f_{n-k}	$\exp(2\pi ikm/N)\tilde{f}_m$
Inversion	$\mathbb{I}_k\mathbf{f}$	f_{N+2k-n}	$\exp(4\pi ikm/N)\tilde{f}_{N-m}$
	$\mathbb{K}_l\mathbf{f}$	$f_{N+2k-n+1}$	$\exp[4\pi i(k + \frac{1}{2})m/N]\tilde{f}_{N-m}$
Second difference	$\Delta\mathbf{f}$	$f_{n+1} - 2f_n + f_{n-1}$	$-4\sin^2(\pi m/N)\tilde{f}_m$
Complex conjugation		f_n^*	$\tilde{f}_{N-m}^*$
Convolution (Section 3.1)	$\mathbf{f}\,(\varepsilon)\,\mathbf{g}$	$f_n g_n$	$N^{-1/2}\sum_r \tilde{f}_r \tilde{g}_{m-r}$
	$\mathbf{f}\,(\varphi)\,\mathbf{g}$	$N^{-1/2}\sum_s f_s g_{n-s}$	$\tilde{f}_m \tilde{g}_m$
Correlation (Section 3.2)	$\mathbf{f}\,c\,\mathbf{g}$	$N^{-1/2}\sum_s f_s^* g_{n+s}$	$\tilde{f}_m^* \tilde{g}_m$

[a] In all cases n and m appear mod N.

2

The Application of Fourier Analysis to the Uncoupling of Lattices

We shall apply here Fourier analysis and other vector space and symmetry concepts introduced in Chapter 1 to the study of certain coupled systems which have simple mechanical realizations as one-dimensional crystalline lattices. In Section 2.1 we define the constituents of such systems and their corresponding solution so that we may pose the problem of uncoupling lattices of such elements in Section 2.2. A rather detailed study of the basic solutions is made in Section 2.3 for a simple lattice and in Section 2.4 for more complicated ones which can be described by second- or farther-neighbor interaction in crystals or as molecular or diatomic chains. We go to a more general setting in studying energy and other phase-space concepts which belong properly to analytical mechanics. Sections 2.5 and 2.6 can be read after the first two sections if the reader so prefers. Although examples drawn from Sections 2.3 and 2.4 are used to illustrate examples of the theory, the reader should be able to follow the general presentation easily.

2.1. Mechanical and Electric Analogies

We shall study here the elements which constitute coupled systems of a rather general type, exemplified by mechanical and electric networks. The former are constituted by masses, restitution forces (springs), driving forces, and viscous damping; the latter will consist of a standard *RLC* circuit plus electromotive forces. The differential equations which describe the time

evolution of these two systems point out analogies between their constituent elements.

2.1.1. Masses, Springs, and Damping

The equation of motion of the simple mechanical system in Fig. 2.1 can be found from the following considerations. The external (time-dependent) force $F(t)$ will produce the following: (a) an acceleration $\ddot{f}(t)$ of the *mass* M, where $\ddot{f}(t) \coloneqq d^2f(t)/dt^2$; (b) a stretching $f(t)$ of the spring with *Hooke's constant* k; and (c) if the system is immersed in a "perfect" viscous fluid, when moving it will experience a *velocity-dependent* drag $c\dot{f}(t)$, where c is the *damping constant* of the medium ($c \geqslant 0$). Setting action equal to reaction, we can write the mechanical equation of motion as

$$M\ddot{f}(t) + c\dot{f}(t) + kf(t) = F(t). \tag{2.1}$$

This is an inhomogeneous second-order *linear* differential equation with constant coefficients, whose solution is quite simple. Of course, actual mechanical systems do not exhibit a constant k for all deformations $f(t)$ since the spring must be finite; the viscous damping does not, for all velocities, have the simple $c\dot{f}(t)$ behavior, and frictional forces—constant and opposite to the direction of motion—can certainly be present. Nevertheless, Eq. (2.1), besides being a good model for actual mechanical situations, lends itself admirably to the modeling of other apparently unrelated systems. It also has the advantage of mathematical simplicity.

2.1.2. Inductances, Capacitors, and Resistance

The electric *RLC* circuit of Fig. 2.2 consists of a series connection of a resistance R, an inductance L, a capacitor C, and an applied electromotive

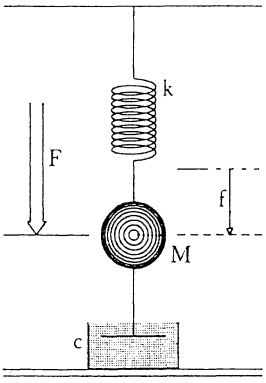


Fig. 2.1. A driven, damped oscillator. An inertial mass M (with elongation f) is subject to a restitution spring with Hooke's constant k, a viscous damping device of constant c, and a driving force F.

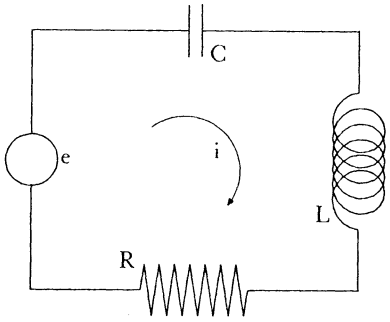


Fig. 2.2. A simple *RLC* circuit. The current i flows through an inertial inductance L, a "spring" capacitor C, and a damping resistance R and is driven by an electromotive source e.

force $e(t)$. If the circulating change is $q(t)$ and the current is $i(t) = dq(t)/dt =: \dot{q}(t)$, Kirchhoff's second law leads to the equations

$$L\ddot{q}(t) + R\dot{q}(t) + C^{-1}q(t) = \dot{e}(t), \tag{2.2a}$$

$$C\ddot{q}(t) + RCL^{-1}\dot{q}(t) + L^{-1}q(t) = CL^{-1}\dot{e}(t), \tag{2.2b}$$

where we have multiplied the first by CL^{-1} to obtain the second. Equations (2.1) and (2.2) are of the same form and lead to analogies between mechanical and electric elements. The spring elongation $f(t)$ and velocity are identified with the circulating charge $q(t)$ and current, while mass, restitution, and viscous drag are identified with either L, C^{-1}, and R or C, L^{-1}, and RC/L. The first analogy is perhaps the more intuitive one, as kinetic and potential mechanical energy are made to correspond with magnetic and electrostatic forms of energy. The second set leads to a correspondence between a class of electric networks and mechanical lattices, as has been presented in the classic book by Brillouin (1946). We shall henceforth refer only to mechanical lattices in illustrating the concepts of complex vector spaces and the Fourier transform. Standing or traveling waves, for instance, are easier to visualize in a mechanical device than in the dials of an array of meters in a circuit. The methods and results can be applied without undue extra effort to the electric case.

2.1.3. Longitudinal and Transverse Mechanical Vibrations

Since many of the models mentioned above make use of longitudinal as well as transverse vibrations of lattices, it is important to point out the difference between the two. Longitudinal vibrations in lattices will be described in the next section and follow the elementary system in Fig. 2.1 and the ensuing solution. For transverse vibrations there is more than Eq. (2.1) to the problem, so we propose the following:

Exercise 2.1. Consider transverse vibrations of the mass M under the action of two springs each of constant $\frac{1}{2}k$ as depicted in Fig. 2.3. Let the *unstretched*

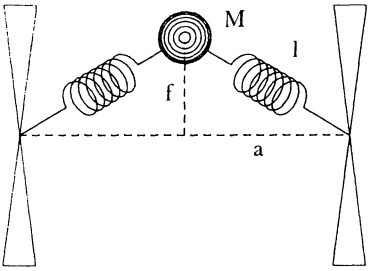


Fig. 2.3. A mass allowed to perform transverse vibrations under the influence of two springs.

length of the springs be a_0. Show that this leads to the *nonlinear* differential equation

$$M\ddot{f}(t) + c\dot{f}(t) + 2kf(t)[1 - a_0(a^2 + f(t)^2)^{-1/2}] = F(t). \tag{2.3}$$

Exercise 2.2. Show that in Eq. (2.3) we can make two approximations: (a) Assume that the stretched length l (Fig. 2.3) is much longer than the natural length a_0. (b) Assume that the oscillations are small, so that $[a^2 + f(t)^2]^{1/2} \simeq a$. In each case one obtains a linear differential equation. They are not identical though.

2.1.4. Solutions to the Equations of Motion with Initial Conditions

In the absence of external forces, Eqs. (2.1)–(2.2) admit solutions of the general type

$$f(t) = a \exp(i\omega t), \tag{2.4}$$

where a is a constant and ω can be found by substituting (2.4) into (2.1):

$$-M\omega^2 + ic\omega + k = 0, \tag{2.5}$$

i.e., we have *two* possible values of ω, given by

$$\omega^{\pm} = \frac{ic}{2M} \pm \left[\frac{k}{M} - \left(\frac{c}{2M}\right)^2\right]^{1/2} =: i\Gamma \pm \omega^e \tag{2.6a}$$

$$\Gamma := \frac{c}{2M}, \qquad \omega^e := (k/M - \Gamma^2)^{1/2}. \tag{2.6b}$$

Hence, the general solution of the homogeneous equation (2.1) can be written as

$$f(t) = \exp(-\Gamma t)[a \exp(i\omega^e t) + b \exp(-i\omega^e t)] \tag{2.7}$$

for a and b arbitrary constants. The latter can be determined from two known data about $f(t)$ and/or its derivatives. Typically, if we know the value and derivative of $f(t)$ at some initial time t_0, $f_0 := f(t_0)$ and $\dot{f}_0 := df(\tau)/d\tau|_{\tau=t_0}$, Eq. (2.7) for $t = t_0$ allows us to solve for a and b as

$$a = -(2\omega^e)^{-1} \exp(-i\omega^+ t_0)(\omega^- f_0 + i\dot{f}_0), \tag{2.8a}$$

$$b = (2\omega^e)^{-1} \exp(-i\omega^- t_0)(\omega^+ f_0 + i\dot{f}_0). \tag{2.8b}$$

Replacement into (2.7) yields

$$f(t) = (2\omega^e)^{-1}\{-\omega^- \exp[i\omega^+(t - t_0)] + \omega^+ \exp[i\omega^-(t - t_0)]\}f_0 + i(2\omega^e)^{-1}\{-\exp[i\omega^+(t - t_0)] + \exp[i\omega^-(t - t_0)]\}\dot{f}_0. \quad (2.9)$$

Reducing further, we can bring the solution to the form

$$f(t) = [\dot{G}(t - t_0) + 2\Gamma G(t - t_0)]f_0 + G(t - t_0)\dot{f}_0, \quad (2.10)$$

where for ω^e real we have defined

$$G(\tau) \coloneqq (\omega^e)^{-1} \exp(-\Gamma\tau) \sin \omega^e\tau \qquad \text{(oscillatory)} \quad (2.11a)$$

and its time derivative

$$\dot{G}(\tau) = -\Gamma G(\tau) + \exp(-\Gamma\tau) \cos \omega^e\tau. \quad (2.11b)$$

As $G(\tau)$ depends on c, M, and k, it will serve us to denote it occasionally by $G^{c,M,k}(\tau)$. Clearly, $G(\tau)$ and $\dot{G}(\tau)$ are themselves solutions of the original differential equation (2.1) with no external forces present.

2.1.5. Critical and Overdamped Cases

The structure of the general solution given by (2.10) is quite transparent. If the damping is small with respect to the restitution spring (more precisely, for $c^2 < 4Mk$), ω^e is a real number, playing the role of the *effective angular frequency*, and the nature of (2.10)–(2.11) is that of a *damped oscillation*. See Fig. 2.4.

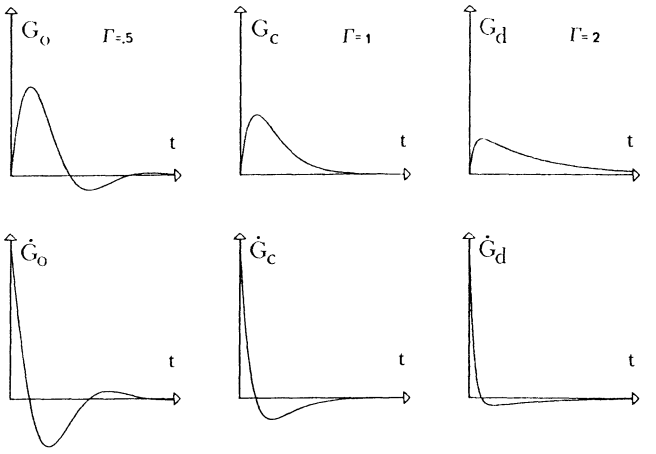


Fig. 2.4. The functions $G(t)$ and $\dot{G}(t)$ for the oscillatory (o), critical (c), and overdamped (d) cases. Time units of $(M/k)^{1/2}$ are used, the t-axis representing the interval from 0 to 10. The vertical axes of the figures have height 1. Damping constants in each case are chosen as $\Gamma = 0.5$, 1, and 2.

If the damping constant increases, the effective angular frequency will decrease and reach zero when $c^2 = 4Mk$. In this case (*critical damping*), the solution (2.10) retains its form, but, as $(\omega^e)^{-1} \sin \omega^e \tau \to \tau$, the function $G(\tau)$ is now given by

$$G(\tau) = \tau \exp(-\Gamma\tau) \qquad \text{(critical)} \tag{2.12}$$

and $\dot{G}(\tau)$ accordingly. See Fig. 2.4 (curves G_c and $\dot{G}_c$). Finally, for $c^2 > k4M$ we have the *overdamped* situation when the solution is (2.9) with

$$G(\tau) = (w^e)^{-1} \exp(-\Gamma\tau) \sinh w^e\tau \qquad \text{(overdamped)}, \tag{2.13a}$$

$$iw^e := \omega^e = i(\Gamma^2 - k/M)^{1/2}. \tag{2.13b}$$

See Fig. 2.4 (curves G_d and $\dot{G}_d$). As $|w^e| < \Gamma$ for all $k > 0$, the solutions fall to zero exponentially, while no proper oscillation takes place.

2.1.6. Some Further Remarks and Exercises

The solution of (2.1) in the presence of an external driving force is a sum of the general solution of the homogeneous part of the differential equation seen above plus a particular solution of (2.1). The general construction of the solution to the inhomogeneous equation (2.1) will be made using the techniques of Fourier and Laplace transforms in Sections 7.4 and 8.1. The methods in this part are not significantly dependent on the presence of external forces so we shall henceforth work only with the *homogeneous* equation (2.1), which represents a damped-oscillator equation of motion with initial conditions.

Among the systems whose models are lattices constituted by such elements we have the oscillations of natural crystals and electric circuits in a larger network; in fact, it is the very model of an elastic ether as conceived in his time by Newton and followed for several centuries which led to Maxwell's equations for the electromagnetic field.

Exercise 2.3. Refer to Exercise 2.2. Denote by ω_a the angular frequency of approximation (a) [simply $\omega_a = \omega^e$ in (2.6b)] and ω_b that of approximation (b) [as above but replacing the spring constant k by $k_b := k(1 - a_0/a)$]. Show that in approximation (b) the longitudinal and transverse oscillation frequencies are not equal but that

$$\omega_a/\omega_b = [(1 - a_0/a) - c^2/2Mk]^{1/2}.$$

Hence, when drawing transverse oscillations and using the mathematical language of longitudinal ones, we are referring to approximation (b).

Exercise 2.4. Follow the developments in this section for the undamped case $c = 0$. Find $G^{0mk}(\tau)$ and the form (2.10).

Exercise 2.5. Consider the case when no spring is present ($k = 0$). In that case $\omega^+ = ic/M$, $\omega^- = 0$, and we are always in the overdamped case with $w = \Gamma = c/2M$. Show that the general solution is (2.10) with

$$G^{cM0}(\tau) = (2\Gamma)^{-1}[1 - \exp(-2\Gamma\tau)], \qquad \dot{G}^{cM0}(\tau) = \exp(-2\Gamma\tau), \tag{2.14}$$

i.e.,

$$f(t) = f_0 + (2\Gamma)^{-1}\{1 - \exp[-2\Gamma(t - t_0)]\}\dot{f}_0. \tag{2.15}$$

Exercise 2.6. Examine the situation where no damping or spring is present. You can solve the problem either directly or by considering (2.14)–(2.15) as $\Gamma \to 0$. Show that the solution can still be written in the form (2.10) with

$$G^{0M0}(\tau) = \tau, \qquad \dot{G}^{0M0}(\tau) = 1, \tag{2.16}$$

so that

$$f(t) = f_0 + (t - t_0)\dot{f}_0, \tag{2.17}$$

i.e., simple inertial motion.

Exercise 2.7. Follow the development in this section when $M = 0$, so the second-derivative term in (2.1) vanishes. The oscillating body looses its inertia, and only restitution and viscous forces act. Show that the solution, in terms of the initial displacement at t_0, is

$$f(t) = f_0 \exp[-k(t - t_0)/c]. \tag{2.18}$$

Exercise 2.8. Verify that the solution (2.18) can also be obtained from (2.10) and (2.13) by letting $M \to 0$. Note that although Γ, $w^e \to \infty$, their difference $\omega^- \to -ik/c$. Similarly, although $G^{c0k}(\tau)$, $\dot{G}^{c0k}(\tau) \to 0$, the term $2\Gamma G^{c0k}(\tau)$ in (2.10) survives and gives rise to the form (2.18).

2.2. The Equation of Motion of Coupled Systems and Solution

A system of N interacting elements will be called a *lattice*. In its simplest one-dimensional mechanical realization, it is a set of N masses interacting through spring-like forces. This interaction can be nonzero for a pair of "nearest neighbors" only or can include "farther" masses as well. Each particle by itself, in addition, can be subject to viscous and external forces. When the nearest-neighbor interaction is the most significant, it is convenient to arrange the mass points on a line where the first-neighbor relation is manifest. Further, as we assume every mass to have two first neighbors, the points in the lattice will close in a circle. See Fig. 2.5. This model is also useful to describe second- and farther-neighbor harmonic oscillator interactions.

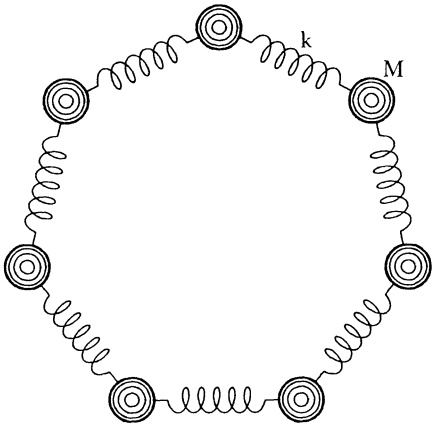


Fig. 2.5. Mechanical lattice composed of masses M and springs k with first-neighbor interaction only.

2.2.1. Inertial, Interaction, and Dissipation Operators

Let f_n denote the displacement of the nth mass M_n relative to its equilibrium position. Unless the lattice is at rest, it will be a function of time: $f_n = f_n(t)$. For the purpose of the model we assume here the vibrations in the lattice to be longitudinal only. Let k_{nm} be the spring constant between particles n and m; then the force acting on the nth mass is $k_{nm}(f_n - f_m)$ in the direction from mass n to mass m. (See Fig. 2.6 for first-neighbor interactions.) If we add the possibility of having a spring k_{nn} between M_n and its equilibrium position, the total force on M_n due to the interaction among the lattice elements is thus

$$\begin{aligned}\sum_{m\neq n} k_{nm}(f_n - f_m) + k_{nn}f_n &= -\sum_{m\neq n} k_{nm}f_m + f_n \sum_m k_{nm} \\ &= \sum_m \left[-k_{nm} + \delta_{n,m}\left(k_{nn} + \sum_r k_{nr}\right)\right] f_m =: \sum_m \kappa_{nm} f_m. \end{aligned} \tag{2.19}$$

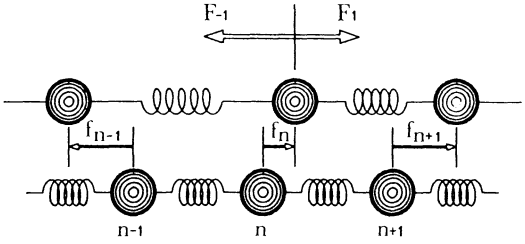


Fig. 2.6. Longitudinal vibrations in a linear lattice. Positions, elongations, and acting forces of the deformed lattice (above) are shown vis-à-vis the undeformed situation (below).

We assume, as in Section 1.6, that the lattice is closed (Fig. 2.5) so that its elements are numbered modulo N. Hence f_k and f_{k+mN} (m integer) describe the same displacement. If, finally, the damping constant for the nth element is c_n and $F_n = F_n(t)$ is the external force, the equation of motion for the nth particle in the lattice is

$$M_n\ddot{f}_n + c_n\dot{f}_n + \sum_m \kappa_{nm} f_m = F_n, \qquad n = 1, 2, \ldots, N. \tag{2.20}$$

2.2.2. Equation of Motion in Operator Form and the Problem of Uncoupling

The N equations (2.20) can be combined into a single vector equation if we identify f_n with the nth coordinate of a vector $\mathbf{f}$ in some (for definiteness, the orthonormal $\boldsymbol{\varepsilon}$-) basis, as was done in Section 1.6, and the same for F_n. The coefficients κ_{nm} can be arranged into a matrix $\mathbf{K} = \|\kappa_{nm}\|$ in the same basis, representing an *interaction* operator $\mathbb{K}$. Similarly, M_n and c_n can be taken to be the elements of diagonal matrices $\mathbf{M} = \|M_n\delta_{nm}\|$ and $\mathbf{C} = \|c_n\delta_{nm}\|$ representing the *inertial* and *dissipation* operators $\mathbb{M}$ and $\mathbb{C}$. Equations (2.20) can then be written as

$$\mathbb{M}\ddot{\mathbf{f}} + \mathbb{C}\dot{\mathbf{f}} + \mathbb{K}\mathbf{f} = \mathbf{F}. \tag{2.21}$$

This form is *basis independent* and in a sense hides the fact that it was obtained from N *coupled* differential equations (2.20): The solution f_n for the nth particle depends through the interaction term on the solution for the other f_m's, which in turn depend on other ones until all N coordinates are involved. This is what Fig. 2.5 tells us. If the interaction operator $\mathbb{K}$ had a basis where it was represented by a diagonal matrix, and in that basis $\mathbb{M}$ and $\mathbb{C}$ also had diagonal representatives, Eq. (2.21) would yield a set of N *uncoupled* equations which could be solved independently, thereby reducing the problem to that of last section. This may not be possible in general, though it will be for the case when $\mathbb{M}$ and $\mathbb{C}$ are multiples of the identity operator—$\mathbb{M} = M\mathbb{1}$, $\mathbb{C} = c\mathbb{1}$—for then they are represented by diagonal matrices in any basis, meaning in particular that all masses and damping constants are equal. In that case we need only direct our efforts toward finding the eigenbasis of $\mathbb{K}$. In that basis, $\mathbb{K}$ will be represented by a diagonal matrix, and the system of equations will uncouple. Such an eigenbasis does exist, as shown through the following.

Exercise 2.9. The action of the mth mass on the nth through the spring with constant k_{nm} should equal the action of the nth on the mth; hence $k_{nm} = k_{mn}$. Show that this implies that $\mathbb{K}$ is a self-adjoint operator. We proved in Section 1.7 that all such operators have a complete eigenbasis. Notice that if $k_{nm} = 0$ and $k_{mn} \neq 0$ this means that mass m is acted upon by but does not influence mass n. This is a "servomechanism" whereby the position of mass n is monitored as an external force on mass m.

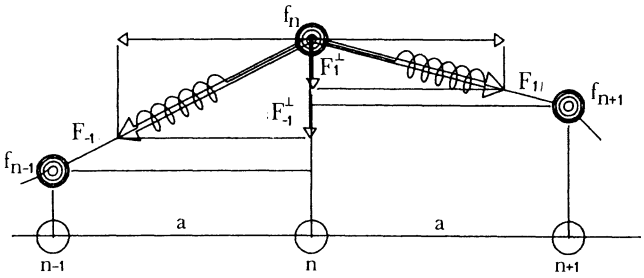


Fig. 2.7. Transverse vibrations in a linear lattice. The longitudinal components of the spring tension forces acting on each mass are equal and opposite. Net force on the mass is the sum of the transverse components.

Exercise 2.10. Consider plane transverse vibrations of the lattice. Show that, within the approximations developed in Exercises 2.1 and 2.2 [(a) and/or (b)], they lead to equations of motion similar to (2.20). Refer to Fig. 2.7.

2.2.3. The Interaction Eigenbasis

Let $\bar{\mathbf{K}} := \|\kappa_n \delta_{nm}\|$ be the diagonal matrix representing $\mathbb{K}$ in its own eigenbasis $\{\psi_n\}_{n=1}^N$, $\{\kappa_n\}_{n=1}^N$ being the eigenvalues. Letting $\bar{f}_n$ be the coordinates of $\mathbf{f}$ in this basis, Eq. (2.21) becomes

$$M\ddot{\bar{f}}_n + c\dot{\bar{f}}_n + \kappa_n \bar{f}_n = \bar{F}_n, \qquad n = 1, 2, \ldots, N, \tag{2.22}$$

which is that of a set of *uncoupled* oscillators with spring constants κ_n, $n = 1, 2, \ldots, N$. As the solution of (2.22) was studied in the last section, we only need to know explicitly the transformation linking the $\boldsymbol{\varepsilon}$- with the $\mathbb{K}$-eigenbasis $\boldsymbol{\psi}$ in order to translate the solutions of (2.22) into the solutions of (2.20). This is easier said than done, so the remainder of Section 2.2 will deal with a simple case where the eigenbasis of $\mathbb{K}$ is one which has been studied before.

2.2.4. The Simple Equal-Mass Lattice

Consider the lattice in Fig. 2.5, where all masses and springs are equal, the viscous and external forces are absent ($\mathbb{C} = \mathbb{0}$, $\mathbf{F} = \mathbf{0}$), and only first-neighbor interactions are considered. As $k_{nm} = k(\delta_{n,m+1} + \delta_{n,m-1})$ and $k_n = 0$, Eq. (2.19) yields

$$\kappa_{nm} = -k(\delta_{n,m+1} + \delta_{n,m-1} - 2\delta_{nm}), \tag{2.23}$$

i.e., *the interaction operator is a multiple k of the second-difference operator* (Section 1.5),

$$\mathbb{K} = -k\mathbb{\Delta}, \tag{2.24}$$

and the vector equation of motion (2.21) then reads

$$M\ddot{\mathbf{f}} - k\Delta\mathbf{f} = \mathbf{0}. \tag{2.25}$$

In the ε-basis, this is represented by the N equations

$$M\ddot{f}_n = k(f_{n+1} - 2f_n + f_{n-1}), \qquad n = 1, 2, \ldots, N, \tag{2.26}$$

which tell us that the acceleration of the nth particle is proportional to the *curvature* of the displacement coordinate around the nth position. In Fig. 2.7 this is manifest: the larger the angle between the $(n-1)-(n)$ and $(n)-(n+1)$ springs, the greater the force and hence the acceleration in the direction of concavity.

2.2.5. Uncoupling and Solution

Equation (2.25) in the φ-*basis* (see Section 1.4) appears simpler than (2.26), since Δ is diagonal there and the component equations uncouple:

$$M\ddot{\tilde{f}}_m - k\lambda_m\tilde{f}_m = 0, \tag{2.27a}$$

$$\lambda_m := -4\sin^2(\pi m/N), \qquad m = 1, 2, \ldots, N. \tag{2.27b}$$

Equations (1.51) relate the *normal* coordinates $\{\tilde{f}_m\}_{m=1}^N$ to the lattice displacements $\{f_n\}_{n=1}^N$. The general solution of Eqs. (2.27) in terms of the $2N$ initial conditions is thus of the oscillatory type [see Eqs. (2.6)–(2.11) for $c, \Gamma = 0$]:

$$\tilde{f}_m(t) = \dot{\tilde{G}}_m(t - t_0)\tilde{f}_m(t_0) + \tilde{G}_m(t - t_0)\dot{\tilde{f}}_m(t_0), \tag{2.28a}$$

$$\tilde{G}_m(\tau) := \omega_m^{-1}\sin\omega_m\tau, \qquad \dot{\tilde{G}}_m(\tau) = \cos\omega_m\tau, \tag{2.28b}$$

$$\omega_m := (-k\lambda_m/M)^{1/2} = 2(k/M)^{1/2}|\sin(\pi m/N)| = \omega_{N-m}, \tag{2.28c}$$

where $\tilde{f}_m(t_0)$ and $\dot{\tilde{f}}_m(t_0)$ are the φ-basis coordinates of the initial displacement and velocity vectors $\mathbf{f}_0 := \mathbf{f}(t_0)$ and $\dot{\mathbf{f}}_0 := \dot{\mathbf{f}}(t_0)$. We have given an apparently redundant absolute value to the last member in (2.28c); this will be seen to be convenient when we exploit the identification $m \equiv n \bmod N$. One case we have "overlooked" is the solution of (2.27) for $m = N$, as there $\lambda_N = 0$ so the Nth normal coordinate is that of a springless "oscillator." This case has been referred to before in Exercise 2.6 and leads to a solution of the type (2.17), i.e.,

$$\tilde{f}_N(t) = \tilde{f}_N(t_0) + (t - t_0)\dot{\tilde{f}}_N(t_0), \tag{2.28d}$$

which can still be correctly incorporated into Eq. (2.28a) since for $\omega_N \to 0$ we have $\tilde{G}_N(\tau) \to \tau$ and $\dot{\tilde{G}}(\tau) \to 1$.

2.2.6. Green's Operator of Time Evolution

The solutions (2.28) can now be integrated back to vector form as

$$\mathbf{f}(t) = \dot{\mathbb{G}}(t - t_0)\mathbf{f}_0 + \mathbb{G}(t - t_0)\dot{\mathbf{f}}_0, \tag{2.29}$$

where $\mathbb{G}(\tau)$ is *Green's operator*, represented in the $\boldsymbol{\varphi}$-basis by the diagonal matrix $\tilde{\mathbf{G}}(\tau) = \|\delta_{mn}\tilde{G}_m(\tau)\|$, and $\dot{\mathbb{G}}(\tau) = d\mathbb{G}(\tau)/d\tau$ similarly. (Recall Exercise 1.29 where $\mathbb{G}$ explicitly denoted the case $c = 0$, $M = 1$, $k = 1$.)

Exercise 2.11. Show that the Green's operator appearing in (2.29) and its time derivative are *self-adjoint* and that they commute with $\mathbb{A}$.

Exercise 2.12. Using the fact that $\mathbf{f}_0$ and $\dot{\mathbf{f}}_0$ in (2.29) are constant, arbitrary vectors, show that Green's operator $\mathbb{G}(\tau)$ satisfies the lattice equation of motion (2.25):

$$M\ddot{\mathbb{G}}(\tau) = k\mathbb{A}\mathbb{G}(\tau). \tag{2.30}$$

Exercise 2.13. Let Eq. (2.29) give the solution at time t in terms of initial conditions at time t_1. The latter, however, may be due to still earlier conditions at some time $t_0 < t_1$. Show that this implies that the Green's operator must satisfy

$$\mathbb{G}(t - t_0) = \dot{\mathbb{G}}(t - t_1)\mathbb{G}(t_1 - t_0) + \mathbb{G}(t - t_1)\dot{\mathbb{G}}(t_1 - t_0), \tag{2.31a}$$

and, in particular, that

$$\mathbb{G}(0) = \mathbb{0}, \qquad \dot{\mathbb{G}}(0) = \mathbb{1}. \tag{2.31b}$$

The subject of time evolution will be taken up in more detail in Section 2.6.

Equation (2.29), written in the $\boldsymbol{\varepsilon}$-basis, will provide us with the solution of the original equation (2.26) for the displacements. Indeed,

$$f_n(t) = \sum_m \dot{G}_{nm}(t - t_0)f_m(t_0) + \sum_m G_{nm}(t - t_0)\dot{f}_m(t_0), \qquad n = 1, 2, \ldots, N, \tag{2.32}$$

where the coefficients are the elements of *Green's operator* in the $\boldsymbol{\varepsilon}$-basis:

$$\begin{aligned} G_{nm}(\tau) &:= (\boldsymbol{\varepsilon}_n, \mathbb{G}(\tau)\boldsymbol{\varepsilon}_m) = [\mathbf{F}\tilde{\mathbf{G}}(\tau)\mathbf{F}^\dagger]_{nm} \\ &= \sum_k F_{nk}\tilde{G}_k(\tau)F^*_{mk} \\ &= N^{-1}\sum_k \omega_k^{-1} \sin \omega_k\tau \exp[2\pi ik(m - n)/N] \\ &= N^{-1}\sum_k \omega_k^{-1} \sin \omega_k\tau \cos[2\pi k(m - n)/N], \end{aligned} \tag{2.33}$$

$$\dot{G}_{nm}(\tau) = N^{-1}\sum_k \cos \omega_k\tau \cos[2\pi k(m - n)/N]. \tag{2.34}$$

Thus, although in working out the solution we slipped into the field $\mathscr{C}$ of complex numbers and unitary transformations, in the end we see that if the

$2N$ initial conditions are real, since $G_{nm}(\tau)$ and $\dot{G}_{nm}(\tau)$ are real functions, the solutions $f_n(t)$ are real, as one should expect.

Exercise 2.14. Verify that the special expression for $\tilde{G}_N(\tau)$ causes no trouble in (2.32)–(2.34) if we take care to make $\omega_N^{-1} \sin \omega_N \tau = \tau$.

2.2.7. Properties of the Green's Operator

The elements of Green's matrix $G_{nm}(\tau)$ in (2.33) and its time derivative (2.34) have several manifest properties: (a) $G_{nm}(\tau)$ and its time derivative are functions of $|n - m|$. This embodies the principle of *reciprocity*: the effect on mass n of a given initial condition at site m is the same as the effect on mass m of that same initial conditions at n. (b) The effect, moreover, depends only on their *relative* distance $|n - m|$, not on their absolute position n or m. In other words, the system is *translationally invariant*: If $\mathbf{f}(t)$ is a solution with initial conditions $\mathbf{f}_0$ and $\dot{\mathbf{f}}_0$, then the translated initial conditions $\mathbb{R}^k\mathbf{f}_0$ and $\mathbb{R}^k\dot{\mathbf{f}}_0$ give rise to the solution $\mathbb{R}^k\mathbf{f}(t)$, as follows from the observation that $\mathbb{R}^k\mathbb{G}(\tau) = \mathbb{G}(\tau)\mathbb{R}^k$. (In the $\boldsymbol{\varphi}$-basis, both operators are represented by diagonal matrices.) (c) Similarly, inversion through $\mathbb{I}_l$ (and $\mathbb{K}_l$ when N is even) of the initial conditions produces a correspondingly inverted solution, as $\mathbb{I}_l$ (and $\mathbb{K}_l$) also commute with the simple lattice Green's operator. The system is correspondingly *invariant under inversions*. We must emphasize in (b) and (c) that translational invariance and inversion invariance refer to the *simple lattice equations of motion* and *time evolution* embodied by $\mathbb{A}$ and $\mathbb{G}(\tau)$, *not* to the *initial conditions*, which may be arbitrary and not at all invariant under $\mathbb{R}^k$ or $\mathbb{I}_l$. These observations *do* imply, however, that *if* a given set of initial conditions has definite symmetry under some operation (as, i.e., $\mathbb{I}_0\mathbf{f}_0 = \sigma\mathbf{f}_0$ and $\mathbb{I}_0\dot{\mathbf{f}}_0 = \sigma\,\dot{\mathbf{f}}_0$, for $\sigma = 1$ or -1), *then* the resulting solution $\mathbf{f}(t)$ will have the same symmetry [i.e., $\mathbb{I}_0\mathbf{f}(t) = \sigma\mathbf{f}(t)$] for all time. We shall have opportunity to use these facts at the end of next section in order to describe lattices with fixed ends.

Exercise 2.15. Prove the preceding statements in detail.

The solution (2.29) to the simple lattice looks neat and compact. It will serve us, however, to dedicate all of Section 2.3 to describing certain particular solutions in the "physical" $\boldsymbol{\varepsilon}$-basis so as to get a firmer understanding of the processes involved. This will be useful when we extend the treatment of this section to more general lattices.

Exercise 2.16. Repeat the analysis of the simple lattice (Fig. 2.5) to include viscous forces. Assuming they are equal for all particles in the lattice and using the results of Section 2.1, prove that the generalization of (2.29) is

$$\mathbf{f}(t) = [\dot{\mathbb{G}}^\Gamma(t - t_0) + 2\Gamma\mathbb{G}^\Gamma(t - t_0)]\mathbf{f}_0 + \mathbb{G}^\Gamma(t - t_0)\dot{\mathbf{f}}_0, \tag{2.35}$$

where the Green's operator $\mathbb{G}^\Gamma(\tau)$ is represented in the φ-basis by a diagonal matrix with elements

$$\tilde{G}_m{}^\Gamma(\tau) = (\omega_m{}^e)^{-1} \exp(-\Gamma\tau) \sin \omega_m{}^e\tau \qquad \text{(oscillatory)}, \tag{2.36}$$

$$\Gamma := c/2M, \qquad \omega_m{}^e := [4(k/M) \sin^2(\pi m/N) - \Gamma^2]^{1/2}, \tag{2.37}$$

and corresponding expressions for the critical and overdamped cases.

Exercise 2.17. Consider the limit when damping is much larger than inertia, so that $c/2M = \Gamma \to \infty$ while c and k remain finite. Refer to Exercise 2.8. In that case, using the overdamped expression for (2.35)–(2.37), show that $\mathbb{G}^\Gamma(\tau)$, $\dot{\mathbb{G}}^\Gamma(\tau) \to \mathbb{0}$. The operator $2\Gamma\mathbb{G}^\Gamma(\tau)$ remains finite, however, and (2.35) becomes

$$\tilde{f}_m(t) = \exp[-4(t - t_0)kc^{-1} \sin^2(\pi m/N)]\tilde{f}_m(t_0), \tag{2.38a}$$

so that $\tilde{f}_m(t)$ and hence $f_n(t)$ stop depending on the initial velocity. The solutions are exponentially damped and correspond to the vector equation

$$\mathbf{f}(t) = \exp[(t - t_0)kc^{-1}\mathbb{\Delta}]\mathbf{f}(t_0). \tag{2.38b}$$

Compare with Eqs. (1.72). The function (2.38a) appears in Fig. 3.5(a).

Exercise 2.18. As a continuation of Exercise 2.17, define the "total heat" of the damped massless lattice as

$$Q := \sum_n f_n. \tag{2.39}$$

Using (2.38b), show that Q at time t is the same as at time t_0. Refer to Exercise 1.28.

2.3. Fundamental Solutions, Normal Modes, and Traveling Waves

The general solution of a coupled system represented by a simple lattice was obtained in Section 2.2. Here we shall filter out the information which is relevant and extendable to more general cases.

2.3.1. Fundamental Solutions

The expression (2.29) for $t_0 = 0$,

$$\mathbf{f}(t) = \dot{\mathbb{G}}(t)\mathbf{f}_0 + \mathbb{G}(t)\dot{\mathbf{f}}_0, \tag{2.40}$$

gives the state vector for the lattice at time t in terms of the initial displacements $\mathbf{f}_0$ and velocities $\dot{\mathbf{f}}_0$. Assume the lattice starts from rest ($\dot{\mathbf{f}}_0 = \mathbf{0}$) with the mth mass displaced by one unit ($\mathbf{f}_0 = \boldsymbol{\varepsilon}_m$). The ensuing time development of the lattice is then given by the state vector

$$\dot{\boldsymbol{\varepsilon}}^m(t) := \dot{\mathbb{G}}(t)\boldsymbol{\varepsilon}_m \tag{2.41a}$$

with components

$$\dot{\varepsilon}_n{}^m(t) = (\boldsymbol{\varepsilon}_n, \dot{\boldsymbol{\varepsilon}}^m(t)) = \dot{G}_{nm}(t), \qquad n = 1, 2, \ldots, N, \tag{2.41b}$$

given explicitly by Eq. (2.34). Assume now that the initial condition of the lattice is $\mathbf{f}_0 = \mathbf{0}, \dot{\mathbf{f}}_0 = \boldsymbol{\varepsilon}_m$, i.e., the mth mass is moving through its equilibrium position with unit velocity. The corresponding solution state vector is

$$\boldsymbol{\varepsilon}^m(t) := \mathbb{G}(t)\boldsymbol{\varepsilon}_m \tag{2.42a}$$

with components

$$\varepsilon_n{}^m(t) = \big(\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}^m(t)\big) = G_{nm}(t), \qquad n = 1, 2, \ldots, N \tag{2.42b}$$

[see Eqs. (2.33)]. We shall refer to (2.41) and (2.42) as the *fundamental solutions* of the N-point lattice. In Figs. 2.8(a) and (b) we have drawn the solutions (2.41) and (2.42) for fixed m. The most general initial condition $\mathbf{f}_0 = \sum_m f_m \boldsymbol{\varepsilon}_m$, $\dot{\mathbf{f}}_0 = \sum_m \dot{f}_m \boldsymbol{\varepsilon}_m$ will then give rise to a state vector

$$\mathbf{f}(t) = \sum_m f_m \dot{\boldsymbol{\varepsilon}}^m(t) + \sum_m \dot{f}_m \boldsymbol{\varepsilon}^m(t), \tag{2.43}$$

which is a *superposition* of the fundamental solutions (2.41) and (2.42). Note that there are $2N$ *parameters* in (2.43): N for the components of $\mathbf{f}_0$ and N for those of $\dot{\mathbf{f}}_0$. The set of solutions (2.43) thus fit a $2N$-dimensional vector space which will be seen in Section 2.6 to be the *phase space* of the system. Meanwhile, we shall only point to the fact that there are $2N$ independent solutions for the N-particle lattice and that the most general solution can be expressed as a linear combination of them.

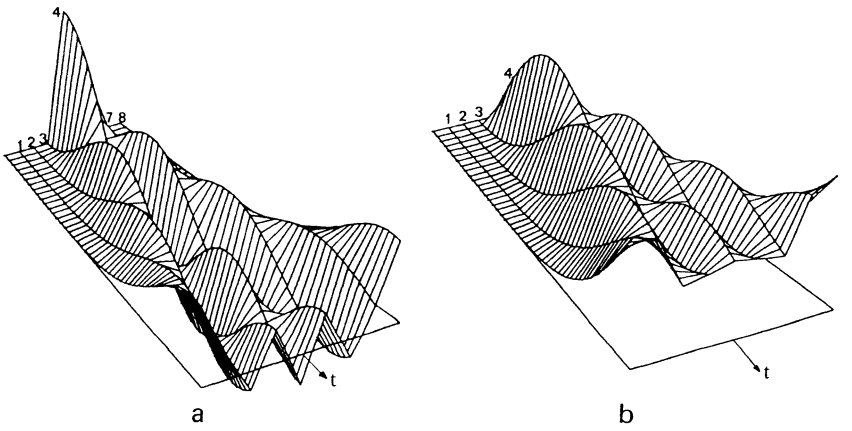


Fig. 2.8. Fundamental solutions for the eight-mass linear closed lattice. (a) The fourth mass starts with unit elongation, and (b) the fourth mass starts with unit velocity. All other fundamental solutions are translated versions of these, numbered modulo 8. Note that for small t a "propagation velocity" for the disturbance can be seen and loosely defined. As the spring mass is zero, however, every mass in the lattice feels the disturbance instantaneously. (Refer to the discussion in Section 5.3 for the infinite lattice.)

Exercise 2.19. Show that the set of fundamental solutions is *not* orthonormal for all t. Green's operator is self-adjoint but *not* unitary.

2.3.2. A Real Orthonormal Basis

Figures 2.8(a) and (b) are neat, but the information they contain is quite structureless. Since the uncoupling of the lattice equations in Section 2.2 was the key step in solving the system and the solutions were those of single harmonic oscillators, we should be asking for fundamental solutions in the $\mathbb{G}$-basis, that is, for the time development of initial conditions given by $\mathbf{f}_0 = \boldsymbol{\varphi}_m$ and/or $\dot{\mathbf{f}}_0 = \dot{\boldsymbol{\varphi}}_{m'}$. The solutions due to such initial conditions would be complex, however, since from (1.52), $(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_m) = F_{mn}$. To have *real* initial conditions still associated with the $\boldsymbol{\varphi}$-basis, we can use the set of vectors $\boldsymbol{\varphi}_m{}^{\pm}$ defined in (1.115), which we write compactly as

$$\boldsymbol{\varphi}_m{}^{\pm} = \xi_m{}^{\pm} 2^{-1/2}(\boldsymbol{\varphi}_m \pm \boldsymbol{\varphi}_{-m}), \quad m = 0, 1, \ldots, \begin{cases} \tfrac{1}{2}(N-1), & N \text{ odd}, \\ N/2, & N \text{ even}, \end{cases} \tag{2.44a}$$

where we use here and below the convention that the subscripts are considered modulo N, and

$$\begin{aligned} &\xi_m{}^{-} = i, \quad \text{except } \xi_0{}^{-} = 0, \\ &\xi_m{}^{+} = 1, \quad \text{except } \xi_0{}^{+} = 2^{-1/2}, \quad \text{and, when } N \text{ even}, \quad \xi_{N/2}^{+} = 2^{-1/2}. \end{aligned} \tag{2.44b}$$

These vectors also constitute an *orthonormal* basis (see Exercise 1.50), which we shall call the $\boldsymbol{\varphi}^{\pm}$-*basis* for short.

Exercise 2.20. Show that the vectors (1.115) have *real* coordinates in the original $\boldsymbol{\varepsilon}$-basis:

$$(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_m{}^{+}) = \xi_m{}^{+}(N/2)^{-1/2} \cos(2\pi mn/N), \tag{2.45a}$$

$$(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_m{}^{-}) = (N/2)^{-1/2} \sin(2\pi mn/N). \tag{2.45b}$$

Note that $(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_0{}^{+}) = N^{-1/2}$ and $(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_{N/2}^{+}) = N^{-1/2}(-1)^n$.

2.3.3. Normal Modes

We define state vectors analogous to (2.41)–(2.42) whose initial displacements or velocities at $t_0 = 0$ are the vectors of the $\boldsymbol{\varphi}^{\pm}$-basis:

$$\dot{\boldsymbol{\varphi}}^{m\pm}(t) \coloneqq \dot{\mathbb{G}}(t)\boldsymbol{\varphi}_m{}^{\pm}, \tag{2.46a}$$

$$\boldsymbol{\varphi}^{m\pm}(t) \coloneqq \mathbb{G}(t)\boldsymbol{\varphi}_m{}^{\pm}. \tag{2.46b}$$

Solutions (2.46a) start from rest with maximum displacement, while (2.46b) start with the lattice moving through the equilibrium shape. We can find the form of the lattice vibrations represented by (2.46) by calculating

$$\begin{aligned} \dot{\varphi}_n^{m\pm}(t) &= \left(\boldsymbol{\varepsilon}_n, \dot{\boldsymbol{\varphi}}^{m\pm}(t)\right) = \sum_k (\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_k)\left(\boldsymbol{\varphi}_k, \dot{\mathbb{G}}(t)\boldsymbol{\varphi}_m{}^{\pm}\right) \\ &= \xi_m{}^{\pm} 2^{-1/2}[F_{nm}\dot{\bar{G}}_m(t) \pm F_{n,-m}\dot{\bar{G}}_{-m}(t)] \end{aligned} \tag{2.47}$$

and similarly for $\varphi_n^{m\pm}(t)$. Now $F_{n,-m} = F_{mn}^*$, and from (2.28b) and (2.28c) we can see that $\tilde{G}_m = \tilde{G}_{-m}$ and similarly for its time derivative. Hence, after a short calculation the lattice solutions (2.46) are obtained as

$$\varphi_n^{m+}(t) = \xi_m{}^+(2/N)^{1/2} \cos(2\pi nm/N) \cos \omega_m t, \tag{2.48a}$$

$$\varphi_n^{m-}(t) = (2/N)^{1/2} \sin(2\pi nm/N) \cos \omega_m t, \tag{2.48b}$$

$$\varphi_n^{m+}(t) = \xi_m{}^+(2/N)^{1/2} \cos(2\pi nm/N)\omega_m^{-1} \sin \omega_m t, \tag{2.48c}$$

$$\varphi_n^{m-}(t) = (2/N)^{1/2} \sin(2\pi nm/N)\omega_m^{-1} \sin \omega_m t. \tag{2.48d}$$

These have been plotted in Fig. 2.9. In spite of the small complication of the ξ's and the apparent proliferation of indices, the picturing of the solutions—the *normal modes* of the system—is rather simple: they are *standing waves* of the lattice. They are also *separated* functions of n and t; that is, they have the form $\varphi_n(t) = \nu(n)\tau(t)$, the waveform $\nu(n)$ being *modulated* by an oscillating function $\tau(t)$.

Exercise 2.21. Check that there are indeed $2N$ different normal modes in Eqs. (2.48).

Exercise 2.22. Verify that

$$\ddot{\boldsymbol{\varphi}}^{m\pm}(t) = -\omega_m{}^2\boldsymbol{\varphi}^{m\pm}(t). \tag{2.49}$$

Exercise 2.23. Suppose we had started with the N lattice equations of motion (2.26) and *assumed* that the solutions $f_n(t)$ were separable functions $\nu(n)\tau(t)$. Substituting this ansatz into (2.26) and following the usual procedure of separation of variables, show that one arrives at $\tau(t) = c \exp(i\omega t)$, where the $-\omega^2$ are the separation constants, which are solutions of the eigenvalues problem $k\Delta\boldsymbol{\nu} = -M\omega^2\boldsymbol{\nu}$. If this is solved and linear combinations taken to ensure the reality of the solutions, Eqs. (2.48) will be obtained.

2.3.4. The Brillouin Angular Frequency Diagram

The most general initial condition of a vibrating lattice, in the same form as (2.43), can be expanded in the $\boldsymbol{\varphi}^{\pm}$-basis for displacements and velocities with coefficients $f_m{}^{\pm}$ and $\dot{f}_m{}^{\pm}$, respectively [m and $\pm$ taking the values allowed by (2.44)], giving rise to a state vector

$$\mathbf{f}(t) = \sum_{m,\pm} f_m{}^{\pm}\dot{\boldsymbol{\varphi}}^{m\pm}(t) + \sum_{m,\pm} \dot{f}_m{}^{\pm}\boldsymbol{\varphi}^{m\pm}(t). \tag{2.50}$$

In the form (2.50), the solution $\mathbf{f}(t)$ is decomposed into sinusoidal waves such as those in Fig. 2.9, each set of $\boldsymbol{\varphi}$'s with the same value of m vibrating with its own angular velocity ω_m [Eq. (2.28c)]. The $\boldsymbol{\varphi}^m$'s are one-quarter period behind the $\dot{\boldsymbol{\varphi}}^m$'s so they represent essentially the same waveform of the lattice. A very handy representation of the allowed angular frequencies ω_m, very much used

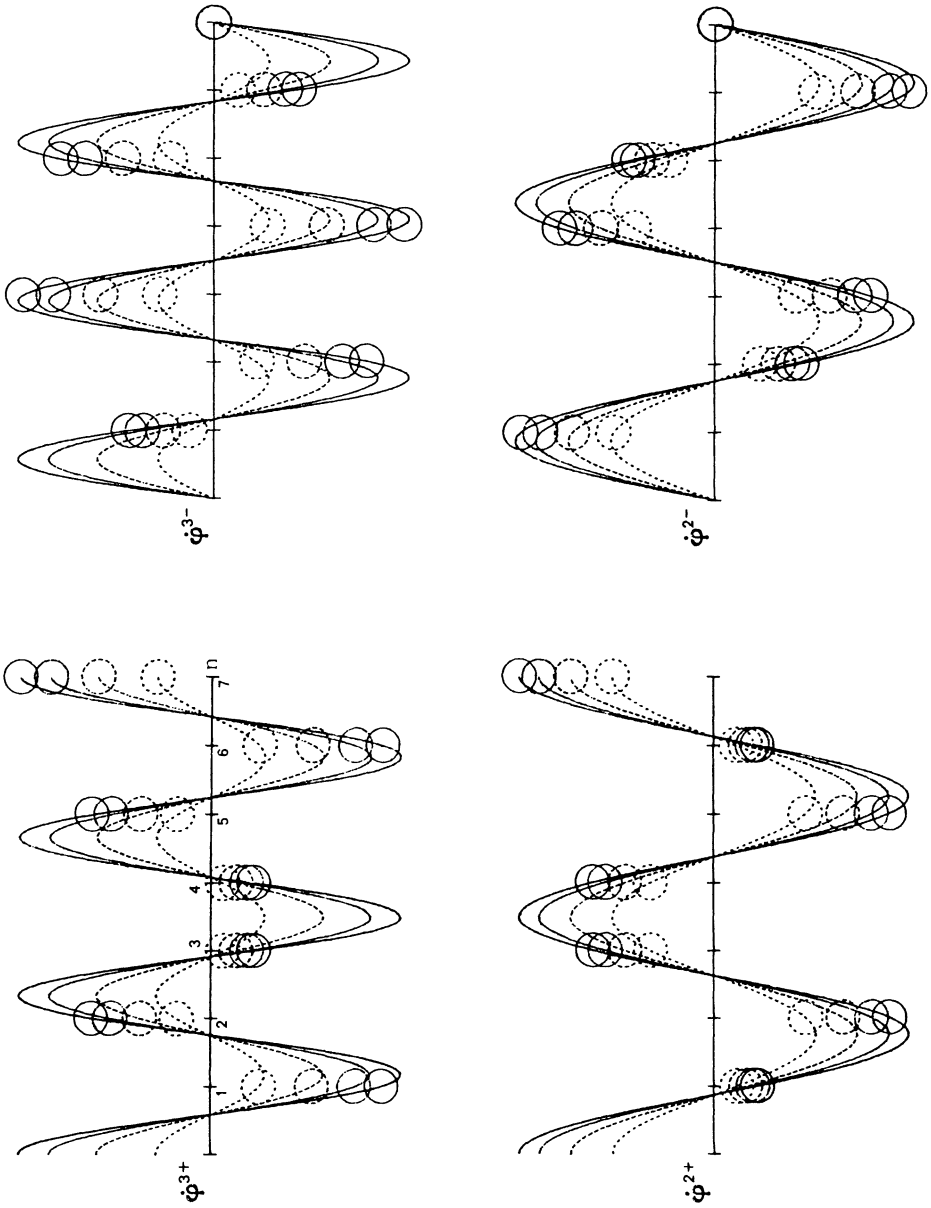

n
7
6
5
4
3
2
1

Fig. 2.9. Normal modes $\varphi^{m\pm}$ and φ^{0} (standing waves) for a seven-mass lattice. The lattice shape has been plotted for real n between 0 and 7, actual masses being indicated by circles. Dotted lines and circles refer to subsequent time snapshots spaced by $\frac{1}{8}$ [in units of $(M/k)^{1/2}$]. It is seen that higher-m waves entail an average higher velocity for the masses. The $\varphi^{m\pm}$ normal modes are similar to the ones depicted in the figures, but they start with zero elongation. The zeroth mode describes undeformed rotation for the whole lattice.

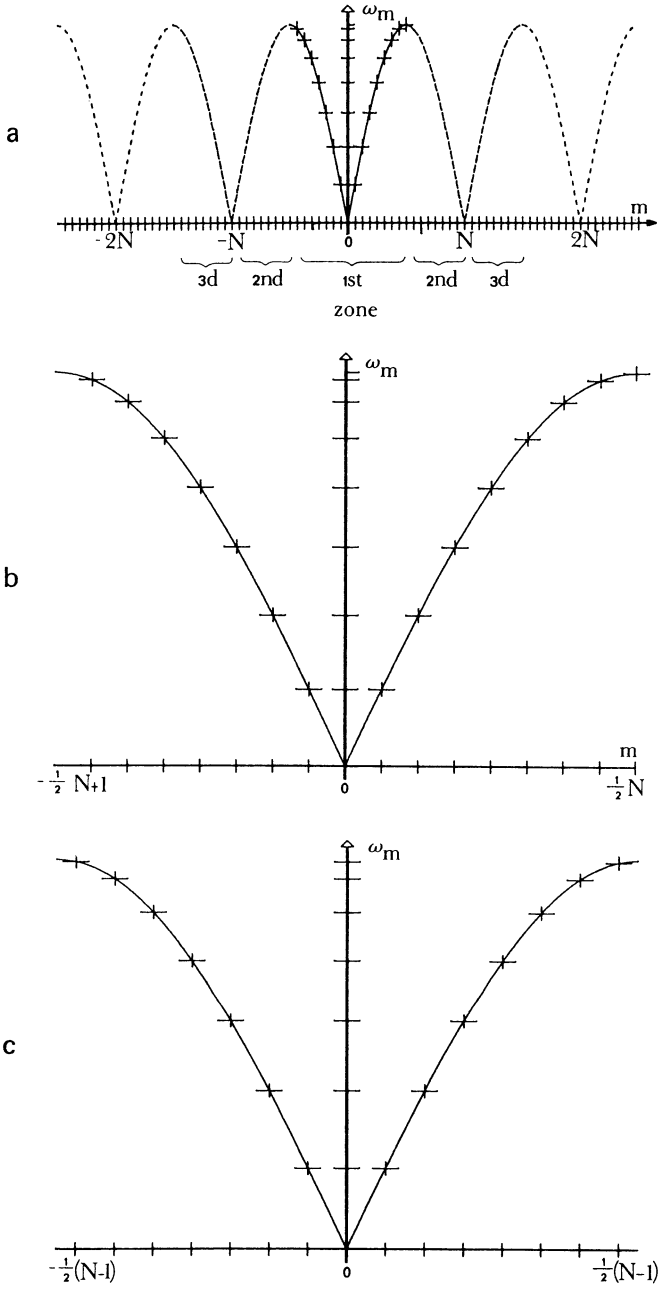


Fig. 2.10. Brillouin frequency diagram plotting the angular frequency ω_m as a function of m: (a) the repeating Brillouin zones; (b) and (c) the central (first) zone for N even and odd. Crosses mark the integer-m allowed frequencies. Note that all ω_m's are doubly degenerate (for $\omega_{\pm m}$) except for ω_0, and, if N is even, $\omega_{N/2}$. This is the difference between (b) and (c).

in solid-state physics, is the *Brillouin* diagram, Fig. 2.10, which plots the ω_m of $\varphi^{m\pm}$ as a function of $\pm m$, taking the interval in m to be centered around $m = 0$. The *first Brillouin zone* for odd $N = 2\nu + 1$ extends over $m = -\nu, -\nu + 1, \ldots, -1, 0, 1, \ldots, \nu - 1, \nu$. When $N = 2\nu'$ is even, it extends over $m = -\nu' + 1, \ldots, -1, 0, 1, \ldots, \nu' - 1, \nu'$. Beyond the ends of these intervals are the second, third, etc., Brillouin zones, which in the case of a one-dimensional lattice are equivalent to the first one. Except for $m = 0$ and $N/2$ (if N is even), two values $\pm m$ correspond to the same value of ω_m, the angular frequency.

Exercise 2.24. Refer to Section 1.7 and note that the $\varphi^{m\pm}(t)$ solutions have *definite parity* under $\mathbb{I}_0$, i.e.,

$$\mathbb{I}_0\varphi^{m\pm}(t) = \pm\varphi^{m\pm}(t) \tag{2.51}$$

for all t. Note that instead of the $\varphi^{\pm}$-basis vectors we could have used any of the eigenbases of $\mathbb{A}$ and $\mathbb{I}_l$ as given in (1.118) and still obtained real solutions. The sine—and cosine—functions of n would have their arguments displaced by $2\pi ln/N$.

2.3.5. Periods and Wavelengths

The period of each set of φ^m's is

$$T_m := 2\pi/\omega_m := (M/k)^{1/2}\pi/|\sin(\pi m/N)|. \tag{2.52}$$

As these periods are in general incommensurable, there will be no periodicity of the total solution $\mathbf{f}(t)$. The normal modes or combinations of the same m-set are the only time-periodic solutions of the vibrating lattice. A representation similar to the Brillouin diagram is shown in Fig. 2.11. Regarding

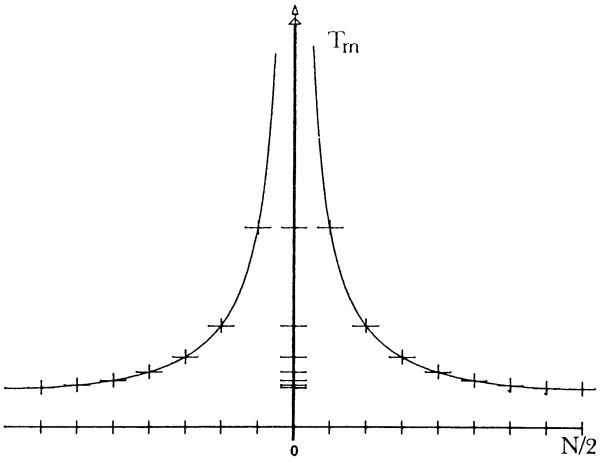


Fig. 2.11. Brillouin diagram for oscillation periods.

the wavelength in units of interparticle separation, it can be seen from (2.48) to be

$$\lambda_m = N/m, \tag{2.53}$$

i.e., there are m wavelengths in the lattice circle. In Fig. 2.12 we plot (2.53) in the Brillouin manner, although λ_m is not a periodic function of m. Had we decided to take $N/(m + N)$, $N/(m \pm 2N)$, etc., we would have been left with the same description of the discrete lattice points; see Fig. 2.13. Some observations on particular normal modes are the following: (a) When N is even, $\varphi^{N/2+}(t)$ and its time derivative [no $\varphi^{N/2-}(t)$ exists] have the largest angular frequency, $\omega_{N/2} = 2(k/M)^{1/2}$, and the smallest period, $T_{N/2} = \pi(M/k)^{1/2}$. The lattice vibrates in such a way that each mass moves in a sense opposite to that of its first neighbors and carries the smallest wavelength: $\lambda_{N/2} = 2$ interparticle separations. (b) When N is odd, the highest frequency corresponds to $m = \pm(N - 1)/2$, as shown in Fig. 2.10. Again, they have the smallest period and wavelength. (c) The "normal mode" $m = 0$ is a bit of a fraud since it does not oscillate at all. Formally, for $\omega_0 = \omega_N$ we had set $(\omega_0)^{-1} \sin \omega_0 t = t$, so, as drawn in Fig. 2.9, $\varphi^0(t) = N^{-1/2}t$, $\dot{\varphi}^0(t) = N^{-1/2}$. It represents a uniform displacement of the full lattice, which by itself is not too interesting. The period and wavelength turn out to be infinite.

Exercise 2.25. When the lattice has an even number of masses one can define an eigenbasis of the $\mathbb{K}_0$ operator proposed in Exercise 1.54 as suggested in (2.51) for $\mathbb{I}_0$—or any $\mathbb{K}_l$ as generalized in Exercise 2.24. Explore the possibilities in this direction. These will be used at the end of this section.

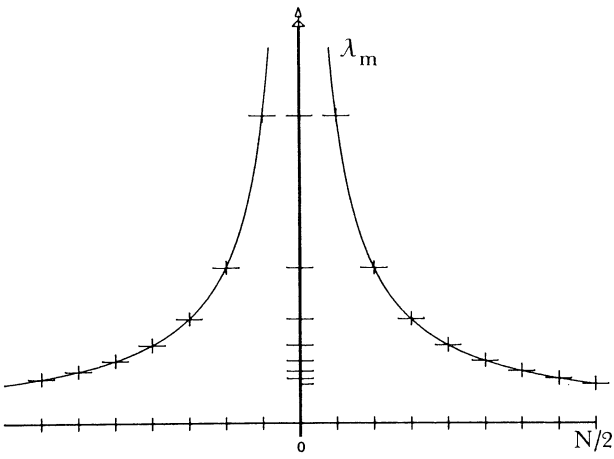


Fig. 2.12. Brillouin diagram for wavelengths.

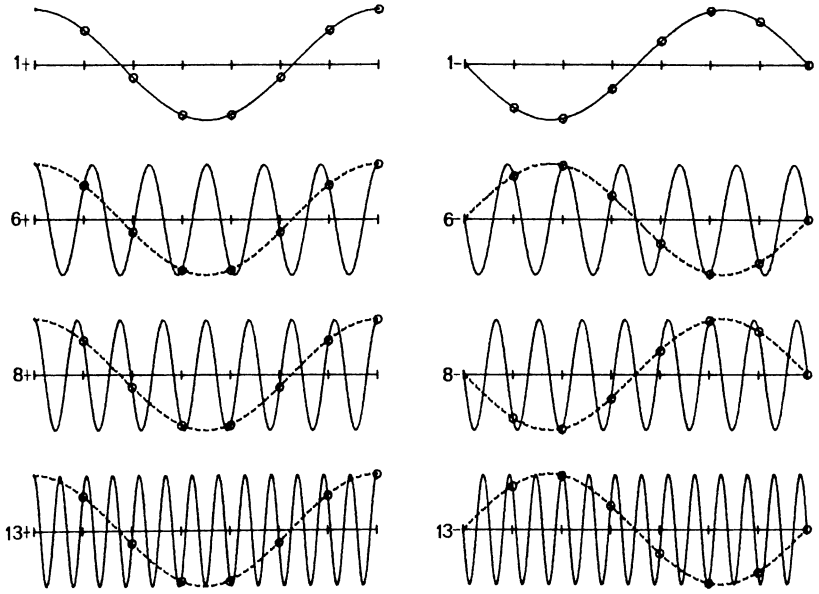


Fig. 2.13. Multiple wavelength degeneracy: $\varphi^{m\pm}$, $\varphi^{N+m\pm}$, ... and $\varphi^{-m\pm}$, $\varphi^{N-m\pm}$, ... describe the same state for the actual lattice masses. All the relevant information is thus contained in the first Brillouin zone.

2.3.6. Traveling Waves

In exploring the fundamental solutions and the normal modes we examined situations in which the initial conditions were either nonzero displacements or nonzero velocities. There is a third set of interesting solutions, *traveling waves*, where both sets of initial conditions are nonzero albeit correlated. From the trigonometric functions appearing in the normal modes (2.48) we can see interesting combinations. Let

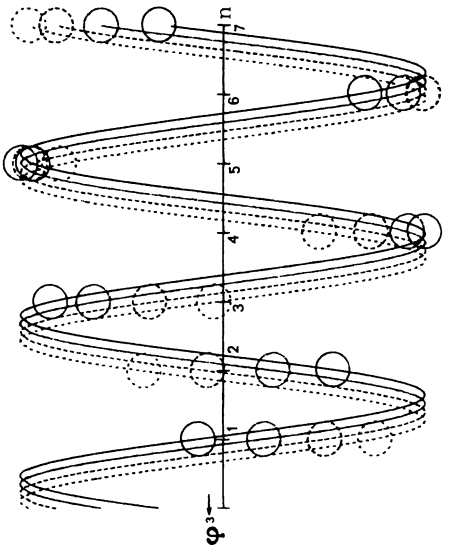
$$\varphi^{m\rightleftarrows}(t) \coloneqq (\omega_m)^{-1}\dot{\varphi}^{m-}(t) \mp \varphi^{m+}(t), \tag{2.54a}$$

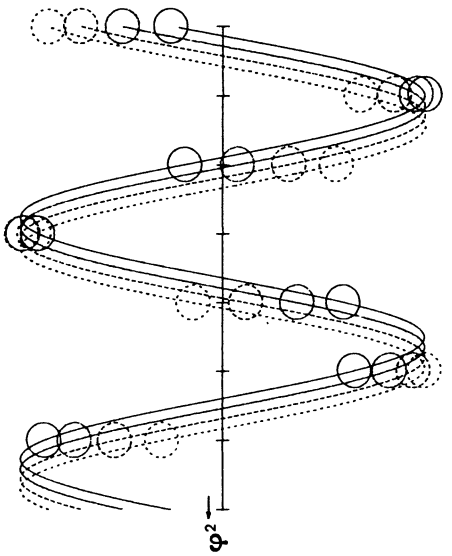
$$\dot{\varphi}^{m\rightleftarrows}(t) \coloneqq \mp\dot{\varphi}^{m+}(t) + \omega_m\varphi^{m-}(t), \tag{2.54b}$$

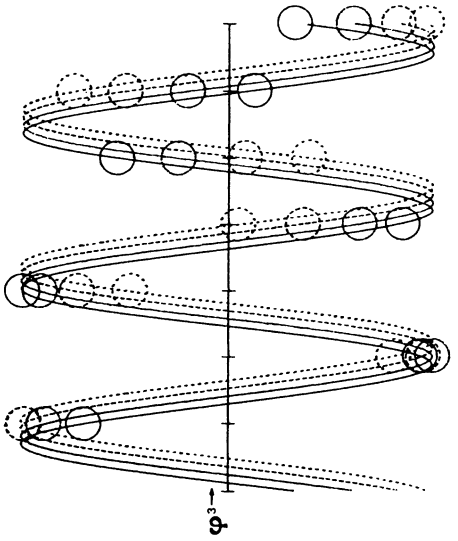
where the ranges of m and $\rightleftarrows$ will be detailed below. The lattice vibrations described by these state vectors (which are solutions of the lattice since the $\varphi^{m\pm}$'s are too) are given by their coordinates in the ε-basis, which can easily be found from (2.48):

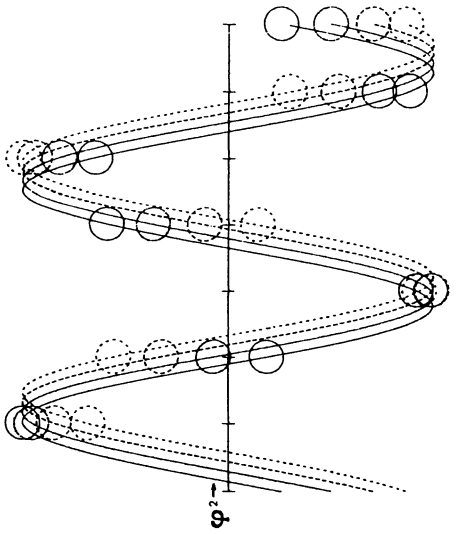
$$\varphi_n^{m\rightleftarrows}(t) = \xi_m{}^{+}(2/N)^{1/2}(\omega_m)^{-1}\sin(2\pi nm/N \mp \omega_m t), \tag{2.55a}$$

$$\dot{\varphi}_n^{m\rightleftarrows}(t) = \mp\xi_m{}^{+}(2/N)^{1/2}\cos(2\pi nm/N \mp \omega_m t). \tag{2.55b}$$









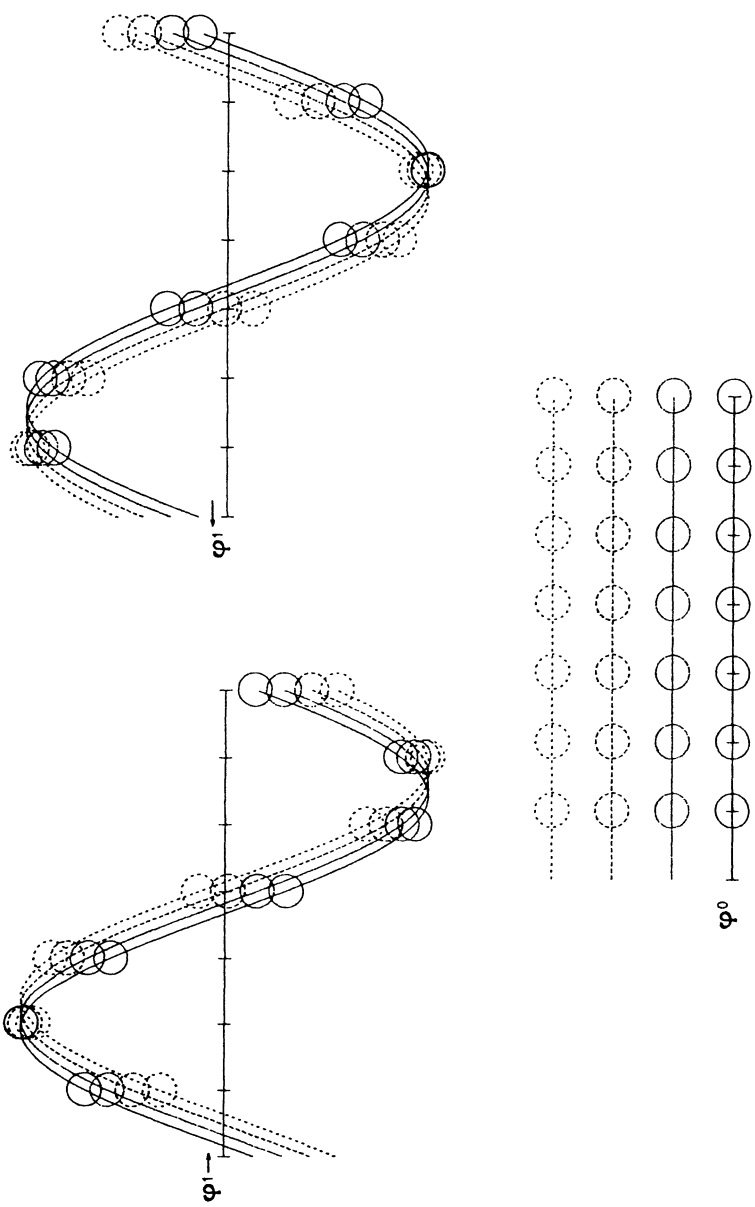


Fig. 2.14. Traveling waves for a seven-mass lattice. As in Fig. 2.9 the lattice shape has been plotted for real n, dotting subsequent time snapshots spaced by $\frac{1}{8}$ [in units of $(M/k)^{1/2}$]. It can be seen that in $\varphi^{m\rightleftarrows}$ the higher values of m entail a greater average movement of the actual masses, although their wave velocity is smaller.

The dependence of $\varphi_n^{m\rightleftarrows}$ on n and t is in the form $2\pi nm/N \mp \omega_m t$, i.e., it is *constant* for

$$n = \pm N\omega_m t/2\pi m. \tag{2.56}$$

With advancing time, the sinusoidal lattice shape represented by $\varphi_n^{m\rightleftarrows}(t)$ will shift to the right and left, respectively, thus describing a right- or left-moving waveform. See Fig. 2.14.

2.3.7. Propagation Velocity

The velocity of this traveling wave is, from (2.56),

$$v_m^{\rightleftarrows} = \pm N\omega_m/2\pi m \tag{2.57}$$

in units of interparticle separation per unit time. The wavelength of the traveling waves is still (2.53), as this is the characteristic of the m-set of states. In Fig. 2.15 we have plotted à la Brillouin the absolute value of the velocities (2.57) as a function of m. This will also clarify the ranges and "extreme" cases of the indices m and $\rightleftarrows$ in (2.54)–(2.55). (a) When N is even, we saw that only $\boldsymbol{\varphi}^{N/2+}$ existed, so here we conclude that $\boldsymbol{\varphi}^{N/2\rightarrow} = -\boldsymbol{\varphi}^{N/2\leftarrow}$. Inspection of (2.55) for this case shows that this "traveling" wave has no definite *sense* of motion, although its velocity (2.57) is $v_{N/2} = 2(k/M)^{1/2}/\pi$. It is the slowest of the waves. (b) When N is odd, the slowest waves correspond to $m = (N-1)/2$. For all other m's down to $m = 1$ both left- and right-traveling waves exist until (c) for $m = 0$, $\boldsymbol{\varphi}^{0\leftarrow} = -\boldsymbol{\varphi}^{0\rightarrow} = \boldsymbol{\varphi}^{0+}$. Again this "wave"

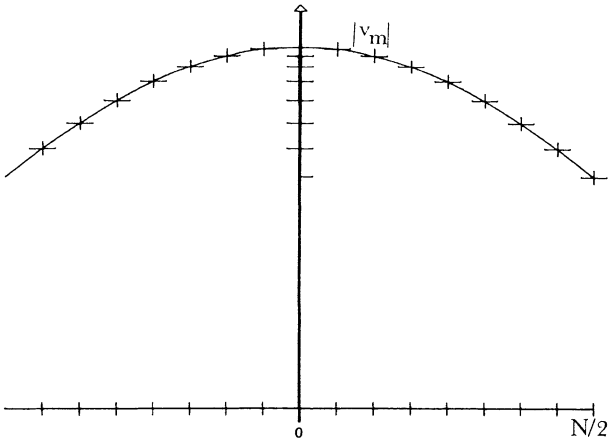


Fig. 2.15. Brillouin diagram for velocities.

is a freak, as it has no sense of motion, although it defines an upper limit for propagation velocities in the lattice. From (2.28c) and for $m \to 0$ this is

$$v_0 = (k/M)^{1/2} \tag{2.58}$$

in units of interparticle separation. Note that this quantity depends only on the lattice parameters of mass and spring.

Exercise 2.26. Show that the traveling waves satisfy

$$\frac{\partial}{\partial t}\boldsymbol{\varphi}^{m\rightleftarrows} = \pm\sigma\omega_m \mathbb{R}^{\sigma N/4m}, \qquad \sigma = \pm 1. \tag{2.59}$$

These are the "square roots" of the second-order differential equation (2.49). Are there "square root" forms for the lattice equation of motion (2.25) for solutions consisting only of right-moving (or left-moving) waves? Why not?

2.3.8. Initial Conditions and Dispersion

Again, the most general state vector describing the lattice can be written in terms of traveling waves as

$$\mathbf{f}(t) = \sum_{m,\rightleftarrows} f_m{}^{\rightleftarrows}\dot{\boldsymbol{\varphi}}^{m\rightleftarrows}(t) + \sum_{m,\rightleftarrows} \dot{\mathbf{f}}_m{}^{\rightleftarrows}\boldsymbol{\varphi}^{m\rightleftarrows}(t). \tag{2.60}$$

This is the analogue of Eqs. (2.43) and (2.50) for the traveling wave $\boldsymbol{\varphi}^{\rightleftarrows}$-*basis*.

Exercise 2.27. Find explicitly the linear combination coefficients in (2.60) in terms of the initial displacements and velocities of the lattice points.

For any set of linear combination constants, Eq. (2.60) tells us that any vibration state of the lattice can be decomposed into $2N$ traveling waves. As each $m^{\rightleftarrows}$-set of waves travels with its own velocity (2.57), any initial shape of the lattice, even if it is composed only of waves traveling in one direction, will be changed: different constituent waves travel with different velocities. A discrete lattice therefore cannot carry definite "signals" other than pure sinusoidal forms, as their shape is eventually lost. Such media are called *dispersive*.

2.3.9. Lattice Models for Dispersive Media

Since crystals are physical systems modeled by lattices with a very large number of masses N, one can ask how and when the dispersion of signals appears. Note that the velocity diagram, Fig. 2.15, has the same shape for all N, except for the "actual" points corresponding to integer values of m, which come closer together as N increases. The curve v_m, for very small values of m/N, can be approximated by the constant v_0 in Eq. (2.58). If our

signal is composed only of low-m partial waves, whose wavelengths are very much larger than the interparticle separation in the lattice, the signal will propagate, to a good approximation, with no loss of shape, as all constituent waves have the same propagation velocity. In this *linear approximation*, dispersion is absent. The dispersion of signals—mechanical or electromagnetic—gives some information of the "granularity" of the medium. This statement still holds (with the appropriate adaptations) even when the "microscopic" model of a system which "in the large" satisfies the wave equation is not that of a vibrating lattice. Sound propagation in gases or amorphous materials, for instance, can rely on different microscopic models.

As the preceding discussion may suggest, when a mechanical lattice is proposed as a microscopic model for a system, the relevant information is mostly that of the spectrum of oscillation frequencies, transmittable wavelengths, and the like. There is little experimental content in specifying arbitrary initial conditions or following the vibration of individual atoms. In this sense, the Brillouin diagram and its three-dimensional version for various crystalline lattices contain much information, and accordingly we shall time and again cast our results in these terms.

Exercise 2.28. Assume the lattice is damped. Follow the discussion in this section for this case. Note that little is changed except for the fact that the oscillation frequencies ω_m become complex. Generally, there will be overdamped as well as oscillatory solutions, the former ones for small values of m and the latter ones for large m's.

Exercise 2.29. Consider a one-dimensional lattice with *fixed ends*. This can mean that the first and last masses are held fixed [Fig. 2.16(a)] or that the midpoints of two springs are constrained [Fig. 2.16(b)]. Show that the "method of images" appears as a natural way to phrase the problem: Assume that a free N-point lattice (N even) has initial conditions which are *odd* under inversions through $\mathbb{I}_0$ or $\mathbb{K}_0$, as then, for all t, the resulting state vector $\mathbf{f}(t)$ will have the same property. If $\mathbb{I}_0\mathbf{f}(t) = -\mathbf{f}(t)$, masses N and $N/2$ are fixed, while if $\mathbb{K}_0\mathbf{f}(t) = -\mathbf{f}(t)$, the midpoint of the springs joining the mass pairs $(N,1)$ and $(\frac{1}{2}N, \frac{1}{2}N - 1)$ pass through the equilibrium position. The actual lattice (Fig. 2.16) is one-half of the proposed free lattice.

Exercise 2.30. Examine the allowed normal modes which can be present in the above "extended" lattice: In Eq. (2.50) only f_m^- and $\dot{f}_m^-$ can be nonzero for Fig. 2.16(a) and analogously (see Exercise 2.24) for the lattice in Fig. 2.16(b). In terms of traveling waves, show that only combinations of $\varphi^{m\rightarrow} + \varphi^{m\leftarrow}$ are allowed to appear in the former. What about the corresponding combinations in the latter?

Exercise 2.31. What happens with the Brillouin and similar diagrams for the lattice with fixed ends? Show that over the "physical" half-lattice orthogonality and completeness for the odd modes still hold.

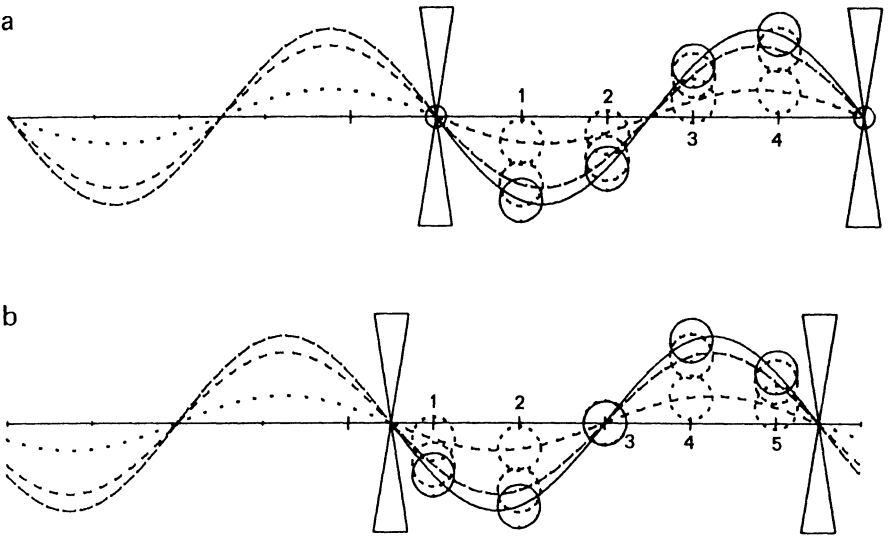


Fig. 2.16. Lattices with two fixed (a) masses, (b) string midpoints. These can be accommodated into a lattice with double the number of masses with restrictions on the allowed vibration modes. Half of the lattice will serve as a "negative mirror image" of the original.

Exercise 2.32. We can consider lattices where the two endpoints are *free*. See that this is well represented, as before, by a closed lattice whose state vectors are *even* under reflection by $\mathbb{I}_0$. A similar analysis follows.

In this part we have for generality concentrated on the description of closed lattices and relegated the study of the fixed-endpoint system to the foregoing exercises. In Part II, the study of the vibrating string will be done almost exclusively on the fixed-endpoint problem.

2.4. Farther-Neighbor Interaction, Molecular and Diatomic Lattices

The concepts developed in Section 2.3 for the simple lattice with only first-neighbor interactions and equal springs and masses will be applied now to systems where each one of these restrictions in turn is lifted in order to examine the features which characterize these extensions.

2.4.1. Farther-Neighbor Interaction and Uncoupling

Lattices with farther-than-first-neighbor interactions (see Fig. 2.17) are certainly relevant in crystallography where the interaction between the

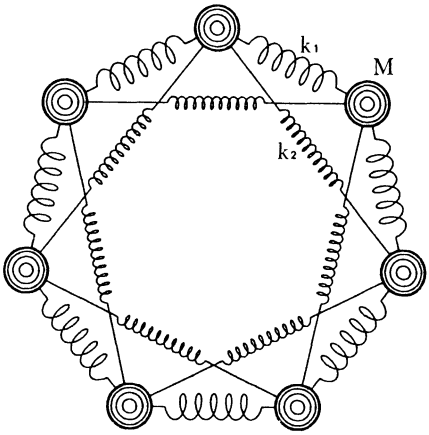


Fig. 2.17. Mechanical model of a linear, closed lattice with first- and second-neighbor interactions.

lattice atoms is electromagnetic and a first-neighbor "spring" model is at best only a good approximation. When describing the interaction term in the lattice equation of motion [Eqs. (2.19)–(2.22)] we allowed for pth neighbor forces through springs of Hooke's constant $k_{n,n\pm p}$ and noted only that $k_{nm} = k_{mn}$ is the requirement of action–reaction equality. Here we shall restrict the lattice to have the same Hooke's constant between all pth neighbors (as shown in Fig. 2.17 for $p = 1$ and $p = 2$) so that $k_p := k_{n,n\pm p}$ is independent of n. The simple lattice has only $k_1 \neq 0$, while in the general case we can consider k_p for p from zero (each mass attached to its equilibrium position by a spring k_0) up to $p = \pi(N)$ [$\pi(N) := (N-1)/2$ for N odd, and $\pi(N) = N/2$ for N even, taking care to note that in this case *two* springs $k_{N/2}$ join opposite masses]. In this general case, the interaction operator $\mathbb{K}$ of Eq. (2.21) is represented in the $\boldsymbol{\varepsilon}$-basis by a matrix $\mathbf{K}$ with elements

$$\kappa_{nm} = -k_{|n-m|} + 2\delta_{nm} \sum_{p=0}^{\pi(N)} k_p. \tag{2.61}$$

[See Eq. (2.19), recalling that row and column indices are taken modulo N.] The matrix $\mathbf{K}$ therefore has entries $k_0' := k_0 + 2\sum_{p=1}^{\pi(N)} k_p$ along the main diagonal and $-k_p$ on diagonals p units on both sides of the main one. For representation purposes it is convenient to write $\mathbf{K}$ in terms of the dihedral matrix representatives [Eq. (1.88)] as

$$\mathbf{K} = k_0'\mathbf{1} - \sum_{p=1}^{\pi(N)} k_p(\mathbf{R}^p + \mathbf{R}^{-p}) \tag{2.62}$$

and correspondingly for the operators themselves. In this way, it is easily

seen that $\mathbb{K}$ is represented by a diagonal matrix in the φ-basis, since the $\mathbb{R}$'s are so represented [Eq. (1.91)]. Quite simply, then,

$$\begin{aligned}\tilde{K}_{mn} &= \delta_{mn}\left\{k_0' - \sum_{p=1}^{\pi(N)} k_p[\exp(2\pi ipm/N) + \exp(-2\pi ipm/N)]\right\} \\ &= \delta_{mn}\left[k_0' - 2\sum_{p=1}^{\pi(N)} k_p \cos(2\pi pm/N)\right] \\ &= \delta_{mn}\left[k_0 + 4\sum_{p=1}^{\pi(N)} k_p \sin^2(\pi pm/N)\right] =: \delta_{mn}\kappa_m. \end{aligned} \tag{2.63}$$

2.4.2. Brillouin Frequency Diagram

The lattice then uncouples into N oscillators with constants $\kappa_m := \tilde{K}_{mm}$ [Eq. (2.22)], and the allowed oscillation frequencies of the system are given by

$$\omega_m = (\kappa_m/M)^{1/2} = 2\left[k_0/4M + \sum_{p=1}^{\pi(N)} (k_p/M)\sin^2(\pi pm/N)\right]^{1/2} \tag{2.64}$$

[compare with Eqs. (2.27) and (2.28)]. The development of Sections 2.2 and 2.3 applies *verbatim* to this lattice with only a change in the values of the allowed angular frequencies (2.64). A Brillouin diagram for this lattice is shown in Fig. 2.18.

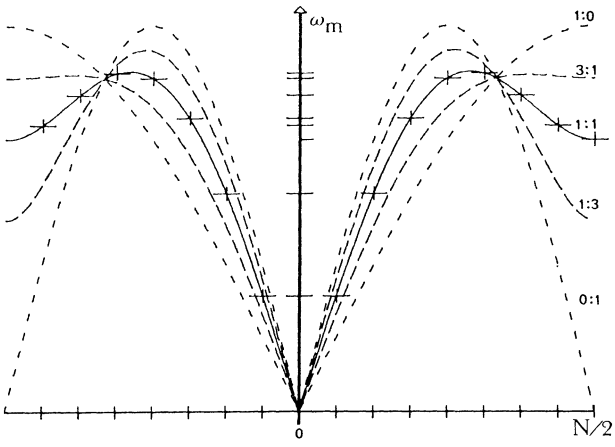


Fig. 2.18. Brillouin frequency diagram for a lattice with first- and second-neighbor interactions through spring constants k_1 and k_2. Curves are plotted for various ratios $k_1:k_2$. If $k_1:k_2 :: 1:0$, we obtain the first-neighbor case (Fig. 2.10). In the other extreme, if $k_1:k_2 :: 0:1$, we obtain two uncoupled lattices of the former type, which results in a doubling of the simple lattice first Brillouin zone.

Exercise 2.33. Note that if $k_0 \neq 0$ the zeroth mode becomes a true oscillation mode. What is the effect on the Brillouin diagram in Fig. 2.18?

Exercise 2.34. Describe the fundamental solutions, elements of Green's matrix, and normal modes of this lattice.

Exercise 2.35. Find the propagation velocities of the traveling waves.

Exercise 2.36. Note that instead of expanding $\mathbf{K}$ in powers of $\mathbf{R}$ as was done in Eq. (2.62), one could expand it in powers of $\boldsymbol{\Delta}$. For the case of first- and second-neighbor interaction only, this leads to $\mathbf{K} = -(k_1 + 4k_2)\boldsymbol{\Delta} - k_2\boldsymbol{\Delta}^2$. Arrive at the result (2.64) for this case and the more general pth-neighbor interaction case.

Exercise 2.37. Suppose only $k_2 \neq 0$. Show that if N is even the lattice uncouples into two $N/2$-mass lattices. What if N is odd?

Exercise 2.38. Introduce viscous damping into the problem.

2.4.3. Molecular Lattices

We consider now a lattice with two kinds of first-neighbor interaction: one with Hooke's constant k_1 between masses N and 1, 2 and 3, etc., up to $N-2$ and $N-1$ (note that N is even) and another with k_2 between 1 and 2, etc., up to $N-1$ and N, as in Fig. 2.19. Such a system is said to be a *molecular* lattice.

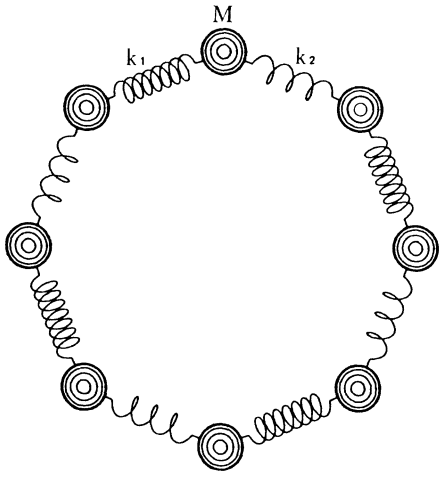


Fig. 2.19. Molecular lattice. Springs with constants k_1 and k_2 alternate between the masses.

The interaction operator will no longer be represented by a matrix constant along the diagonals as in (2.62) but, from (2.19), by

$$\mathbf{K} = \begin{pmatrix} k_1 + k_2 & -k_2 & & & 0 & & -k_1 \\ -k_2 & k_1 + k_2 & -k_1 & & & & 0 \\ & -k_1 & k_1 + k_2 & -k_2 & & & \\ & & -k_2 & \ddots & \ddots & & \\ 0 & & & \ddots & \ddots & & -k_2 \\ & & & & & & \\ -k_1 & & 0 & & & -k_2 & k_1 + k_2 \end{pmatrix}. \tag{2.65}$$

In terms of simpler matrices which have appeared before [Eqs. (1.67a) and (1.88a)], we can write (2.65) as

$$\mathbf{K} = (k_1 + k_2)\mathbf{1} - k_1(\mathbf{E}_1\mathbf{R} + \mathbf{R}^{-1}\mathbf{E}_1) - k_2(\mathbf{E}_1\mathbf{R}^{-1} + \mathbf{R}\mathbf{E}_1) \tag{2.66}$$

and correspondingly for the represented operators. Manifestly, (2.65) is a hermitian matrix, while in (2.66) the hermiticity is also evident, as $\mathbf{E}_1$ is hermitian and $\mathbf{R}$ unitary. The dihedral symmetry D_N of the original simple lattice is broken, and we are left only with invariance transformations which are powers of $\mathbb{R}^2$ and the $\mathbb{K}$'s (Section 1.6) which by themselves form a subgroup of D_N. The odd powers of $\mathbb{R}$ and the $\mathbb{I}$'s will exchange springs k_1 and k_2.

2.4.4. The Interaction Matrix and First Uncoupling

Following earlier treatments of the D_N-symmetric lattices, let us write the equation of motion $\mathbb{M}\ddot{\mathbf{f}} + \mathbb{K}\mathbf{f} = 0$ in the $\boldsymbol{\varphi}$-basis. In this we can aid ourselves with Eqs. (1.67), which have four diagonal blocks, and (1.91), which is completely diagonal, in order to arrive, after some calculation, at

$$\tilde{\mathbf{K}} = \begin{pmatrix} 2(k_1 + k_2)\|\delta_{mn}\sin^2(\pi m/N)\| & i(k_2 - k_1)\|\delta_{mn}\sin(2\pi m/N)\| \\ -i(k_2 - k_1)\|\delta_{mn}\sin(2\pi m/N)\| & 2(k_1 + k_2)\|\delta_{mn}\cos^2(\pi m/N)\| \end{pmatrix}, \tag{2.67}$$

where $\|\delta_{mn}\nu(n)\|$ are $N/2 \times N/2$ diagonal submatrices with $\nu(n)$, $n = 1, 2, \ldots, N/2$, along the diagonal. The matrix (2.67) is thus hermitian, as it should be, and composed of *four diagonal blocks*. The Fourier transform has failed here to produce a completely diagonal matrix. It has, however, considerably simplified the problem since the original equations of motion $M\ddot{f}_n = -\sum_k K_{nk}f_k$ were fully coupled, whereas now $M\ddot{\tilde{f}}_m = -\sum_k \tilde{K}_{mk}\tilde{f}_k$, due to the form (2.67) of $\tilde{\mathbf{K}}$, consists of $N/2$ uncoupled pairs of equations. These are

$$M\ddot{\tilde{f}}_m = -2(k_1 + k_2)\sin^2(\pi m/N)\tilde{f}_m - i(k_2 - k_1)\sin(2\pi m/N)\tilde{f}_{m+N/2}, \tag{2.68a}$$

$$M\ddot{\tilde{f}}_{m+N/2} = i(k_2 - k_1)\sin(2\pi m/N)\tilde{f}_m - 2(k_1 + k_2)\cos^2(\pi m/N)\tilde{f}_{m+N/2}, \quad m = 1, 2, \ldots, N/2 - 1, \tag{2.68b}$$

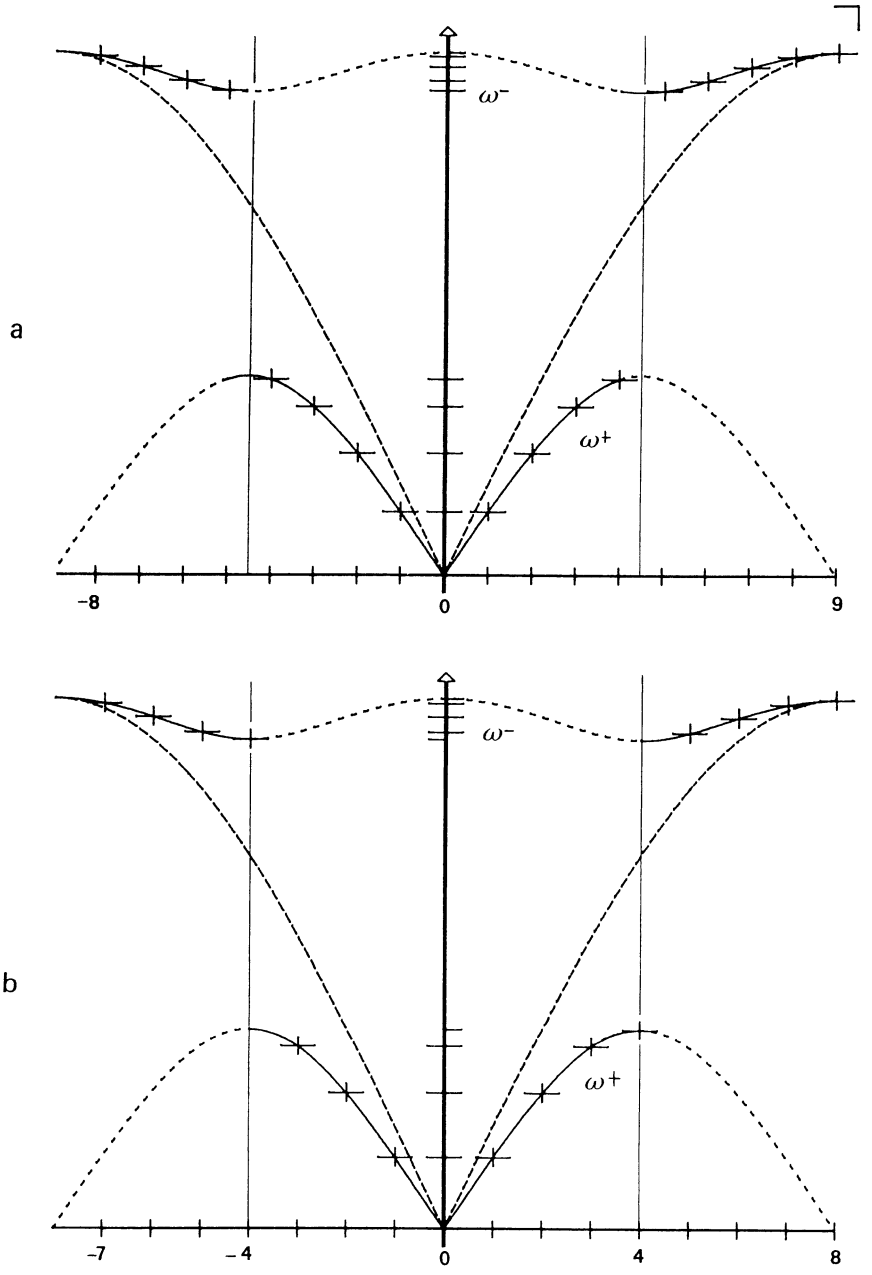


Fig. 2.20. "Extended" Brillouin diagram for the frequencies of a molecular lattice of N masses where (a) $N/2$ is odd ($N = 18$) and (b) $N/2$ is even ($N = 16$) for a ratio $k_\delta/k_\sigma = \frac{1}{2}$. The dotted line represents the Brillouin diagram of an equal-spring lattice. The allowed frequencies, roots of Eq. (2.70) [$\omega_m{}^\pm \sim (-\alpha_m{}^\pm)^{1/2}$; see Eq. (2.80)], thus become the double-period "optic" and "acoustic" branches of the diagram.

and

$$M\ddot{\tilde{f}}_{N/2} = -2(k_1 + k_2)\tilde{f}_{N/2}, \qquad M\ddot{\tilde{f}}_N = 0. \tag{2.68c}$$

Notice first that Eqs. (2.68c) correspond exactly to (2.27) for $m = N/2$ and $m = N$ *for a simple lattice with spring constant* $k_\sigma := (k_1 + k_2)/2$. The solutions will be given then by Eqs. (2.28) for these values of m and k, so we can start drawing our new Brillouin diagram for the molecular lattice by fixing these two values of λ'_m, eigenvalues of $-k_\sigma^{-1}\mathbb{K}$. See Fig. 2.20 for $m = 0$ and $m = N/2$, the dotted line representing the simple lattice with $k_\sigma := (k_1 + k_2)/2$.

2.4.5. Complete Uncoupling

For Eqs. (2.68a)–(2.68b), some further uncoupling is necessary: using the λ_m, $m = 1, 2, \ldots, N$, eigenvalues of $\mathbb{A}$, we can write them as

$$M\ddot{\tilde{\mathbf{f}}}^{(m)} = k_\sigma \tilde{\mathbf{A}}^{(m)}\tilde{\mathbf{f}}^{(m)} \tag{2.69a}$$

with

$$\tilde{\mathbf{f}}^{(m)} := \begin{pmatrix} \tilde{f}_m \\ \tilde{f}_{m+N/2} \end{pmatrix},$$

$$\tilde{\mathbf{A}}^{(m)} := \begin{pmatrix} \lambda_m & i(k_\delta/k_\sigma)(\lambda_m\lambda_{m+N/2})^{1/2} \\ -i(k_\delta/k_\sigma)(\lambda_m\lambda_{m+N/2})^{1/2} & \lambda_{m+N/2} \end{pmatrix}, \tag{2.69b}$$

where $k_\delta := (k_2 - k_1)/2$ and k_σ as before. The 2×2 hermitian matrix $\tilde{\mathbf{A}}^{(m)}$ can be diagonalized exactly [see Eqs. (1.119) and (1.120)], obtaining for its eigenvalues

$$\begin{aligned} \alpha_m{}^{\pm} &:= (\lambda_m + \lambda_{m+N/2})/2 \pm \{[(\lambda_m - \lambda_{m+N/2})/2]^2 + (k_\delta/k_\sigma)^2\lambda_m\lambda_{m+N/2}\}^{1/2} \\ &= -2 \pm 2[\cos^2(2\pi m/N) + (k_\delta/k_\sigma)^2 \sin^2(2\pi m/N)]^{1/2} \\ &= \alpha^{\pm}_{N/2-m}. \end{aligned} \tag{2.70}$$

Comparing with the equal-spring system ($k_\delta \to 0$), we recognize that $\alpha_m{}^+ \to \lambda_m = \lambda_{N-m}$ and $\alpha_m{}^- \to \lambda_{N/2-m} = \lambda_{N/2+m}$. Reflection symmetry under the exchange $m \leftrightarrow N/2 - m$ holds from (2.70). For $m = 0$, the cases (2.68c) are also correctly reproduced in (2.70). We can thus denote the eigenvalues of $-\mathbb{K}$ as $k_\sigma\lambda'_m$, $m = 1, 2, \ldots, N$ [in analogy with those of $\mathbb{A}$; see Eq. (2.27b)], where

$$\lambda'_m = \lambda'_{N-m} = \alpha_m{}^+ = \alpha^+_{N/2-m}, \tag{2.71a}$$

$$\lambda'_{N/2-m} = \lambda'_{N/2+m} = \alpha_m{}^- = \alpha^-_{N/2-m},$$

$$m = 0, 1, 2, \ldots, \begin{cases} N/4 - 1 & \text{for } N/2 \text{ even}, \\ (N-2)/4 & \text{for } N/2 \text{ odd}, \end{cases} \tag{2.71b}$$

and

$$\lambda'_{N/2} = \alpha^{+}_{N/4}, \qquad \lambda'_{3N/4} = \alpha^{-}_{N/4} \quad \text{when } N/2 \text{ even.} \tag{2.71c}$$

2.4.6. Oscillation Frequencies and Shifts

The meaning of the rather involved numbering used above should be apparent in Figs. 2.20(a) and (b) for odd and even $N/2$, respectively. The spectrum of $\mathbb{K}$ modifies that of $-k\mathbb{\Delta}$ in that (a) the eigenvalues λ'_m divide into two sets: those due to the α^+'s and those due to the α^-'s, as

$$0 = \lambda'_0 \leqslant |\alpha_m{}^+| \leqslant 2 - 2|k_\delta/k_\sigma| \leqslant 2 + 2|k_\delta/k_\sigma| \leqslant |\alpha_m{}^-| \leqslant |\lambda'_{N/2}| = 4; \tag{2.72}$$

in between, there is a *gap* of height $4|k_\delta/k_\sigma|$; (b) the α^-'s raise "wings," while the α^+'s lower them by the same amount:

$$\alpha_m{}^+ - \lambda_m = \lambda_{N/2-m} - \alpha_m{}^- \geqslant 0. \tag{2.73}$$

The slope of the curve for λ'_m in Fig. 2.20 remains positive for m between 0 and $N/2$ and vanishes for $m = 0$, $N/4$ and $N/2$. The inequality (2.72) holds for all values of $|k_\delta/k_\sigma|$, preventing the "wings" from topping $\lambda'_{N/2}$.

Exercise 2.39. Show that for small $|k_\delta/k_\sigma|$

$$\alpha_m{}^+ - \lambda_m \simeq (k_\delta/k_\sigma)^2 \sin^2(2\pi m/N). \tag{2.74}$$

Exercise 2.40. When one of the springs vanishes ($k_2 \to 0$) we are left with $N/2$ simple oscillators. What happens with the spectrum of $\mathbb{K}$?

2.4.7. Optic and Acoustic Modes

The eigenvectors of the submatrix $\tilde{\mathbf{A}}^{(m)}$ which involves the m and $(N/2 + m)$ rows and columns of the interaction matrix $\tilde{\mathbf{K}}$ will now be found. For

$$\tilde{\mathbf{A}}^{(m)}\mathbf{x}^{m\pm} = \alpha_m{}^{\pm}\mathbf{x}^{m\pm}, \qquad \mathbf{x}^{m\pm} = \begin{pmatrix} x_1^{m\pm} \\ x_2^{m\pm} \end{pmatrix}, \tag{2.75}$$

the ratios of the components can be conveniently written, using (2.69b), (2.70), (2.73), and identities between the λ's, as

$$-i\rho_m := \frac{x_2^{m+}}{x_1^{m+}} = -i\frac{k_\sigma}{k_\delta}\frac{\alpha_m{}^+ - \lambda_m}{2\sin(2\pi m/N)} = -i\frac{k_\sigma}{k_\delta}\frac{\lambda_{N/2-m} - \alpha_m{}^-}{2\sin(2\pi m/N)} = \frac{x_1^{m-}}{x_2^{m-}}, \tag{2.76}$$

where $0 \leqslant \rho_m < 1$. In this form it is manifest that as the springs become equal ($k_\delta \to 0$, $\rho_m \to 0$), $\mathbf{x}^{m+}$ has a vanishing lower component and $\mathbf{x}^{m-}$ a vanishing upper one. In this case $\tilde{f}_m\varphi_m$ and $\tilde{f}_{m+N/2}\varphi_{m+N/2}$ in (2.69) give, for

their coefficients $\tilde{f}_m(t)$ and $\tilde{f}_{m+N/2}(t)$, uncoupled differential equations. In general, however, the eigenvectors of the molecular lattice will be a superposition of φ_m and $\varphi_{m+N/2}$ with the ratio (2.76). We can thus define, corresponding to the eigenvalues $-k_\sigma \alpha_m{}^{\pm}$ of the interaction operator,

$$\psi_m{}^{+} \coloneqq x_1^{m+}\varphi_m + x_2^{m+}\varphi_{m+N/2} = x_1^{m+}(\varphi_m - i\rho_m\varphi_{m+N/2}) \qquad \text{for } \alpha_m{}^{+}, \quad (2.77a)$$

$$\psi_m{}^{-} \coloneqq x_1^{m-}\varphi_m + x_2^{m-}\varphi_{m+N/2} = x_2^{m-}(-i\rho_m\varphi_m + \varphi_{m+N/2}) \qquad \text{for } \alpha_m{}^{-}, \quad (2.77b)$$

which constitute an orthonormal basis for $\mathscr{V}^N$ once the proper coefficients x_1^{m+} and x_2^{m-} are determined:

$$|x_1^{m+}| = (1 + \rho_m{}^2)^{-1/2} = |x_2^{m-}|. \quad (2.77c)$$

[To keep the index bureaucracy straight, we remark that the range of indices in (2.77) follows that in (2.71) and that in the case $m = 0$ or $N/2$, ρ_m is undefined, as we have only $\psi_0{}^{+} = \varphi_N$ and $\psi_{N/2}^{-} = \varphi_{N/2}$.] Expanding now the sought for solution $\mathbf{f}(t)$ in terms of the $\psi^{\pm}$-basis (2.77),

$$\mathbf{f}(t) = \sum_{m,\pm} \bar{f}_{m,\pm}(t)\psi_m{}^{\pm}, \quad (2.78)$$

the equation of motion for the molecular lattice [Eq. (2.21) with the interaction matrix (2.65)] uncouples completely as

$$M\ddot{\bar{f}}_{m,\pm} + k_\sigma \alpha_m{}^{\pm}\bar{f}_{m,\pm} = 0. \quad (2.79)$$

Its solutions were worked out before in Section 2.1 and are of the purely oscillating type (2.7), with angular frequencies

$$\omega_m{}^{\pm} = (k_\sigma/M)^{1/2}(-\alpha_m{}^{\pm})^{1/2}. \quad (2.80)$$

2.4.8. Brillouin Diagrams

We have drawn the Brillouin diagram corresponding to (2.80) in Fig. 2.21, where, as is customary, only the range of m between $\pm N/4$ is represented. Figure 2.21 shows that the oscillator frequencies divide into two sets: the so-called *acoustical band* for the ω^{+}'s, which involves low frequencies, and the *optical band* for the ω^{-}'s, which involves a range of higher frequencies. They are separated by the gap which is called the *stopping* band. This nomenclature stems from solid-state physics and refers to the fact that in actual crystals the frequencies correspond, respectively, to mechanical acoustic vibrations and electromagnetically induced oscillating fields in the optical range which the crystal is able to carry or transmit. It is opaque for frequencies outside these bands. Electric circuits acting as low-pass or high-pass filters work on the same principles.

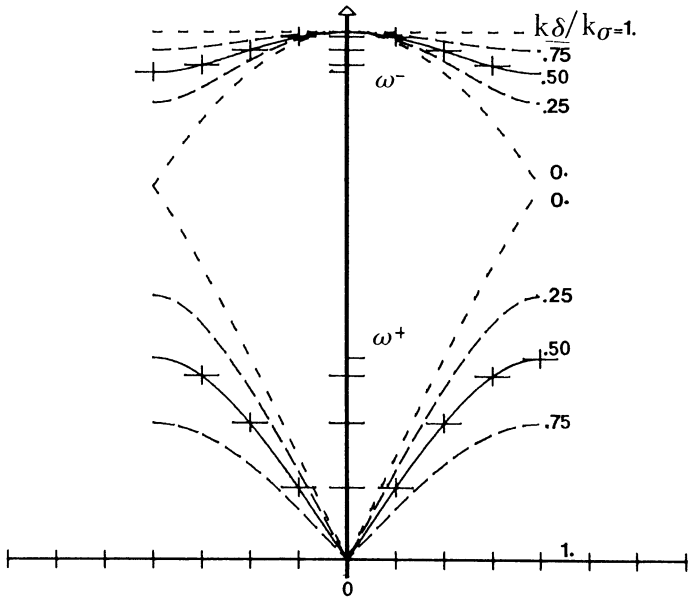


Fig. 2.21. Usual Brillouin frequency diagram for a molecular (and diatomic) lattice extending on integer values within $\pm N/4$. It has been plotted for various values of k_δ/k_σ. If this ratio is zero, the simple lattice diagram is regained; on the other extreme, if $k_1 = 0$, the lattice breaks up into $N/2$ two-mass dumbbells. As each has only zero and its natural oscillation frequency, we obtain two clusters of $N/2$-fold degenerate frequencies.

2.4.9. General Description of the Solutions

In spite of the rather lengthy derivation, the orthonormal $\psi^{\pm}$-basis in Eqs. (2.77) is clearly the "natural" basis for the description of the molecular lattice. Most of the developments of Section 2.2 and 2.3 follow unchanged as follows: (a) Once the solution for the coordinates $\bar{f}_m(t)$ is found in terms of initial conditions, it assumes precisely the form (2.28) in terms of functions $\bar{G}_m(\tau)$ and their time derivatives, where the proper oscillation frequencies (2.80) appear. These constitute the $\psi^{\pm}$-basis representative of the self-adjoint *Green's operator* $\mathbb{G}(\tau)$, whose expression in other bases—notably the "physical" ε-basis—can be calculated leading to the general form (2.29) of the solution. (b) *Fundamental solutions*, for initial conditions of single vectors in the ε-basis, can be found. (c) The basis vectors $\psi_m^{\pm}$ do not have purely real coordinates in the ε-basis, so in order to produce *normal modes* we must find a more appropriate basis. We can consider an eigenbasis of $\mathbb{K}_0$ (the dihedral operator, using the results of Exercises 1.54 and 1.57) and replace the φ_m's in (2.77) by the $\varphi_m'^{\pm}$'s of that basis. We can also build *real* eigenvectors out of (2.77), recalling that complex conjugation in the φ-basis is defined through

$\varphi_m^* := \varphi_{N-m}$. Consideration of initial conditions given by single vectors in this real basis will lead to normal modes as (2.48) with the new ω_m's and two trigonometric summands in place of one.

Exercise 2.41. Find explicitly the unitary transformation linking the ε- and the $\psi^{\pm}$-bases.

Exercise 2.42. When obtaining the nth coordinate in the ε-basis of $\psi_m{}^{\pm}$, you will notice that they behave like $\exp(-2\pi imn/N)$ times $[1 - (-1)^n i\rho_m]$ for the acoustical band eigenvectors and like the same function times $[-i\rho_m + (-1)^n]$ for the optical band eigenvectors. In the latter modes, then, first neighbors oscillate—on the average—on opposite sides of the equilibrium line, while for the acoustical modes they tend to be on the same side. See Fig. 2.22.

Exercise 2.43. Will the Green's matrix in the ε-basis be an even function of $|n - m|$ as it was in (2.33)? What should be its main characteristics?

Exercise 2.44. Can you find an eigenbasis related to (2.77) which is also an eigenbasis of $\mathbb{I}_0$? Why not?

Exercise 2.45. Consider finding *traveling* wave solutions for the molecular lattice.

Exercise 2.46. Introduce viscous damping into the problem.

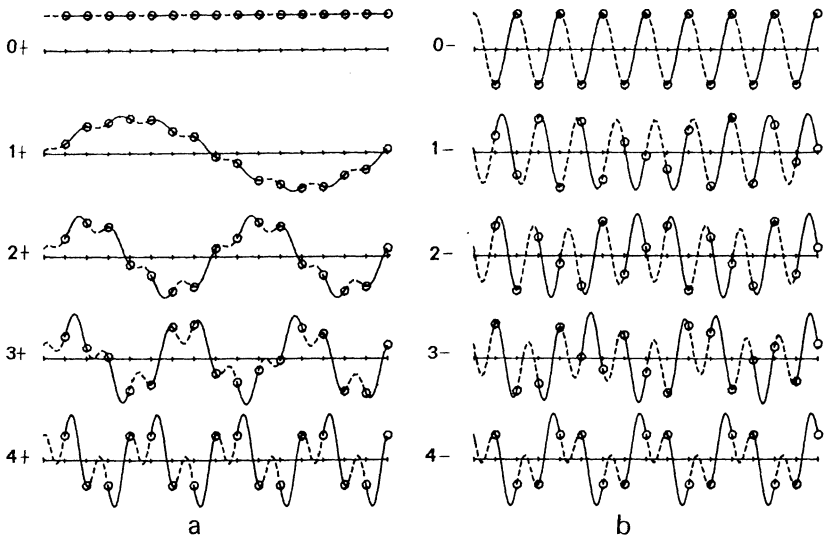


Fig. 2.22. (a) Acoustic, and (b) optic oscillation modes for a molecular lattice with 16 masses (circles). Springs k_1 and k_2 are represented by broken and unbroken lines, plotted for real values of the abscissa. The spring ratio is $k_\delta/k_\sigma = \frac{1}{2}$.

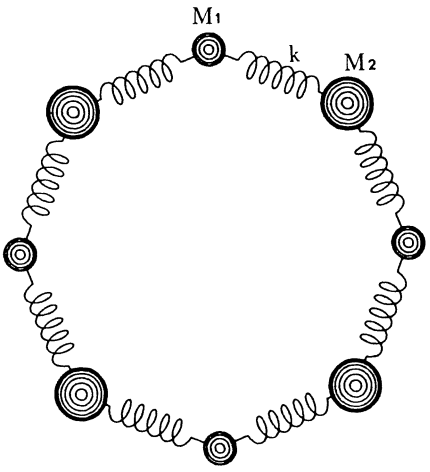


Fig. 2.23. Diatomic lattice. Masses M_1 and M_2 alternate.

2.4.10. Diatomic Lattices

The *diatomic* lattice (see Fig. 2.23) is a lattice with two alternating masses M_1 and M_2. It has several features in common with the molecular lattice and some differences as well. The intertial operator was up to now a multiple M of the unit operator [Eq. (2.21)]. For the diatomic lattice, it will be represented in the $\boldsymbol{\varepsilon}$-basis by a diagonal $N \times N$ matrix (N even) with M_1 in the odd and M_2 in the even position. In terms of matrices we have introduced before [Eqs. (1.67)], we can write

$$\mathbf{M} = \begin{pmatrix} M_1 & & & & 0 \\ & M_2 & & & \\ & & M_1 & & \\ & & & \ddots & \\ 0 & & & & M_2 \end{pmatrix} = M_1\mathbf{E}_1 + M_2\mathbf{E}_2, \tag{2.81}$$

and the (undamped) equation of motion can be written as

$$\ddot{\mathbf{f}} + \mathbb{M}^{-1}\mathbb{K}\mathbf{f} = 0. \tag{2.82}$$

2.4.11. Diagonalization of a Nonhermitian Matrix

Our procedure up to now has been to find the eigenvectors and -values of the interaction operator in order to find a basis of $\mathscr{V}^N$ where the lattice equations uncouple. The problem with Eq. (2.82) is that $\mathbb{M}^{-1}\mathbb{K}$ is *not* a hermitian operator. Although the two factors *are* hermitian, they do not

commute. Yet $\mathbb{M}^{-1}\mathbb{K}$ is not too "far" from being hermitian; in the φ-basis it is represented by

$$(M_1\tilde{\mathbf{E}}_1 + M_2\tilde{\mathbf{E}}_2)^{-1}\tilde{\mathbf{K}} = (M_1^{-1}\tilde{\mathbf{E}}_1 + M_2^{-1}\tilde{\mathbf{E}}_2)\tilde{\mathbf{K}}$$

$$= \begin{pmatrix} \mu_\sigma \| \delta_{mn}\kappa_m \| & \mu_\delta \| \delta_{mn}\kappa_{m+N/2} \| \\ \mu_\delta \| \delta_{mn}\kappa_m \| & \mu_\sigma \| \delta_{mn}\kappa_{m+N/2} \| \end{pmatrix}, \qquad \begin{cases} \mu_\sigma := (\mu_1^{-1} + \mu_2^{-1})/2, \\ \mu_\delta := (\mu_2^{-1} - \mu_1^{-1})/2, \end{cases} \tag{2.83}$$

where we have used the result (1.67) on the $\tilde{\mathbf{E}}_i$ and Eq. (2.63) for the form of the general pth-neighbor equal-spring interaction matrix. We are representing an $N/2 \times N/2$ diagonal matrix with elements $\nu(n)$ by $\| \delta_{nm}\nu(m) \|$ as in Eq. (2.67). All 2×2 submatrices formed by taking the intersections of the nth and mth row and column are diagonal and hermitian except when $m = n + N/2$.

Exercise 2.47. Show that $\mathbb{M}^{-1}\mathbb{K}$, in its ε-basis representation, has two $N/2 \times N/2$ hermitian submatrices: those constituted by the even- or odd-rowed and -columned elements of the original matrix.

The nondiagonal 2×2 submatrices are

$$\tilde{\mathbf{K}}^{(m)} := \begin{pmatrix} \mu_\sigma\kappa_m & \mu_\delta\kappa_{m+N/2} \\ \mu_\delta\kappa_m & \mu_\sigma\kappa_{m+N/2} \end{pmatrix} =: \mu_\sigma k_1 \tilde{\mathbf{B}}^{(m)}. \tag{2.84}$$

Their eigenvalues can be found by applying (1.120) and extracting the factor $\mu_\sigma k_1$:

$$k_1\beta_m^{\pm} = (\kappa_m + \kappa_{m+N/2})/2 \pm \{[(\kappa_m - \kappa_{m+N/2})/2]^2 + (\mu_\delta/\mu_\sigma)^2\kappa_m\kappa_{m+N/2}\}^{1/2}. \tag{2.85}$$

The spectrum of (2.84) and (2.85) looks very much like the molecular lattice spectrum (2.70). Indeed, for first-neighbor interactions only, we have $\kappa_m = k_1\lambda_m$, and the expressions for $\beta_m^{\pm}$ in the two-mass case and $\alpha_m^{\pm}$ for the molecular case in (2.70) become *identical* under the formal substitution

$$\frac{k}{M_1} \to \frac{k_1}{M}, \qquad \frac{k}{M_2} \to \frac{k_2}{M}, \qquad \text{i.e.,} \quad \frac{\mu_\delta}{\mu_\sigma} \to \frac{k_\delta}{k_\sigma}. \tag{2.86}$$

2.4.12. Oscillation Frequencies

The Brillouin diagram for the diatomic first-neighbor interaction lattices is then given by Fig. 2.21 with the same eigenvalue numbering and the appropriate label changes: for $M_2 \to M_1$, $\mu_\delta \to 0$ and $k_1\beta_m^{+} \to \kappa_m$, $k_1\beta_m^{-} \to \kappa_{m+N/2}$. For the pth-neighbor interacting lattice another property of the

molecular case carries over: the raising of the optical band "wings" equals the lowering of the acoustical band ones,

$$k_1\beta_m{}^+ - \kappa_m = \kappa_{m+N/2} - k_1\beta_m{}^- \geqslant 0. \tag{2.87}$$

For the general diatomic lattice, the Brillouin diagram can thus be constructed based on the monatomic one in Fig. 2.18.

2.4.13. Optic and Acoustic Modes

Finding the eigenvectors $\mathbf{y}^{m\pm}$ of (2.84) corresponding to $\beta_m{}^\pm$ is an exercise parallel to (2.75)–(2.76). Indeed, using analogous notation,

$$\begin{aligned} \rho_m{}^+ &:= \frac{y_2^{m+}}{y_1^{m+}} = \frac{\mu_\sigma}{\mu_\delta}\frac{k_1\beta_m{}^+ - \kappa_m}{\kappa_{m+N/2}} \geqslant 0, \\ \rho_m{}^- &:= \frac{y_1^{m-}}{y_2^{m-}} = \frac{\mu_\sigma}{\mu_\delta}\frac{k_1\beta_m{}^- - \kappa_{m+N/2}}{\kappa_m} \geqslant 0. \end{aligned} \tag{2.88}$$

It follows that the eigenvectors of $\mathbb{M}^{-1}\mathbb{K}$ are

$$\hat{\psi}_m{}^+ := y_1^{m+}\varphi_m + y_2^{m+}\varphi_{m+N/2} = y_1^{m+}(\varphi_m + \rho_m{}^+\varphi_{m+N/2}), \tag{2.89a}$$

$$\hat{\psi}_m{}^- := y_1^{m-}\varphi_m + y_2^{m-}\varphi_{m+N/2} = y_1^{m-}(\rho_m{}^-\varphi_m + \varphi_{m+N/2}), \tag{2.89b}$$

where we still have to fix y_1^{m+} and y_2^{m-} adequately for normalization. Now, the set of vectors (2.89) constitutes a basis for $\mathscr{V}^N$, but not a completely orthonormal one. From the remarks on the "not far from hermitian" matrix (2.83) it follows that $(\hat{\psi}_m, \hat{\psi}_{m'}) = 0$ for $m \neq m'$. When $m = m'$ the acoustical and optical modes (2.89a) and (2.89b), although linearly independent, are *not* orthogonal. The natural description of the diatomic lattice is thus in terms of a nonorthogonal basis. This is not too inconvenient from the point of view of a good qualitative picture of the workings of such lattices, in particular the two-band structure of the frequency spectrum and the identification of "optical" (or "acoustical") modes with vibrations where the two unequal masses are preferentially on opposite sides (or on the same side) of the equilibrium position.

Exercise 2.48. Starting from the equation of motion of the diatomic lattice in the ε-basis $\mathbf{M}\ddot{\mathbf{f}} = -\mathbf{K}\mathbf{f}$, perform a *nonunitary* transformation $\mathbf{f} = \mathbf{M}^{-1/2}\mathbf{g}$, where $\mathbf{M}^{-1/2}$ is a well-defined diagonal matrix, and multiply the whole equation by $\mathbf{M}^{-1/2}$. Thus arrive at $\ddot{\mathbf{g}} = -\mathbf{K}'\mathbf{g}$, $\mathbf{K}' = \mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}$ *hermitian*. Note that for first-neighbor interactions in $\mathbf{K}$, $\mathbf{K}'$ represents a first-neighbor interaction plus two different zero-order interaction springs.

Exercise 2.49. A nonunitary transformation linking the two-band and diatomic lattices can also be set up comparing the eigenvectors $\mathbf{x}^{m\pm}$ in (2.75) and $\mathbf{y}^{m\pm}$ for (2.84). The question is to find a 2×2 matrix $\mathbf{T}^{(m)}$ (for fixed m) such that

$\mathbf{x}^{m\pm} = \mathbf{T}^{(m)}\mathbf{y}^{m\pm}$, i.e., $\tilde{\mathbf{A}}^{(m)}\mathbf{T}^{(m)} = \mathbf{T}^{(m)}\tilde{\mathbf{B}}^{(m)}$. Show that such a matrix is diagonal with elements $t_m := \exp(i\pi/4)\tan^{1/2}(\pi m/N)$ and t_m^{-1}, $m = 1,2, \ldots, N/2 - 1$.

Exercise 2.50. Find the most general solution vector $\mathbf{f}(t)$ for the diatomic lattice expressed in terms of the nonorthogonal eigenbasis (2.89). Identify Green's matrix in the ψ-basis. See that upon transforming back to the "physical" ε-basis the Green's operator matrix representative becomes *nonhermitian.*

2.4.14. Short Survey of Other Lattice Systems

Having worked on different sample cases in this section, we can see that, generally speaking, the Fourier transform takes us from the fully coupled "physical" basis to a mathematically simpler one. Immediate extensions involve lattices with q different springs or masses which repeat a pattern r times (so $N = qr$). These can be treated and the problem reduced to diagonalizing $q \times q$ matrices, which in turn divide the spectrum into q bands which raise and lower "wings" with respect to the equal-spring or -mass case. For an overall view and physical application we warmly recommend the classic book by Brillouin (1946). This book is mainly concerned with actual three-dimensional crystals of infinite extent. Very readable articles dealing with finite lattices with different types of constraints and characteristics have been written by Louck (1962), Merchant and Brill (1973), and Chaturvedi and Baijal (1974). A very interesting problem whose treatment departs from our line of work but which nevertheless is important in the physics of semiconductors is that of a *mass defect* in the lattice, i.e., one mass being different from the others. Articles on this subject have been written by Weinstock (1970, 1971) and Maradudin *et al.* (1963). Variants of this problem include molecular lattices with atomic or bond defects: See Dettmann and Ludwig (1965), Dean (1967), and Munn (1969). A qualitative description of the behavior of a linear crystal when mass defects are introduced one at a time is given by Alonso *et al.* (1973) and, for the threshold oscillation frequencies of a diatomic lattice, by Valladares (1975). On the more philosophical aspects of lattice couplings in very general systems, an article and book by Capra (1974a, 1974b) are a must for the interested reader.

2.5. Energy in a Lattice

In this section we shall describe the energy present in a vibrating N-mass lattice. In the absence of damping we expect the total energy to be conserved. Moreover, when we uncouple the system in its eigenbasis, we shall find that the individual energies associated with the normal modes are conserved as well.

2.5.1. Kinetic and Potential Energy in Each Particle

Consider an N-element lattice described by the vector equation

$$\mathbb{M}\ddot{\mathbf{f}} + \mathbb{C}\dot{\mathbf{f}} + \mathbb{K}\mathbf{f} = \mathbf{0}, \tag{2.90}$$

where, as detailed in Section 2.2, $\mathbb{M}$, $\mathbb{C}$, and $\mathbb{K}$ are the inertial, dissipation, and interaction operators. In the "physical" $\boldsymbol{\varepsilon}$-basis the coordinates of $\mathbf{f}$, $f_n(t)$ describe the displacements of the lattice points, while $\mathbb{M}$ and $\mathbb{C}$ are represented by diagonal matrices $\|M_n\|$ and $\|c_n\|$, M_n being the mass and c_n the damping constant of the nth lattice element. The interaction operator $\mathbb{K}$ is self-adjoint and represented by $\|\kappa_{mn}\|$ [see Eq. (2.19)].

At some time t, the kinetic energy of the nth mass is

$$E_n^{\,k}(t) := \tfrac{1}{2}M_n(\dot{f}_n)^2, \tag{2.91}$$

while its potential energy can be found by integrating the force to which the particle is subject, Eq. (2.19), along a segment from its equilibrium position to its actual position $f_n(t)$, all other lattice elements being fixed:

$$E_n^{\,p}(t) := \int_0^{f_n} dx\left(\sum_{m\neq n}\kappa_{nm}f_m + \kappa_{nn}x\right) = \sum_{m\neq n}\kappa_{nm}f_nf_m + \tfrac{1}{2}\kappa_{nn}f_n^{\,2}. \tag{2.92}$$

No other forms of energy being present in the lattice, the total energy of the nth particle is

$$E_n(t) = E_n^{\,k}(t) + E_n^{\,p}(t). \tag{2.93}$$

Substitution of a solution $\mathbf{f}(t)$ as found in the last sections into (2.91)–(2.93) should give $E_n(t)$ for each of the individual particles. The description obtained in this fashion, however, is not too illuminating. Since the particles are coupled, as the lattice motion proceeds in time, potential energy is exchanged between the lattice constituents so that none of the individual $E_n(t)$'s is constant. As before, a simpler description of the quantities involved is obtained through writing them in a vector-basis-independent form applied to the whole lattice.

2.5.2. Total Energy and Its Conservation

The total kinetic energy can be written as

$$E^k(t) := \sum_n E_n^{\,k}(t) = \tfrac{1}{2}\sum_n \dot{f}_n^{*}M_n\dot{f}_n = \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}), \tag{2.94}$$

using the inner product defined in Section 1.2. The $E^k(t)$ thus defined is positive even for complex $\dot{f}_n(t)$.

The total potential energy will be the sum of the $E_n^p(t)$ in (2.93) over all n. In setting up this expression we have to be careful in order not to double-count the cross terms $f_n f_m$ which appear twice. Halving these, we obtain the sum

$$E^p(t) := \sum_n E_n^p(t) = \tfrac{1}{2} \sum_{m,n} f_n^* \kappa_{nm} f_m = \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\mathbf{f}), \tag{2.95}$$

where again we have used the inner product form. The total energy present in the lattice is thus the sum of (2.94) and (2.95):

$$E = \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}) + \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\mathbf{f}). \tag{2.96}$$

This expression is both compact and useful, as we can find the effect of dissipation on the expected conservation of total energy. Indeed, using the hermiticity of $\mathbb{M}$, $\mathbb{K}$, and $\mathbb{C}$, the reality of (2.94) and (2.95), and Eq. (2.90), we find that

$$\begin{aligned} \frac{d}{dt} E &= \tfrac{1}{2}(\ddot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}) + \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\ddot{\mathbf{f}}) + \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{K}\mathbf{f}) + \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\dot{\mathbf{f}}) \\ &= (\dot{\mathbf{f}}, \mathbb{M}\ddot{\mathbf{f}} + \mathbb{K}\mathbf{f}) = -(\dot{\mathbf{f}}, \mathbb{C}\dot{\mathbf{f}}). \end{aligned} \tag{2.97}$$

The conclusion of (2.97) is that *in the absence of dissipation, the total energy (2.96) of the lattice is conserved.*

2.5.3. Energy in the Normal Modes

Our original description in terms of the energy in each lattice element was inconvenient because potential energy exchange is taking place. As we saw in the last sections, however, the more natural description of the lattice is in terms of the eigenvectors of the operator $\mathbb{M}^{-1}\mathbb{K}$. In what follows, as in Section 2.2, we shall consider all masses equal $\mathbb{M} = M\mathbb{1}$ and similarly for all dissipation coefficients $\mathbb{C} = c\mathbb{1}$. Let $\{\boldsymbol{\psi}_n\}_{n=1}^N$ be the orthonormal eigenbasis of the self-adjoint interaction operator. Then, for

$$\mathbf{f}(t) = \sum_n \bar{f}_n(t)\boldsymbol{\psi}_n, \qquad \mathbb{K}\boldsymbol{\psi}_n = \kappa_n \boldsymbol{\psi}_n, \tag{2.98}$$

Eq. (2.90) leads to

$$M\ddot{\bar{f}}_n + c\dot{f}_n + \kappa_n \bar{f}_n = 0, \tag{2.99}$$

and the solutions for $\bar{f}_n(t)$ were given in Section 2.1. Now, substitution of (2.98) into the expression for the total energy (2.96) yields

$$\begin{aligned} E &= \tfrac{1}{2} \sum_{m,n} \dot{\bar{f}}_m^* \dot{\bar{f}}_n (\boldsymbol{\psi}_m, \mathbb{M}\boldsymbol{\psi}_n) + \tfrac{1}{2} \sum_{m,n} \bar{f}_m^* \bar{f}_n (\boldsymbol{\psi}_m, \mathbb{K}\boldsymbol{\psi}_n) \\ &= \tfrac{1}{2} \sum_m (M|\dot{\bar{f}}_m|^2 + \kappa_m |\bar{f}_m|^2) = \sum_m E_m^{\psi}, \end{aligned} \tag{2.100}$$

where we have defined the energy associated with the mth mode (relative to the ψ-basis):

$$E_m^{\psi} := \tfrac{1}{2}(M|\dot{\bar{f}}_m|^2 + \kappa_m|\bar{f}_m|^2). \tag{2.101}$$

As this depends only on the mth component of the state vector $\mathbf{f}$ and cross terms are absent, we conjecture (and prove below) that *there is no energy exchange between the different modes of the interaction operator eigenbasis.* Moreover, *in the absence of dissipation, each of the mode energies (2.101) is conserved.* Parallel to our proof of (2.97) from (2.96) and (2.90), we can show that the energy loss of the mth mode (2.101) is due only to its own dissipation term. Using the equation of motion (2.99) for each mode, we obtain

$$\frac{d}{dt}E_m^{\psi} = \tfrac{1}{2}M(\ddot{\bar{f}}_m\dot{\bar{f}}_m^* + \dot{\bar{f}}_m\ddot{\bar{f}}_m^*) + \tfrac{1}{2}\kappa_m(\dot{\bar{f}}_m\bar{f}_m^* + \bar{f}_m\dot{\bar{f}}_m^*) = -c|\dot{\bar{f}}_m|^2. \tag{2.102}$$

Exercise 2.51. In the expression for the total energy (2.96), assume that not all masses are equal, so $\mathbb{M}$ is not a multiple $M\mathbb{1}$ and does not commute with $\mathbb{K}$. Then, in finding the eigenbasis of $\mathbb{M}^{-1}\mathbb{K}$ [as in the case of the diatomic lattice, Eq. (2.82)] we have $\mathbb{K}\psi_n = \gamma_n\mathbb{M}\psi_n$ for the eigenbasis, and the expression for the total energy analogous to (2.100) becomes

$$E = \tfrac{1}{2}\sum_{m,n}(\dot{\bar{f}}_m^*\dot{\bar{f}}_n + \gamma_n\bar{f}_m^*\bar{f}_n)(\psi_m, \mathbb{M}\psi_n), \tag{2.103}$$

which shows there is energy exchange between modes. Examine the options for defining conserved "partial" energies in cases when $(\psi_m, \mathbb{M}\psi_n)$ is zero except for subsets of ψ's.

2.6. Phase Space, Time Evolution, and Constants of Motion

In our description of the time evolution of a lattice of mechanical elements we have seen that both $\mathbf{f}(t)$ and its time derivative $\dot{\mathbf{f}}(t)$ entered as initial conditions, basically because the equations of motion are differential equations of second order. Our account of the lattice energy, moreover, suggests that $\mathbf{f}(t)$ and $\dot{\mathbf{f}}(t)$ should be taken on equal footing. The appearance of two (or more) quantities intertwined in this way strongly indicates that vector space concepts give the most economical description of the system. That this is so will be seen in this section. The concept to be developed is that of the *phase space* of a system and the insight it gives into its time evolution and conservation laws.

2.6.1. Phase Space of a System

In our mechanical representation of a coupled system by mass-and-spring lattices, $\mathbf{f}(t) \in \mathscr{V}^N$ stands for the displacement vector. We define the *momentum vector*,‡ closely related to the velocity vector $\dot{\mathbf{f}}(t)$, as

$$\mathbf{g}(t) \coloneqq \mathbb{M}\dot{\mathbf{f}}(t), \tag{2.104}$$

where $\mathbb{M}$ is, as before, the inertia operator. In the "physical" $\boldsymbol{\varepsilon}$-basis, where $f_n = (\boldsymbol{\varepsilon}_n, \mathbf{f})$ are the individual mass displacements, $\mathbb{M}$ is represented by a diagonal matrix $\mathbf{M} = \|M_n\|$, where $\{M_n\}_{n=1}^N$ are the N particle masses. We now construct the $2N$-dimensional *phase space* of N-mass systems, $\mathscr{V}_{\text{II}}^N$, as a vector space with elements

$$\boldsymbol{\zeta} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}, \qquad \mathbf{f}, \mathbf{g} \in \mathscr{V}^N. \tag{2.105}$$

In the canonical column-vector realization, $\boldsymbol{\zeta} \in \mathscr{V}_{\text{II}}^N$ is represented by $2N$ components, the first being those of $\mathbf{f}$ and the second those of $\mathbf{g}$; $\mathscr{V}_{\text{II}}^N$ is then said to be the *direct sum* of two $\mathscr{V}^N$ spaces ($\mathscr{V}_{\text{II}}^N = \mathscr{V}^N \oplus \mathscr{V}^N$).

2.6.2. The Simple Harmonic Oscillator

It will help us to get a better grasp of the phase space $\mathscr{V}_{\text{II}}^N$ if we consider the one-dimensional oscillator problem examined in Section 2.1 whose complete solution is (2.10) and, to start with, disregard damping. As there, phase space is two-dimensional, $\mathscr{V}_{\text{II}}^1 = \mathscr{V}^2$. We can plot the motion of the oscillator in this plane as in Fig. 2.24. If the appropriate scales are chosen for f and g, the system is described by a point which moves clockwise in a circle. The radius of this circle is proportional to the energy ($\frac{1}{2}M^{-1}g^2 + \frac{1}{2}kf^2$), while the angular velocity is $(k/M)^{1/2}$, the same for all radii. The initial position of the phase-space point is f_0, g_0. In Fig. 2.25 we have represented a similar but damped oscillator.

2.6.3. The Lattice Equations of Motion in Phase Space

The free lattice equation of motion, Eq. (2.90), may be written as a *vector* equation in $\mathscr{V}_{\text{II}}^N$ as

$$\begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & -\mathbb{C}\mathbb{M}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}. \tag{2.106}$$

Indeed, the first row is only (2.104), which identifies $\mathbf{g}$ as the momentum

‡ Note that in the presence of viscous drag, $g_n(t)$ is *not* the momentum *canonically conjugate* to $f_n(t)$ as defined, for instance, in Goldstein (1950, Chapter 6).

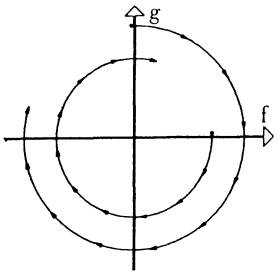


Fig. 2.24. Motion in phase space of harmonic oscillators with nonzero elongation and velocity. Distances between arrows represent equal time intervals.

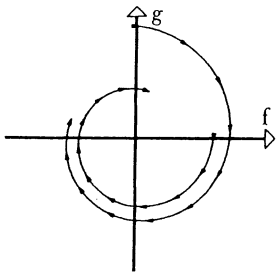


Fig. 2.25. Motion in phase space of damped harmonic oscillator. Distances between arrows represent equal time intervals.

associated to **f**, while the second row rewrites the original Eq. (2.90) using both **f** and **g**. Equation (2.106) has the simple structure

$$\mathbb{H}_{II}\zeta = \frac{d}{dt}\zeta, \qquad \text{where } \mathbb{H}_{II} := \begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & -\mathbb{C}\mathbb{M}^{-1} \end{pmatrix}; \tag{2.107}$$

i.e., it is a system of differential equations which are of *first order* in time. We shall refer to $\mathbb{H}_{II}$ as the *generator* of the equation of motion.

2.6.4. Time-Evolution Operator

The simplification inherent in the reduction of order of the differential equation of motion is considerable. The reason for this is that *the time evolution becomes a Taylor expansion*:

$$\zeta(t + t_0) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n}{dt'^n} \zeta(t') \Big|_{t'=t_0} =: \exp\left(t \frac{d}{dt'}\right) \zeta(t') \Big|_{t'=t_0}, \tag{2.108}$$

where we can define the exponential of the operator td/dt' in terms of the series expansion of the exponential function. This is in line with our description of functions of operators in terms of functions of the representing matrices in Section 1.5, although here we have exponentiated a *differential* operator. The validity of the definition depends here on the validity of the Taylor expansion of $\zeta(t)$: we must assume $\zeta(t)$ to be a set of $2N$ *analytic* functions of t, i.e., to have a convergent Taylor expansion for all finite t. The explicit solutions obtained from Section 2.1 onward indicate that this is valid. Now, the vector $\zeta(t)$ must satisfy the equation of motion (2.107), which states that $(d/dt')^n \zeta(t') = \mathbb{H}_{II}^n \zeta(t')$. The linear combination of such powers of d/dt' in (2.108) thus yields

$$\zeta(t + t_0) = \exp(t\mathbb{H}_{II})\zeta(t_0) \tag{2.109}$$

as the general solution of the equation of motion with initial conditions $\zeta(t_0)$.

2.6.5. The Simple Lattice Case

Equation (2.109) is not only simple-looking but useful as well; it leads to the explicit expressions of time evolution through the Green's operator discussed in Sections 2.2–2.4. Indeed, consider first the case of the simple lattice of Section 2.2; $\mathbb{M} = M\mathbb{1}$, $\mathbb{C} = \mathbb{0}$, and $\mathbb{K} = -k\mathbb{\Delta}$. The operator $\mathbb{H}_{II}$ takes the form

$$\mathbb{H}_{II} = \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} \qquad \text{(simple lattice)}. \tag{2.110}$$

Its square is already diagonal,

$$\mathbb{H}_{II}^2 = \begin{pmatrix} M^{-1}k\mathbb{\Delta} & \mathbb{0} \\ \mathbb{0} & M^{-1}k\mathbb{\Delta} \end{pmatrix}, \tag{2.111a}$$

and its even powers can be written as

$$\mathbb{H}_{II}^{2m} = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} (M^{-1}k\mathbb{\Delta})^m. \tag{2.111b}$$

The exponential series can be then evaluated as

$$\begin{aligned} \exp(t\mathbb{H}_{II}) &= \left(\sum_{n=0\,\text{even}}^{\infty} + \sum_{n=1\,\text{odd}}^{\infty} \right) \frac{t^n}{n!} \mathbb{H}_{II}^n \\ &= \sum_{m=0}^{\infty} \frac{t^{2m}}{(2m)!} \mathbb{H}_{II}^{2m} + \mathbb{H}_{II} \sum_{m=0}^{\infty} \frac{t^{2m+1}}{(2m+1)!} \mathbb{H}_{II}^{2m} \\ &= \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} \sum_{m=0}^{\infty} \frac{[t(M^{-1}k\mathbb{\Delta})^{1/2}]^{2m}}{(2m)!} \\ &\quad + \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} [M^{-1}k\mathbb{\Delta}]^{-1/2} \sum_{m=0}^{\infty} \frac{[t(M^{-1}k\mathbb{\Delta})^{1/2}]^{2m+1}}{(2m+1)!}. \end{aligned} \tag{2.112}$$

In the last member we have arranged things so that the cosh x and x^{-1} sinh x power series are manifest, noting that only integer powers of the operator $\mathbb{\Delta}$ are actually involved. This allows us to write

$$\begin{aligned} \mathbb{G}_{II}(t) &:= \exp(t\mathbb{H}_{II}) = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} \cosh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \\ &\quad + \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} (M^{-1}k\mathbb{\Delta})^{-1/2} \sinh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \\ &= \begin{pmatrix} \dot{\mathbb{G}}(t) & M^{-1}\mathbb{G}(t) \\ k\mathbb{\Delta}\mathbb{G}(t) & \dot{\mathbb{G}}(t) \end{pmatrix}, \end{aligned} \tag{2.113}$$

having defined

$$\mathbb{G}(t) := (M^{-1}k\mathbb{\Delta})^{-1/2} \sinh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \tag{2.114a}$$

and

$$\dot{\mathbb{G}}(t) = \cosh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \tag{2.114b}$$

as its time derivative [see Eqs. (1.76)–(1.79)]. The definition (2.114) is not new: it has already appeared in Eq. (1.73) for $M = 1 = k$ and corresponds exactly to the $\mathscr{V}^N$ Green's operator and its time derivative for the simple lattice. We can then write Eqs. (2.109) and (2.113) as

$$\boldsymbol{\zeta}(t) = \mathbb{G}_{II}(t - t_0)\boldsymbol{\zeta}(t_0). \tag{2.115}$$

In terms of the $\mathbf{f}$- and $\dot{\mathbf{f}}$-components and initial conditions,

$$\begin{pmatrix} \mathbf{f}(t) \\ \dot{\mathbf{f}}(t) \end{pmatrix} = \begin{pmatrix} \dot{\mathbb{G}}(t - t_0) & \mathbb{G}(t - t_0) \\ \ddot{\mathbb{G}}(t - t_0) & \dot{\mathbb{G}}(t - t_0) \end{pmatrix} \begin{pmatrix} \mathbf{f}_0 \\ \dot{\mathbf{f}}_0 \end{pmatrix}. \tag{2.116}$$

In the last expression we have used (2.104) and introduced $\ddot{\mathbb{G}}(t - t_0)$ through differentiation of (2.114b) in order to replace the 1-2 element of the matrix (2.113). This is only a restatement of the time-evolution equation (2.29) and its derivative.

2.6.6. Group Properties

Several relations in $\mathscr{V}^N$ between the equation of motion and the Green's operator become simplified in $\mathscr{V}^N_{II}$ where $\mathbb{G}_{II}(t)$ is the sole time-evolution operator. From (2.113) and the composition of two exponential functions of the same operator, Eq. (1.70), it follows that

$$\mathbb{G}_{II}(t_1)\mathbb{G}_{II}(t_2) = \mathbb{G}_{II}(t_1 + t_2) \tag{2.117}$$

as well as

$$\mathbb{G}_{II}(0) = \mathbb{1}, \tag{2.118}$$

where here $\mathbb{1}$ is the unit operator in $\mathscr{V}^N_{II}$. Writing $\mathbb{G}_{II}$ in 2×2 matrix form, we reproduce Eqs. (2.31).

The foregoing two equations and the obvious property of associativity show that the time-evolution operators have the first three properties of a *group* (Section 1.4). The fourth defining property, that of the existence of an *inverse* operator $\mathbb{G}_{II}^{-1}(t)$ for every $\mathbb{G}_{II}(t)$, is also true here. In fact,

$$\mathbb{G}_{II}^{-1}(t) = \mathbb{G}_{II}(-t), \tag{2.119}$$

as can be seen from its definition (2.113), (2.117), or explicit calculation. The set of time-evolution operators $\mathbb{G}_{II}(t)$ for $t \in (-\infty, \infty)$ thus forms a *one-parameter continuous* group of time translations *generated* by $\mathbb{H}_{II}$. As the group elements *commute* [this can be seen by exchanging t_1 and t_2 in (2.117)], the group is said to be *abelian.* Thus far in this section we have been speaking in basis-independent vector and operator language. The physical displacements of the lattice elements and their momenta are the coordinates of $\boldsymbol{\zeta}$ in $\boldsymbol{\varepsilon}$-bases for the displacement and momentum $\mathscr{V}^N$'s in $\mathscr{V}^N_{II} = \mathscr{V}^N \oplus \mathscr{V}^N$. We shall assume that the two $\mathscr{V}^N$'s are described by the same basis.

2.6.7. Evolution Operator in Normal Mode Basis

When it comes to the explicit expression for the time-evolution operator we can make good use of the Fourier transform since $\mathbb{G}_{II}(t)$ is the exponential of $\mathbb{H}_{II}$ and thus will be represented by a matrix with four diagonal blocks whenever $\mathbb{H}_{II}$ is likewise represented. As the operators in the 2×2 matrix form of $\mathbb{H}_{II}$ are, in the simple case (2.110), only multiples of $\mathbb{\Delta}$ and $\mathbb{1}$, this happens in the Fourier φ-basis. The matrix equation then uncouples into N separate 2×2 matrix equations each of the form

$$\begin{pmatrix} \tilde{f}_m(t) \\ \dot{\tilde{f}}_m(t) \end{pmatrix} = \begin{pmatrix} \tilde{G}_m(t - t_0) & \tilde{G}_m(t - t_0) \\ \dot{\tilde{G}}_m(t - t_0) & \dot{\tilde{G}}_m(t - t_0) \end{pmatrix} \begin{pmatrix} \tilde{f}_m(t_0) \\ \dot{\tilde{f}}_m(t_0) \end{pmatrix}.$$

$$m = 1, 2, \ldots, N, \quad (2.120a)$$

where, from (2.114),

$$\tilde{G}_m(t - t_0) = (M^{-1}k\lambda_n)^{-1/2} \sinh[t(M^{-1}k\lambda_n)^{1/2}]. \quad (2.120b)$$

Of course, this is precisely Eqs. (2.28): Recall that the elements of diagonal $\tilde{\Delta}$ are λ_n [see Eqs. (1.62)], and use the identity $(ix)^{-1} \sinh ix = x^{-1} \sin x$.

In terms of $2N$-dimensional phase-space diagrams, the motion in the φ-basis (2.120) appears as in Fig. 2.24 in each of the N Fourier component phase-space planes. The oscillation frequencies are different for different m's.

Exercise 2.52. Differentiating (2.113), show that

$$\mathbb{H}_{II}\mathbb{G}_{II}(t) = \mathbb{G}_{II}(t)\mathbb{H}_{II} = \dot{\mathbb{G}}_{II}(t), \quad (2.121)$$

i.e., the time-evolution operator commutes with its generator and is a solution of the lattice equation of motion. Compare with (2.30).

Exercise 2.53. Write out explicitly the time-evolution operator for a general interaction operator $\mathbb{K}$ (when $\mathbb{M} = M\mathbb{1}$ and $\mathbb{C} = \mathbb{0}$, covering the cases of the farther-neighbor interaction and molecular lattices). Show that you need only replace $k\mathbb{\Delta}$ by $-\mathbb{K}$ in (2.113) and (2.114). All the subsequent equations follow without change; in particular, the Fourier transform continues to provide a basis, where Green's operator is represented by a block-diagonal matrix.

Exercise 2.54. Consider the case of the diatomic lattice in Section 2.4. There, we saw, $\mathbb{M}$ and $\mathbb{K}$ are self-adjoint but do not commute. Carry out the exponentiation of the generator (2.107) (for $\mathbb{C} = \mathbb{0}$) with due care. Show that

$$\mathbb{H}_{II}^{2n} = \begin{pmatrix} (-\mathbb{M}^{-1}\mathbb{K})^n & \mathbb{0} \\ \mathbb{0} & (-\mathbb{K}\mathbb{M}^{-1})^n \end{pmatrix} \quad \text{(general, undamped).} \quad (2.122)$$

Following (2.111)–(2.113), one arrives at the expression

$$\mathbb{G}_{II}(t) = \begin{pmatrix} \dot{\mathbb{G}}(t) & \mathbb{M}^{-1}\mathbb{G}(t)^\dagger \\ -\mathbb{K}\mathbb{G}(t) & \dot{\mathbb{G}}(t)^\dagger \end{pmatrix}, \quad (2.123a)$$

which generalizes (2.113) for noncommuting operators. Here,

$$\mathbb{G}(t) = (-\mathbb{M}^{-1}\mathbb{K})^{-1/2} \sinh[t(-\mathbb{M}^{-1}\mathbb{K})^{1/2}] \quad \text{(general, undamped).} \quad (2.123b)$$

Note that for any well-defined function P,

$$\mathbb{M}^{-1}P(\mathbb{M}^{-1}\mathbb{K})^{\dagger} = \mathbb{M}^{-1}P(\mathbb{K}\mathbb{M}^{-1}) = P(\mathbb{M}^{-1}\mathbb{K})\mathbb{M}^{-1}, \tag{2.124a}$$

$$\mathbb{K}P(\mathbb{M}^{-1}\mathbb{K}) = P(\mathbb{K}\mathbb{M}^{-1})\mathbb{K} = \mathbb{M}P(\mathbb{M}^{-1}\mathbb{K})\mathbb{M}^{-1}\mathbb{K}. \tag{2.124b}$$

This allows one to generate various identities. In particular, it should be noticed that if we have found a basis where $\mathbb{M}^{-1}\mathbb{K}$ is represented by a diagonal matrix, as in the treatment of the diatomic lattice in Section 2.4, Green's operator $\mathbb{G}(t)$ in $\mathscr{V}^N$ and its time derivatives will also be diagonal and easily calculable from (2.123b). However, the block entries of the time-evolution operator (2.123a) involve operators $\mathbb{M}^{-1}\mathbb{G}(t)^{\dagger}$ and $\mathbb{K}\mathbb{G}(t)$ which are *not* diagonal. Not all is lost, however, since the expressions for $\mathbb{M}^{-1}$ and $\mathbb{K}$ are usually simple to calculate if we know the basis explicitly. This is the case for the diatomic lattice, where the basis in which $\mathbb{M}^{-1}\mathbb{K}$ is diagonal is given by (2.89). Try implementing this program in detail.

Exercise 2.55. Allow for damping. One can solve exactly the case when $\mathbb{M} = M\mathbb{1}$ and $\mathbb{C} = c\mathbb{1}$ using the results in Exercises 1.55 and 1.56, transforming $\mathbb{H}_{II}$ to diagonal form, exponentiating, and transforming back [i.e., Eq. (1.71)]. Show that this leads to the time-evolution operator in $\mathscr{V}_{II}^{N}$ given by

$$\mathbb{G}_{II}^{cM}(t) = \begin{pmatrix} \dot{\mathbb{G}}^{cM}(t) + 2\Gamma\mathbb{G}^{cM}(t) & M^{-1}\mathbb{G}^{cM}(t) \\ -\mathbb{K}\mathbb{G}^{cM}(t) & \dot{\mathbb{G}}^{cM}(t) \end{pmatrix}, \tag{2.125a}$$

where

$$\mathbb{G}^{cM}(t) = \exp(-\Gamma t)\mathbb{U}^{-1/2}\sinh t\mathbb{U}^{1/2} \qquad \text{(damped)}, \tag{2.125b}$$

$$\mathbb{U} = \Gamma^2\mathbb{1} - M^{-1}\mathbb{K}, \qquad \Gamma = c/2M. \tag{2.125c}$$

Compare with the results of Exercise 2.16. Notice that here, too, the Fourier φ-basis allows for the explicit solution of the problem.

Exercise 2.56. Following Exercise 2.17, consider the limit of (2.125) when the masses are very small, so damping overwhelms inertia and $\Gamma = c/2M \to \infty$, while c remains finite. The phase-space description breaks down; $\mathbf{f}$ and $\dot{\mathbf{f}}$ become uncoupled as the time-evolution operator (2.125) written in the form (2.116) becomes diagonal. Here again the Fourier φ-basis is the appropriate one.

Exercise 2.57. Given the time-evolution operator $\mathbb{G}^{cM}(t)$ in (2.123) and (2.125), verify that, indeed, it is generated by $\mathbb{H}_{II}$ of Eq. (2.107). To this end, refer to Eqs. (1.76) and (1.79), which are independent of the adjunction properties of the operators involved.

There is another area we should like to present in our study of vector analysis in phase space: the role of the symmetry of a system in finding its constants of motion.

2.6.8. Energy as a Sesquilinear Form

The expression for the energy, Eq. (2.96), can be generalized to a *sesquilinear form* in $\mathscr{V}_{II}^{N}$. Indeed, we can write for the undamped case

$$\begin{aligned} E(\zeta_1, \zeta_2) &:= \tfrac{1}{2}(\mathbf{f}_1, \mathbb{K}\mathbf{f}_2) + \tfrac{1}{2}(\mathbf{g}_1, \mathbb{M}^{-1}\mathbf{g}_2) \\ &= (\mathbf{f}_1^\dagger \quad \mathbf{g}_1^\dagger)\begin{pmatrix} \tfrac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \tfrac{1}{2}\mathbb{M}^{-1} \end{pmatrix}\begin{pmatrix} \mathbf{f}_2 \\ \mathbf{g}_2 \end{pmatrix} =: \zeta_1^\dagger \mathbb{E}_{II}\zeta_2. \end{aligned} \tag{2.126}$$

We shall call $\mathbb{E}_{II}$ the *energy operator*. The adjunction of $\mathscr{V}_{II}^{N}$ vectors and operators is defined in terms of the corresponding adjunction of vectors and matrix representatives in $\mathscr{V}^{N}$: $\zeta^\dagger$ is the row vector whose elements are the complex conjugates of those of ζ in (2.105), and for $\mathscr{V}_{II}^{N}$ operators we transpose the 2×2 matrix and adjoin the $\mathscr{V}^{N}$ operator elements. Clearly, $E(\zeta, \zeta)$ (note $\zeta_1 = \zeta = \zeta_2$) is the energy corresponding to the phase-space state vector ζ. The conservation of the quantity (2.126) under time evolution of the undamped lattice can be proven through calculating

$$\begin{aligned} E(\zeta_1(t), \zeta_2(t)) &= \zeta_1^\dagger(t)\mathbb{E}_{II}\zeta_2(t) \\ &= \zeta_1^\dagger(t_0)\mathbb{G}_{II}^\dagger(t - t_0)\mathbb{E}_{II}\mathbb{G}_{II}(t - t_0)\zeta_2(t_0) \end{aligned} \tag{2.127}$$

and showing that this equals $E(\zeta_1(t_0), \zeta_2(t_0))$, i.e., that

$$\mathbb{G}_{II}^\dagger(t - t_0)\mathbb{E}_{II}\mathbb{G}_{II}(t - t_0) = \mathbb{E}_{II}. \tag{2.128}$$

One can verify directly that (2.128) is true by replacing the expressions for $\mathbb{G}_{II}^\dagger$, $\mathbb{G}_{II}$, and $\mathbb{E}_{II}$ as 2×2 matrices with operator elements from (2.123) and (2.126). It is more illuminating, however, to use an alternative proof which makes use of $\mathbb{H}_{II}$, the generator of $\mathbb{G}_{II}$. Consider infinitesimal time evolution, letting $\delta t := t - t_0$ be as small as we please. We can then use the exponential series in writing

$$\mathbb{G}_{II}(\delta t) = \exp(\delta t \mathbb{H}_{II}) \simeq \mathbb{1} + \delta t \mathbb{H}_{II}, \tag{2.129}$$

where we disregard terms of second and higher order in δt. Substitution into (2.128) yields

$$\mathbb{E}_{II} = (\mathbb{1} + \delta t \mathbb{H}_{II}^\dagger)\mathbb{E}_{II}(\mathbb{1} + \delta t \mathbb{H}_{II}). \tag{2.130}$$

Collecting terms in δt, we obtain

$$\mathbb{H}_{II}^\dagger \mathbb{E}_{II} + \mathbb{E}_{II}\mathbb{H}_{II} = \mathbb{0}. \tag{2.131}$$

This equation is easier to verify than (2.128), as it only involves products of two operators at a time:

$$\begin{aligned} \mathbb{H}_{II}^\dagger \mathbb{E}_{II} &= \begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix}^\dagger \begin{pmatrix} \tfrac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \tfrac{1}{2}\mathbb{M}^{-1} \end{pmatrix} = \begin{pmatrix} \mathbb{0} & -\mathbb{K}^\dagger \\ \mathbb{M}^{-1\dagger} & \mathbb{0} \end{pmatrix}\begin{pmatrix} \tfrac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \tfrac{1}{2}\mathbb{M}^{-1} \end{pmatrix} \\ &= \begin{pmatrix} \mathbb{0} & -\tfrac{1}{2}\mathbb{K}\mathbb{M}^{-1} \\ \tfrac{1}{2}\mathbb{M}^{-1}\mathbb{K} & \mathbb{0} \end{pmatrix} = -\begin{pmatrix} \tfrac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \tfrac{1}{2}\mathbb{M}^{-1} \end{pmatrix}\begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix} \\ &= -\mathbb{E}_{II}\mathbb{H}_{II}. \end{aligned} \tag{2.132a}$$

Now, the validity of (2.131) implies the validity of the original equation (2.128), since for any power n,

$$(\mathbb{H}_{II}^{\dagger})^n \mathbb{E}_{II} = -(\mathbb{H}_{II}^{\dagger})^{n-1} \mathbb{E}_{II} \mathbb{H}_{II} = \cdots = (-1)^n \mathbb{E}_{II} \mathbb{H}_{II}^n, \tag{2.132b}$$

and similarly for any sum of powers. Thus, for any well-defined function P of $\mathbb{H}_{II}$ (see Section 1.5),

$$P(\mathbb{H}_{II}^{\dagger}) \mathbb{E}_{II} = \mathbb{E}_{II} P(-\mathbb{H}_{II}). \tag{2.132c}$$

When $P = \exp$, Eq. (2.128) is proven.

We would like to stress that the invariance of the sesquilinear form for the energy is a consequence of the *operator* equation (2.131). If we can find a basis $\{\psi_n\}_{n=1}^N$ in $\mathscr{Y}^N$ such that $\mathbb{H}_{II}$ be represented by a 2×2 matrix of diagonal $N \times N$ blocks, then $\mathbb{E}_{II}$ will be similarly represented since it is constituted by the same operators. It follows that we will have N conserved "partial" energies since the analogue of Eqs. (2.128)–(2.131) holds for each 2×2 submatrix involving the mth and $(N + m)$th rows and columns. These are the E_m^{ψ} in Eq. (2.101).

2.6.9. Other Conserved Sesquilinear Forms and Symmetry

We can now turn the tables and investigate how to construct conserved sesquilinear forms in $\mathscr{Y}_{II}^N$, i.e., to find operators $\mathbb{F}_{II}$ such that

$$F(\zeta_1, \zeta_2) := \zeta_1^{\dagger} \mathbb{F}_{II} \zeta_2, \qquad \mathbb{F}_{II} = \begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix} \tag{2.133}$$

is a constant of the motion. The form (2.133) will be conserved if and only if Eq. (2.131) holds, $\mathbb{F}_{II}$ replacing the energy operator $\mathbb{E}_{II}$; that is,

$$\begin{pmatrix} \mathbb{0} & -\mathbb{K} \\ \mathbb{M}^{-1} & \mathbb{0} \end{pmatrix} \begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix} = -\begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix} \begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix}. \tag{2.134}$$

This embodies the four equations

$$\mathbb{M}^{-1} \mathbb{F}_a = \mathbb{F}_d \mathbb{K}, \tag{2.135a}$$

$$\mathbb{K} \mathbb{F}_d = \mathbb{F}_a \mathbb{M}^{-1}, \tag{2.135b}$$

$$\mathbb{K} \mathbb{F}_c = -\mathbb{F}_b \mathbb{K}, \tag{2.135c}$$

$$\mathbb{M}^{-1} \mathbb{F}_b = -\mathbb{F}_c \mathbb{M}^{-1}. \tag{2.135d}$$

Note that if we have two operators $\mathbb{F}_{II}^{(1)}$ and $\mathbb{F}_{II}^{(2)}$ satisfying (2.134)–(2.135), any linear combination of them will also be an operator leading to a conserved sesquilinear form. We thus need only look for a *basis* of $\mathbb{F}_{II}$'s satisfying these equations. If we set $\mathbb{F}_b = \mathbb{0} = \mathbb{F}_c$ in (2.135) so that the last two equations are trivially satisfied, one solution to the two first ones is $\mathbb{F}_a = c\mathbb{K}$, $\mathbb{F}_d = c\mathbb{M}^{-1}$ for any constant c. This yields, for $c = \frac{1}{2}$, the energy operator $\mathbb{E}_{II}$.

Consider next setting $\mathbb{F}_a = \mathbb{0} = \mathbb{F}_d$ and $\mathbb{F}_c = -\mathbb{F}_b$. This leaves then the requirement that $\mathbb{F}_b$ *commute* with $\mathbb{K}$ and $\mathbb{M}$. In light of Sections 1.6, 2.3, and 2.4 we see that $\mathbb{F}_b$ may be *any of the operators of the dihedral group which are symmetries of the lattice.*

2.6.10. All Constants of Motion for the Simple Lattice

For definiteness, consider the simple lattice (equal masses and springs) where the symmetry group is constituted by rotations $\mathbb{R}^k$ and inversions $\mathbb{I}_l$ and $\mathbb{K}_m$, letting $\mathbb{D}$ stand for any linear combination of these operators.

The operators we are examining here will thus have the form

$$\mathbb{F}_{II} = \begin{pmatrix} \mathbb{0} & \mathbb{D} \\ -\mathbb{D} & \mathbb{0} \end{pmatrix}, \tag{2.136a}$$

$$\mathbb{D} = \sum_k a_k \mathbb{R}^k + \sum_l b_l \mathbb{I}_l + \sum_m c_m \mathbb{K}_m. \tag{2.136b}$$

The associated conserved quantity for a particular lattice state is the form (2.133) for $\zeta_1 = \zeta = \zeta_2$:

$$\begin{aligned} F(\zeta, \zeta) = \zeta^\dagger \mathbb{F}_{II} \zeta &= (\mathbf{f}, \mathbb{D}\mathbf{g}) - (\mathbf{g}, \mathbb{D}\mathbf{f}) \\ &= \sum_{m,n} D_{mn}(f_m^* g_n - g_m^* f_n) \\ &= \sum_{m,n} \tilde{D}_{mn}(\tilde{f}_m^* \tilde{g}_n - \tilde{g}_m^* \tilde{f}_n). \end{aligned} \tag{2.137}$$

If we now ask the physical displacements and momenta to be real, the next to last member in (2.137) tells us that unless $D_{mn} = -D_{nm}$, the constant (2.137) will vanish. If we look up the matrix elements of the dihedral operators [Eqs. (1.89) and (1.99)],we see that the inversions $\mathbb{I}_l$ and $\mathbb{K}_m$ are symmetric; hence they cannot be in $\mathbb{D}$, which can only consist then of combinations of $\mathbb{R}^k - \mathbb{R}^{-k}$, i.e.,

$$\begin{aligned} F_k^R &:= \sum_{m,n} (\delta_{m,n+k} - \delta_{m,n-k})(f_m g_n - g_m f_n) \\ &= \sum_n (f_n g_{n-k} - g_n f_{n-k}). \end{aligned} \tag{2.138}$$

This form is reminiscent of angular momentum. Out of the constant of motion (2.133) we can also find "partial" conserved quantities. In the φ-basis the operator $\mathbb{R}^k - \mathbb{R}^{-k}$ is represented by a diagonal matrix [Eq. (1.91)] which, when substituted into (2.137), leads to

$$F_k^R = -4 \sum_m \sin(2\pi km/N) \operatorname{Im}(\tilde{f}_m^* \tilde{g}_m). \tag{2.139}$$

Since $\mathbb{F}_{II}$ has diagonal blocks in the φ-basis, it follows that (for k not a divisor of N) the members of the sum (2.139) are separately conserved, that is,

$$F_m := \mathrm{Im}(\tilde{f}_m^* \tilde{g}_m), \qquad m = 1, 2, \ldots, N, \tag{2.140}$$

are N constants of motion which arise because of the invariance of the lattice under rotations. These, together with the partial-wave energies E_m^{Ψ} in (2.101), give $2N$ constants of motion. The lattice with real displacements is expected to have no more constants of motion than the parameters needed to specify its initial condition: a total of $2N$ numbers. (See Exercise 2.60.) In terms of the N-dimensional phase-space diagram in the φ-basis (Fig. 2.24), the partial energies E_m^{Ψ} fix the radii of the circles, while the F_m are related to the angular coordinates of the initial conditions.

Exercise 2.58. Verify directly, using the explicit lattice solutions (2.28), that (2.140) are indeed independent of time.

Exercise 2.59. Using the vector form of the equations of motion, show from the third member of (2.137) that $dF/dt = 0$. The derivation is parallel to (2.97).

Exercise 2.60. When we examined the choice $\mathbb{F}_b = \mathbb{0} = \mathbb{F}_c$ in (2.134) we glossed over pointing out a more general solution to the remaining operators: $\mathbb{F}_a = \mathbb{K}\mathbb{D}$, $\mathbb{F}_d = \mathbb{M}^{-1}\mathbb{D}$, where $\mathbb{D}$ is any operator (2.136b) embodying the symmetry group of the lattice. Follow the argument starting from (2.136) to show that for real constants of motion one needs $\mathbb{D}$'s such that $\tilde{D}_{mn} = \tilde{D}_{nm}^*$. This excludes rotations but allows operators of the kind $\mathbb{I}_l + \mathbb{I}_{-l}$ [see Eq. (1.92)] or $\mathbb{K}$'s when permitted. Show that, as in finding (2.140), this does not bring in new independent constants of motion.

Exercise 2.61. The sesquilinear form $E(\zeta_1, \zeta_2)$ in (2.126) can be thought of as defining an inner product (see Section 1.2) with *metric* $\mathbb{E}_{II}$. Note, however, that this is not a *positive* inner product, since there exists a nonzero vector $\zeta_0 := \binom{\varphi}{0}_N$ such that $E(\zeta_0, \zeta_0) = 0$. This represents the energy of a lattice at rest with all masses having equal displacements. Such a *nonnegative* inner product does not allow for the unique definition of the adjoint of an operator. Nevertheless, one can help oneself with the adjunction in $\mathscr{V}^N$ in order to define a unique adjoint under $E(\zeta_1, \zeta_2)$. The conceptual advantage of this point of view is that Eq. (2.128) becomes the statement that *time evolution is a unitary transformation of phase space*. The generator of this transformation, $\mathbb{H}_{II}$, is such that $i\mathbb{H}_{II}$ is self-adjoint under $E(\zeta_1, \zeta_2)$: Eq. (2.131). In this connection, recall Exercise 1.33.

To sum up, we would like to emphasize the role which the Fourier transform played in the reduction of the description of coupled systems to that of its uncoupled elements. Since *a posteriori* we see that the solutions always involve superpositions of sine waves, it stands to reason that a sine-wave basis of solutions should be the proper approach to the problem. The vector space version of this constitutes the essence of the foregoing sections. Sine waves are not only periodic but have the property that all their deriva-

tives—or even finite differences—are also functions of the same kind. We can expect them to appear in most problems which involve linear difference equations with constant coefficients. When the coefficients are not constant, other functions appear—the special functions of mathematical physics—which lend themselves to analyses which parallel Fourier analysis. We shall have a taste of this in the sections on circular membrane vibration modes and oscillator wave functions.

3

Further Developments and Applications of the Finite Fourier Transform

In actual applications, most mathematical methods have to deal with finite data sets. Thus it is not surprising that the *finite* Fourier transform is the main tool among transforms in applied research. Two topics in communication science have been selected to illustrate the use of the finite Fourier transform: signal filters and windows in Section 3.1 and signal detection in the presence of noise in Section 3.2. These make use of the operations of convolution and correlation. The implementations of these techniques would be impossible without present-day computers and an efficient algorithm for the numerical work. The fast Fourier transform (FFT) operating principles are given in Section 3.3. Finally, in Section 3.4 we let the dimension of the vector space grow without bound. In this way we arrive at the Fourier series and integral transforms which are the subjects of Parts II and III. The sections are mutually independent except for Section 3.2, which relies somewhat on concepts developed in Section 3.1. Otherwise, they can be read in any order. The References should be consulted if the reader wishes a wider picture of the applied technology.

3.1. Convolution: Filters and Windows

The operation of convolution between the components of two vectors in $\mathcal{V}^N$ does not commonly appear in ordinary vector analysis but is quite important in the applications of the Fourier transform to communication

theory and technology. We shall first introduce this operation in a rather general setting and then particularize to the case of interest as applied to signal filtering and windowing.

3.1.1. The Coordinate-by-Coordinate Product Relative to a Basis

Let $\mathbf{f}$ and $\mathbf{g}$ be two vectors in $\mathscr{V}^N$, with coordinates $\{f_n\}_{n=1}^N$ and $\{g_n\}_{n=1}^N$ in the $\boldsymbol{\varepsilon}$-basis (see Sections 1.1 and 1.2). Construct now a vector $\mathbf{h} \in \mathscr{V}^N$ whose coordinates in the same basis are

$$h_n = f_n g_n, \qquad n = 1, 2, \ldots, N, \tag{3.1}$$

i.e., simply the coordinate-by-coordinate product of the first two vectors. We denote thus

$$\mathbf{h} \coloneqq \mathbf{f}(\boldsymbol{\varepsilon})\,\mathbf{g}, \tag{3.2}$$

defining a mapping from $\mathscr{V}^N \times \mathscr{V}^N$ into $\mathscr{V}^N$ which we call the *product* of vectors $\mathbf{f}$ and $\mathbf{g}$ *relative* to the $\boldsymbol{\varepsilon}$-basis. To determine the coordinates $\{\bar{h}_m\}_{m=1}^N$ of $\mathbf{h}$ in (3.2) in any *other* $\bar{\boldsymbol{\varepsilon}}$-basis obtained from the first one through a transformation $\mathbf{V}$ (see Section 1.2), we perform

$$\begin{aligned}
\bar{h}_m &= \sum_n (V^{-1})_{mn} h_n = \sum_n V_{mn}^{-1} f_n g_n \\
&= \sum_n V_{mn}^{-1} \sum_k V_{nk} \bar{f}_k \sum_l V_{nl} \bar{g}_l \\
&= \sum_{k,l} C_{m,k,l}^{(V)} \bar{f}_k \bar{g}_l,
\end{aligned} \tag{3.3}$$

where

$$C_{m,k,l}^{(V)} \coloneqq \sum_n V_{mn}^{-1} V_{nk} V_{nl} \tag{3.4}$$

are the *coupling* coefficients for the $\bar{\boldsymbol{\varepsilon}}$-basis coordinates.

The definition of the product (3.1)–(3.2) is quite simple. It does not appear in ordinary three-dimensional vector analysis since it does not seem to have found any meaningful application. In Fourier analysis, we shall see that it is quite useful.

Exercise 3.1. Show that the *bilinear* product (3.1)–(3.2) is commutative, associative, and distributive with respect to vector addition. Perform the proof in the $\boldsymbol{\varepsilon}$- and $\bar{\boldsymbol{\varepsilon}}$-bases. What symmetries are implied for the coupling coefficients (3.4)?

3.1.2. Coupling Coefficients and Convolution

If the transformation **V** in (3.3)–(3.4) is the Fourier transform, the coupling coefficients are particularly simple:

$$\begin{aligned} C^{(F)}_{m,k,l} &= \sum_n F^*_{nm} F_{nk} F_{nl} \\ &= N^{-3/2} \sum_n \exp[2\pi i n(m - k - l)/N] \\ &= N^{-1/2} \delta_{m,k+l}. \end{aligned} \tag{3.5}$$

The expression for $\tilde{h}_m$ is then called the *convolution* of $\tilde{f}_n$ and $\tilde{g}_n$:

$$\tilde{h}_m = N^{-1/2} \sum_n \tilde{f}_n \tilde{g}_{m-n} = N^{-1/2} \sum_n \tilde{f}_{m-n} \tilde{g}_n =: N^{-1/2} (\tilde{f} * \tilde{g})_m, \tag{3.6}$$

where all indices are counted modulo N.

3.1.3. Product in the Fourier Basis

If the product (3.2) is now made relative to the φ-basis,

$$\mathbf{k} = \mathbf{f}(\varphi)\,\mathbf{g}, \tag{3.7a}$$

namely,

$$\tilde{k}_m = \tilde{f}_m \tilde{g}_m, \qquad m = 1, 2, \ldots, N, \tag{3.7b}$$

then the ε-basis coordinates of the vectors involved can be found using the coupling coefficients (3.4) for the inverse Fourier transform. These are only the complex conjugates of (3.5), so that

$$k_n = N^{-1/2} \sum_m f_m g_{n-m} = N^{-1/2} \sum_m f_{n-m} g_m =: N^{-1/2} (f * g)_n. \tag{3.8}$$

These formulas have been collected in Table 1.1 at the end of Chapter 1.

Exercise 3.2. Using the Schwartz inequality, show that for (3.7)–(3.8)

$$|k_n|^2 \leqslant N^{-1} \|\mathbf{f}\|^2 \|\mathbf{g}\|^2. \tag{3.9}$$

Note for the product (3.1)–(3.2) relative to any basis δ this implies that

$$\|\mathbf{f}(\delta)\mathbf{g}\| \leqslant N^{1/2} \|\mathbf{f}\|\, \|\mathbf{g}\|. \tag{3.10}$$

3.1.4. Signals

In discussing applications in signal filtering we shall first consider the product (3.7) of two vectors relative to the φ-basis and define what we mean

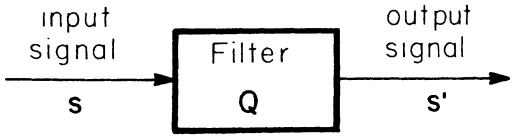


Fig. 3.1. Signal filtering.

here by a *signal vector* **s** and a *filter* $\mathbb{Q}$, showing then that the convolution (3.7)–(3.8) describes the output of the signal through the filter (see Fig. 3.1).

A *signal* **s** is an N-dimensional vector whose coordinates in the ε-basis represent the input data to a "black box" system. This can be a telephone conversation, a space probe coded message, or any other form of information

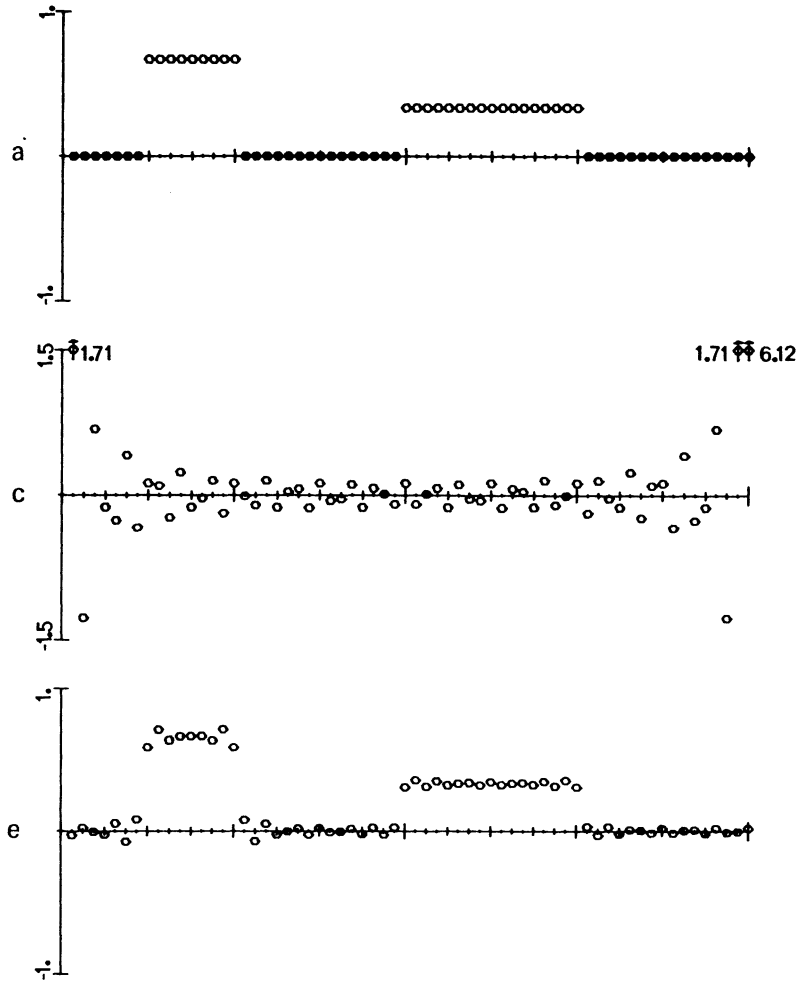
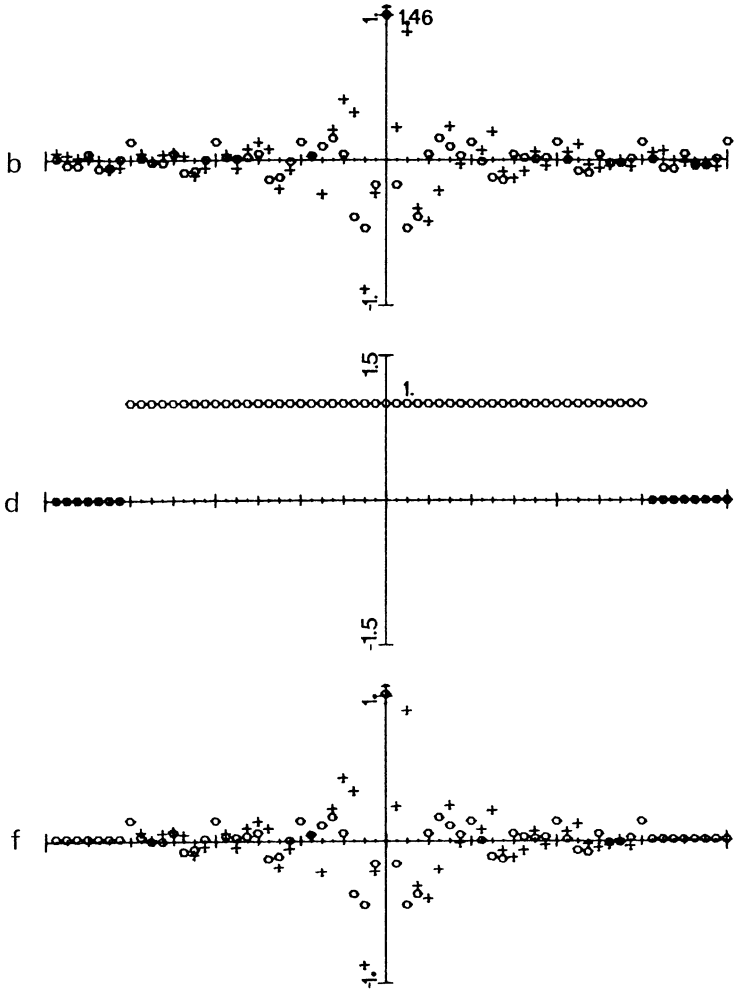


Fig. 3.2. (a) Signal. (b) Fourier transform of the signal. Real components are indicated by open circles, while imaginary components are denoted by crosses. As is customary, we are representing the Fourier-transformed components—the *frequency domain*—as extending on both sides of the $m = 0 \equiv N$ component. (c) Filter. (d) Transfer function of the filter [Fourier transform of (c)]. This is a low-pass filter which annuls the high-frequency components. Its transfer

which has finite length and which from the point of view of experiment can be taken to consist of a finite—albeit large—number of discrete data values. The consideration of discrete rather than continuous signals is here motivated by our mathematical construct but in practice corresponds to the impossibility of experimentally handling an actual infinity of data points. In Fig.



function is real and symmetric under reflections $m \leftrightarrow -m$; correspondingly, (c) exhibits the same characteristics. The product of (b) and (d) is (f), whose inverse Fourier transform is (e), the output filtered signal; (e) is thus the convolution of (a) and (c). Note that the suppression of the high-frequency components of the signal results in oscillations of the output in the neighborhood of its "discontinuities."

3.2(a) we show an example of a signal **s** with coordinates s_n, $n = 1, 2, \ldots, N$. In Fig. 3.2(b) the partial-wave content of **s** is shown: Equation (1.51b) states that

$$s_n = N^{-1/2} \sum_m \tilde{s}_m \exp(-2\pi i m n/N), \tag{3.11}$$

which displays the signal **s** as a sum of waveforms $\boldsymbol{\varphi}_m$ with amplitude proportional to $\tilde{s}_m$ (see Fig. 1.3). The quantities $p_m{}^s := |\tilde{s}_m|^2$ for $m = 1, 2, \ldots, N$ constitute the *power spectrum* of the signal **s**.

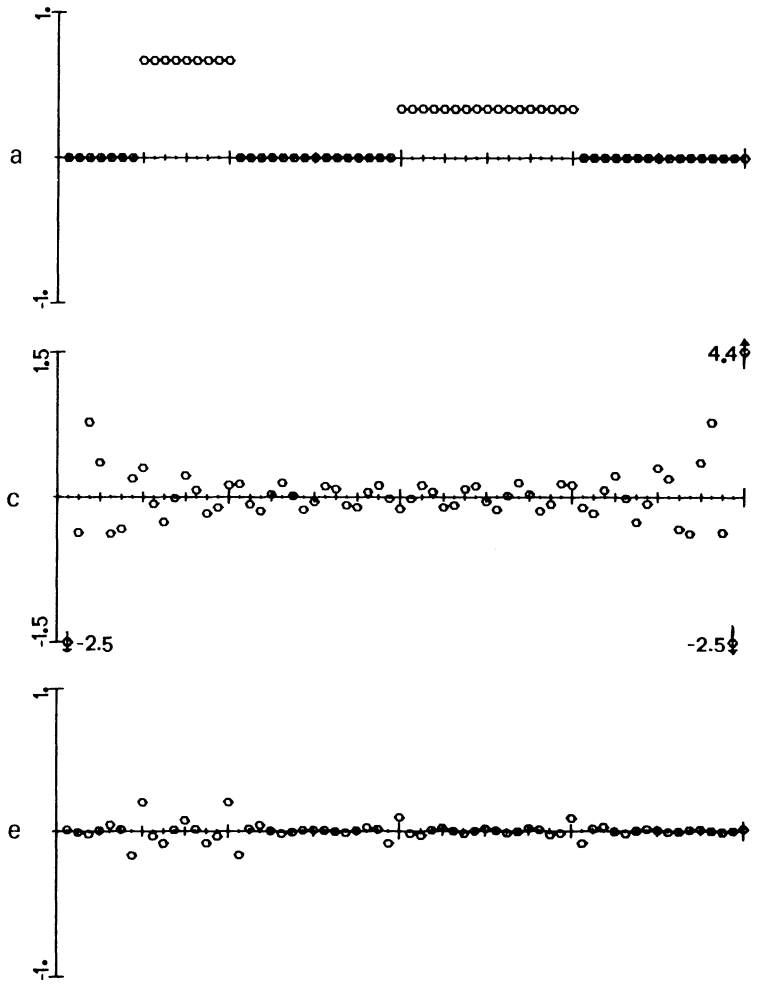
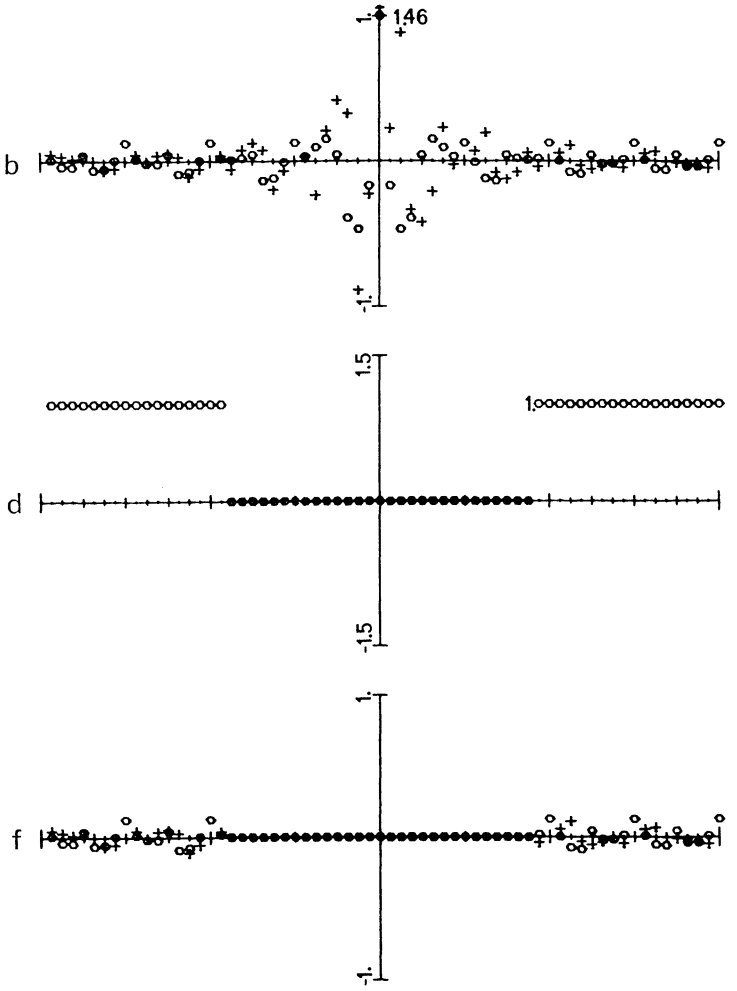


Fig. 3.3. (a) Signal (the same as in Fig. 3.2). (b) Fourier transform. (c) is the high-pass filter and (d) is its Fourier transform, i.e., the transfer function of the filter.

3.1.5. Filters

When the input signal $\mathbf{s}$ is fed into the "black box" signal processor in Fig. 3.1 it is converted into an *output* signal $\mathbf{s}'$. If a linear combination of input signals $\mathbf{s} = c_1\mathbf{s}_1 + c_2\mathbf{s}_2$, $c_1, c_2 \in \mathscr{C}$, is converted into the linear combination of the corresponding output signals $\mathbf{s}' = c_1\mathbf{s}'_1 + c_2\mathbf{s}'_2$, the box acts as a *linear operator* $\mathbb{Q}$ and $\mathbf{s}' = \mathbb{Q}\mathbf{s}$. To find the matrix $\|Q_{nm}\|$ representing $\mathbb{Q}$ in a given basis, we can test the box with *unit pulses*: We let $\mathbf{s} = \boldsymbol{\varepsilon}_n$ for



The product of (b) and (d) is (f). The output filtered signal is (e). The latter shows that under high-pass filtering it is mainly the "discontinuities" of the signal which remain.

$n = 1, 2, \ldots, N$ successively and then find the components $s'_m = (\boldsymbol{\varepsilon}_m, \mathbf{s}')$ of the output signal, thus constructing $Q_{nm} = s'_m$ for $n, m = 1, 2, \ldots, N$. The testing can also be done using the waveforms $N^{-1/2} \exp(-2\pi inm/N)$, which constitute the signal $\mathbf{s}$ in (3.11). In this case, we let $\mathbf{s} = \boldsymbol{\varphi}_n$ for $n = 1, 2, \ldots, N$, find the components $\tilde{s}'_m = (\boldsymbol{\varphi}_m, \mathbf{s}')$, and construct $\mathbb{Q}$ as represented by $\tilde{Q}_{nm} = \tilde{s}'_m$ for $n, m = 1, 2, \ldots, N$. Now, if the black box is such that *waveforms of a given frequency are converted into waveforms of the same frequency*, with only a possible change of amplitude and phase, the device will here be called a *filter*. (In actual technology, the meaning of a *filter* is very often widened to include any linear operator.) In this case, for a given $\mathbf{s} = \boldsymbol{\varphi}_n$ input, we obtain an output $\mathbf{s}' = \tilde{q}_n \boldsymbol{\varphi}_n$, $\tilde{q}_n$ being a complex number, $n = 1, 2, \ldots, N$. The set of coefficients $\{\tilde{q}_n\}_{n=1}^N$ is called the *transfer function* of the filter. It is easy to see that $\mathbb{Q}$ is then represented in the $\boldsymbol{\varphi}$-basis by a *diagonal* matrix $\tilde{\mathbf{Q}} = \|\delta_{nm}\tilde{q}_n\|$, and any input signal (3.11) will produce an output $\mathbf{s}'$ with partial-wave coefficients

$$\tilde{s}'_n = \tilde{q}_n \tilde{s}_n, \qquad n = 1, 2, \ldots, N; \qquad \text{i.e.,} \quad \mathbf{s}' = \mathbf{q}(\boldsymbol{\varphi})\mathbf{s}. \tag{3.12}$$

For a particular wave input $\mathbf{s} = \boldsymbol{\varphi}_n$, when $\tilde{q}_n = 1$, the wave passes through the filter undistorted, while if $|\tilde{q}_n| > 1$ or $|\tilde{q}_n| < 1$, the wave will be enhanced or attenuated.

Exercise 3.3. Show that if $\tilde{q}_n$, the transfer function of a filter, is complex, its phase $\arg \tilde{q}_n$ determines a phase shift in the signal waveform. This shift, in units of data point separation, is $\sigma_n = -(N/2\pi n) \arg \tilde{q}_n$. Devices such that $|\tilde{q}_n| = 1$ and $\sigma_n =$ constant (modulo N) are *delay* filters. Notice that as we are working here with the tools of finite-dimensional spaces, a delay filter would pass the last part of the input to the beginning of the output.

3.1.6. Low- and High-Pass Filters

If low frequencies are enhanced and high frequencies are attenuated, i.e., if $\tilde{q}_n$ is large for n near 0 (recall the coordinates are numbered modulo N and see Fig. 1.3) and small for n near $N/2$, we have a *low-pass* filter. If high frequencies are enhanced and low ones correspondingly suppressed, the filter is a *high-pass* one. In Fig. 3.2(d) we have drawn the transfer function of a "rectangular" low-pass filter and in Fig. 3.2(c) its inverse transform. The output signal partial-wave coefficients (3.12) are shown in Fig. 3.2(f) and the output signal in Fig. 3.2(e). The latter is the *convolution* of the input signal Fig. 3.2(a) and the transform [Fig. 3.2(c)] of the transfer function. In Fig. 3.3 a rectangular high-pass filter has been applied to the same signal. Note that the power spectrum of the output signal (3.12) is simply $p_m^{s'} = p_m^s |\tilde{q}_m|^2$. This is unchanged for delay filters (see Exercise 3.3).

We are generally interested in upgrading the quality of signals, not in degrading it as Figs. 3.2 and 3.3 may suggest. Transmission lines or storing

devices act in many ways as filters which attenuate the high-frequency components which constitute the "fine detail" of a signal. A high-pass filter which enhances these components can be used to restore the signal to its original sharpness. The proper transfer function of this upgrading filter is determined by determining the transfer function of the degrading process. Of course, if some frequencies are entirely suppressed, they cannot be restored; the effect of noise (to be described in Section 3.2) happens also to be most important in the high-frequency region, so practical considerations exist which curtail the possibilities of these devices.

Exercise 3.4. Assume that the input signal is passed through two (or more) filters with different transfer functions $\tilde{q}_n^{(1)}$ and $\tilde{q}_n^{(2)}$. These may be placed in *series* [Fig. 3.4(a)] or in *parallel* [Fig. 3.4(b)] with a signal-summing device. Show that

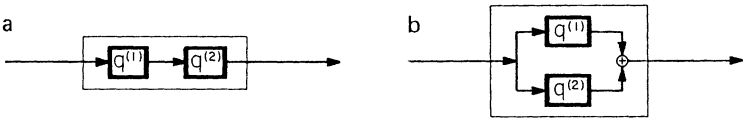


Fig. 3.4.

the filter arrays can be replaced by a single filter whose transfer function is $\tilde{q}_n = \tilde{q}_n^{(1)}\tilde{q}_n^{(2)}$ in the first case and $\tilde{q}_n = \tilde{q}_n^{(1)} + \tilde{q}_n^{(2)}$ in the second.

Exercise 3.5. An *averaging filter* produces an output signal $\mathbf{s}'$ whose components relate to the input signal $\mathbf{s}$ as $s'_m = (s_m + s_{m-1})/2$. Find the transfer function of such a filter to be $\tilde{q}_n = [1 + \exp(2\pi in/N)]/2$, and see that it enhances the lower frequencies. Note that, as an operator, the filter can be expressed by $\mathbb{Q} = (\mathbb{1} + \mathbb{R})/2$, where $\mathbb{R}$ is the rotation operator of Section 1.6. Such a filter will smooth out a signal and can be expected to reduce the noise (see Section 3.2).

Exercise 3.6. A *differencer filter* relates output to input by $s'_m = (s_m - s_{m-1})/2$. Find the transfer function, and see that it enhances the higher frequencies. A differencer filter will pick out *changes* in signal intensity and accentuate boundaries much like a Xerox copier when reproducing gray-tone images. Note that the second-difference operator $\mathbb{\Delta}$ of Sections 1.5 and 2.2 can be used as a filter too. Its spectrum tells us that it also enhances higher frequencies.

3.1.7. Windows

Our presentation of filtering devices has been overly optimistic. We have implied that the signal as a whole can be filtered when needed. A telephone conversation or even a speech spectrogram cannot be conveniently handled in this way. What must be done in these cases, roughly, is to break the full signal into consecutive pieces—time *windows*—each of which consists of a reasonably small set of data points which can be filtered and Fourier-analyzed separately. The process of windowing the signal corresponds mathematically

to multiplying the signal points s_n, $n = 1, 2, \ldots, N$, by a *window* function w_n, $n = 1, 2, \ldots, N$, which admits only data points between n_1 and n_2 and rejects all others: As a first example, we consider a *rectangular* window function:

$$r_n = \begin{cases} 1, & n_1 \leqslant n \leqslant n_2, \\ 0, & \text{otherwise.} \end{cases} \tag{3.13}$$

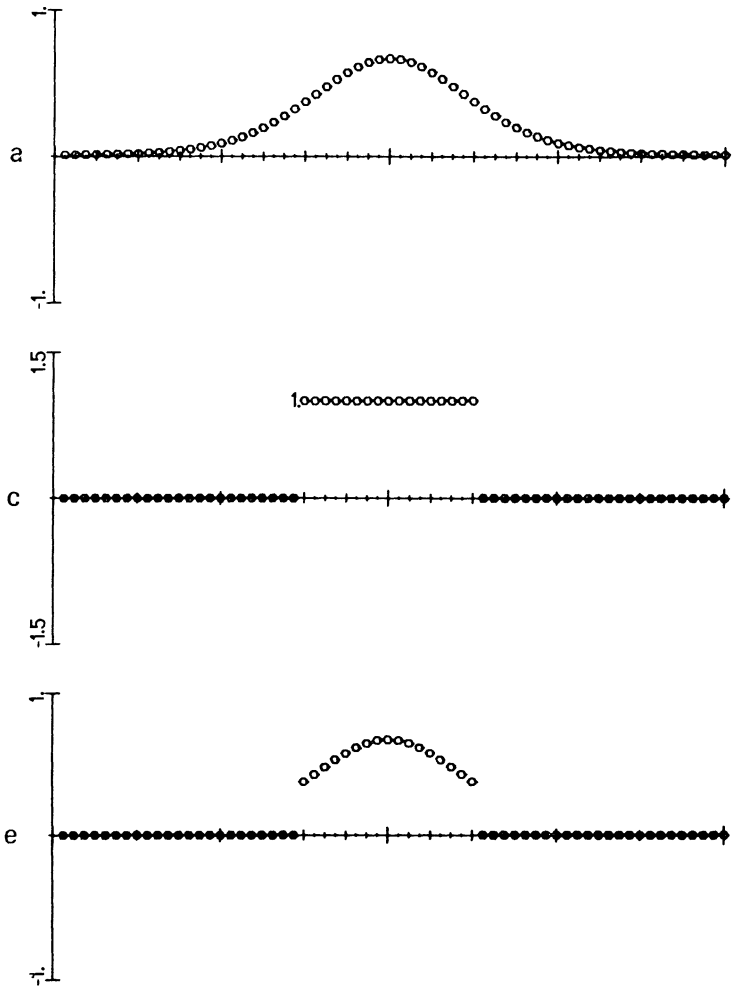
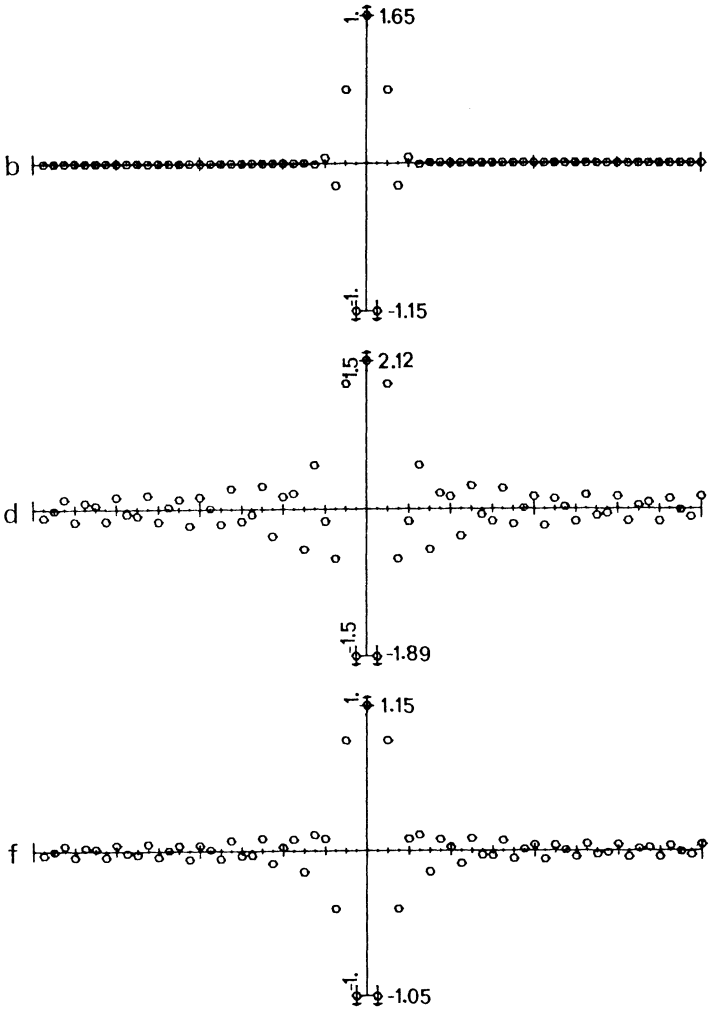


Fig. 3.5. (a) A "smooth" signal [representing the function in Eq. (2.38a)] and (b) its Fourier transform, exhibiting vanishingly small high-frequency components. (c) A rectangular "time window" and (d) its Fourier transform. The latter has

The output signal of such a windowing device is

$$s'_n = r_n s_n, \qquad \text{i.e.,} \quad \mathbf{s}' = \mathbf{r}(\varepsilon)\,\mathbf{s}. \tag{3.14}$$

In Fig. 3.5, we have used the rectangular window function [Fig. 3.5(c)] on a "smooth" signal [Fig. 3.5(a)] with little or no high-frequency components [Fig. 3.5(b)]. In chopping up a signal in this way [Fig. 3.5(e)], we are paying the price, due to the abruptness of the chop, of introducing spurious high-



significant components for all frequencies. (e) The chopped signal [the product of (a) and (c)]. (f) Fourier transform of (e) and convolution of (b) and (d). The appearance of high-frequency components is an artifact of the abrupt window function.

frequency components [Fig. 3.5(f)] which misrepresent the signal. This is an artifact of the window function we have used and can be seen to stem from the fact that the rectangular window function has a Fourier transform which is quite spread out in *side lobes*, with significant high-frequency components. The high-frequency components in Fig. 3.5(f) are a result of $\tilde{s}'_n$ being the convolution of $\tilde{s}_n$ with this spread-out window-transform function. This effect is termed *leakage*. To reduce the leakage effect it is desirable to use a window function whose Fourier transform has side lobes as small as possible.

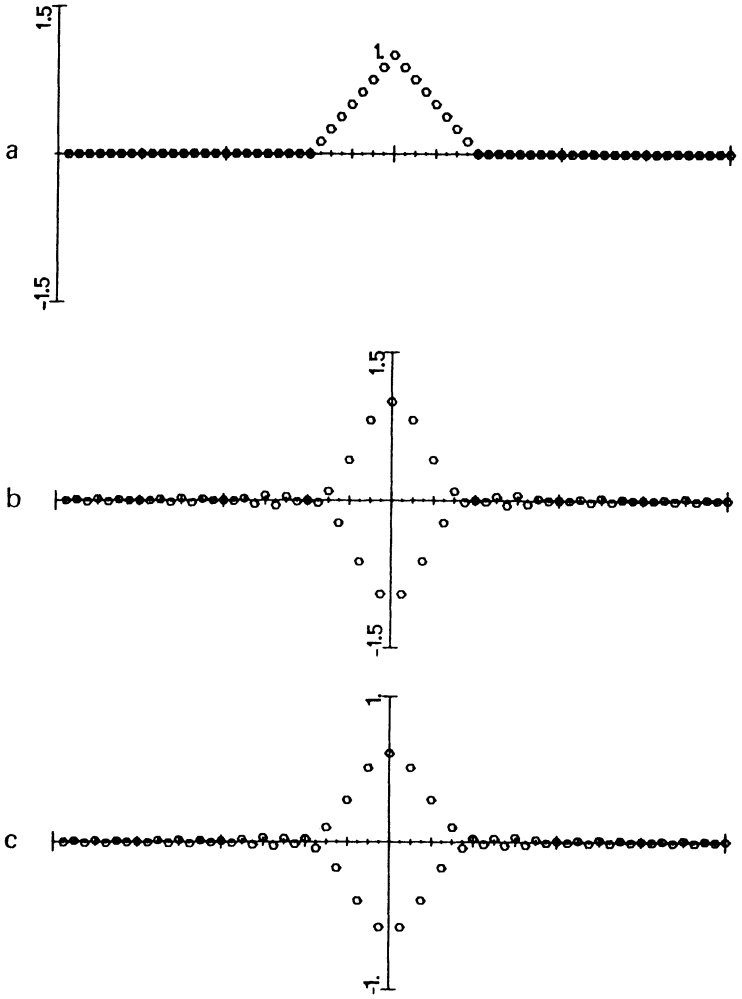


Fig. 3.6. (a) A triangular window function and (b) its Fourier transform. *Side lobes* are smaller here than in Fig. 3.5(d). (c) The smooth signal in Fig. 3.5(a) cut by this window exhibits smaller high-frequency components than in Fig. 3.5(f).

Instead of a rectangular window, a *triangular* function (Fig. 3.6) can be used, as its Fourier transform has smaller side lobes. An even better choice is the *Hanning* function, which has a $(1 - \cos \theta)$ form in its nonzero range (Fig. 3.7). The price paid for these improvements in the smoothing of the window is that there must be some window *overlap* in the description of the signal so that none of the signal components is slighted for falling at the edge of the window.

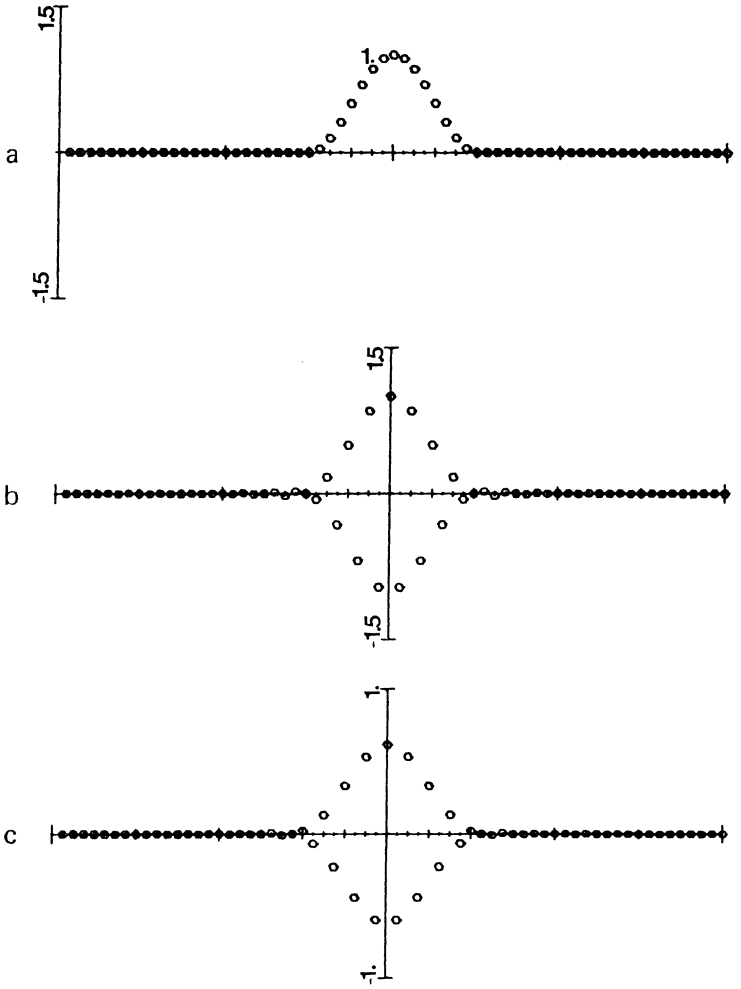


Fig. 3.7. (a) The Hanning function and (b) its Fourier transform. As the latter has negligible side lobes, the windowed "smooth" signal in Fig. 3.5(a), having basically no high-frequency components, (c), is expected to be acceptably "smooth" as well.

Exercise 3.7. Consider *amplitude modulation* of a *carrier wave* φ_c by a signal $\mathbf{s}^0$. The total input signal would then be $\mathbf{s}$,

$$s_n = (\varphi_c)_n s_n^0 = s_n^0 N^{-1/2} \exp(-2\pi i c n/N). \tag{3.15}$$

Show that the partial-wave coefficients of $\mathbf{s}$ are those of $\mathbf{s}^0$ but shifted by c units: $\tilde{s}_{m+c} \sim \tilde{s}_m^0$. Amplitude modulation can be used to transmit a very "smooth" signal, constituted only by low frequencies, through a communication line which strongly attenuates these frequencies. Shortwave AM radio, for instance, uses the transmission properties of electromagnetic waves of appropriately high frequency for the coding of low-frequency signals. FM, on the other hand, codes the signal into the Fourier transform components $\tilde{s}_n$ with proper time windowing.

We have tried to give an inkling of how the Fourier transform and convolution appear in communication. Clearly, to go into more details would take us to a very broad field. The reader interested in this area will definitely benefit from browsing through the books by Lee (1960) and Schwartz and Shaw (1975) and that of Jenkins and Watts (1968) on signal processing and applications of spectral analysis as well as the book by Brigham (1974) on basic Fourier transform applications, which also contains a good list of the source literature. A delightful field of application is that of speech analysis and synthesis. A very readable article by Flanagan (1972) and a book by Flanagan (1971) are suggested.

3.2. Correlation: Signal Detection and Noise

Signal detection in the presence of noise is one of the most important problems in communication. The concepts developed in Fourier analysis will be used to state some of the relevant variables and to broadly outline the strategy of solution. We start by defining the *correlation* of a string of signal data.

3.2.1. Correlation

Consider a sesquilinear operation mapping $\mathscr{V}^N \times \mathscr{V}^N$ into $\mathscr{V}^N$ relative to a basis—for definiteness we shall consider here the φ-basis—as the component-by-component product

$$\tilde{k}_m = \tilde{f}_m^* \tilde{g}_m, \qquad m = 1, 2, \ldots, N, \quad \mathbf{f}, \mathbf{g}, \mathbf{k} \in \mathscr{V}^N, \tag{3.16}$$

Except for the complex conjugation in the first factor, this operation is basically the product introduced in Section 3.1, and its properties are quite similar. The distinct usefulness of (3.16) appears when we translate it to a

relation between the ε-basis coordinates of the vectors involved. These can be found through the inverse Fourier transform

$$k_n = \sum_m F_{nm}\tilde{k}_m = \sum_m F_{nm}\tilde{f}_m^*\tilde{g}_m$$
$$= \sum_m F_{nm}\sum_k F_{mk}f_k^*\sum_l F_{ml}^* g_l. \tag{3.17}$$

Exchanging sums and using (3.5) with an appropriate relabeling of indices, we find

$$k_n = N^{-1/2}\sum_m f_m^* g_{n+m} = N^{-1/2}\sum_m f_{m-n}^* g_m =: N^{-1/2}(fcg)_n,$$
$$n = 1, 2, \ldots, N, \tag{3.18}$$

which we define as the *correlation between* **f** and **g**.

Exercise 3.8. Show that in terms of the rotation operators $\mathbb{R}^n$ of Section 1.6 the correlation (3.18) can be written as

$$k_n = N^{-1/2}(fcg)_n = N^{-1/2}(\mathbf{f}, \mathbb{R}^n\mathbf{g}). \tag{3.19}$$

Exercise 3.9. Using the result of Exercise 3.8, the fact that $\mathbb{R}^n$ is a unitary operator and the Schwartz inequality show that the norm of the correlation vector in (3.18) satisfies

$$\|\mathbf{fcg}\| \leqslant N^{1/2}\|\mathbf{f}\|\,\|\mathbf{g}\|. \tag{3.20}$$

This is the analogue of a similar result on convolution given in (3.10).

The correlation assigns a set of numerical values to the "closeness" between the signal **f** and the signal **g**; if these are real and such that f_m and g_m have generally the same sign, $(fcg)_0$ will be a sum of generally positive terms and hence large. If we find some component l among the $(fcg)_n$ to be unusually large in comparison with the others, we can conclude either that f_m and g_{m-l} have generally the same sign or that a large component or components in **f** have met its or their counterpart in **g**. The number l gives the *lag* between the two.

3.2.2. Autocorrelation

Examine now the case when $\mathbf{f} = \mathbf{g}$, the *autocorrelation* function of **f** being the k_n in (3.18). Of course

$$k_0 = N^{-1/2}(fcf)_0 = N^{-1/2}\|\mathbf{f}\|^2, \tag{3.21}$$

but what happens to k_n for n "close" to 0? If the signal **f** is such that the f_m are a "smooth" or slowly varying function of m, $f_{m\pm1}$ will still have generally the same phase and magnitude as f_m, and so will $f_{m\pm2}$, etc. The correlation function k_n is thus expected to have a more or less broad real peak around

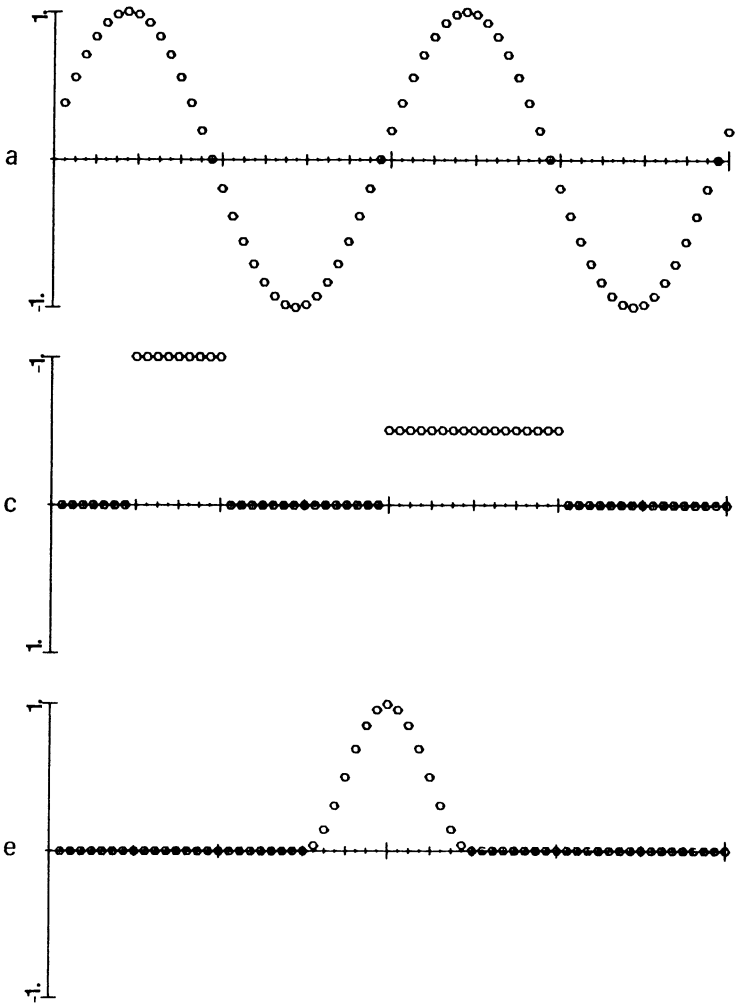


Fig. 3.8. (a) Periodic signal and (b) its autocorrelation. (c) "Two-peak" signal [Fig. 3.2(a)] and (d) its autocorrelation. (e) "Smooth" nonperiodic signal and (f) its autocorrelation.

$n = 0$. The width is determined by the distance j at which $f_{m\pm j}$ still has the same phase on the average as f_m, before sign cancellations start occurring in the sum (3.18). If now the signal f_m is *periodic* in m with period P (P divisor of N), then $f_m = f_{m+lP}$ for l integer and $k_{lP} = k_0$. The correlation function will exhibit peaks spaced by P units and will itself be periodic. In Fig. 3.8(a) is a periodic signal and in Fig. 3.8(b) its correlation function; other signals [Figs. 3.8(c) and (e)] also have characteristic correlation functions [Figs. 3.8(d) and (f)].

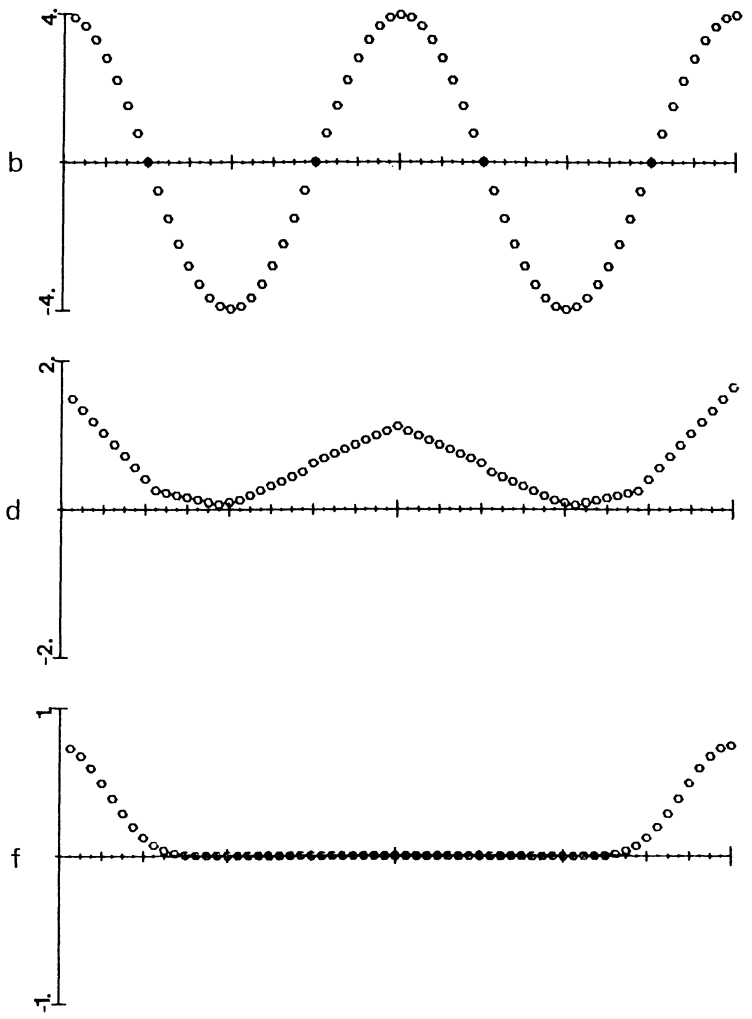


Fig. 3.8 (*continued*)

Exercise 3.10. Show that the autocorrelation function $k_n = (fcf)_n$ is even in n and cannot have a value *larger* than k_0 in (3.21). You can use the Schwartz inequality on (3.19).

Exercise 3.11. Show that *the Fourier transform of the autocorrelation function is the power spectrum* $p_n{}^f = |\tilde{f}_n|^2$ of **f**.

The autocorrelation function k_n, we have seen, gives a numerical value of the "degree of similarity" between a signal and its image shifted

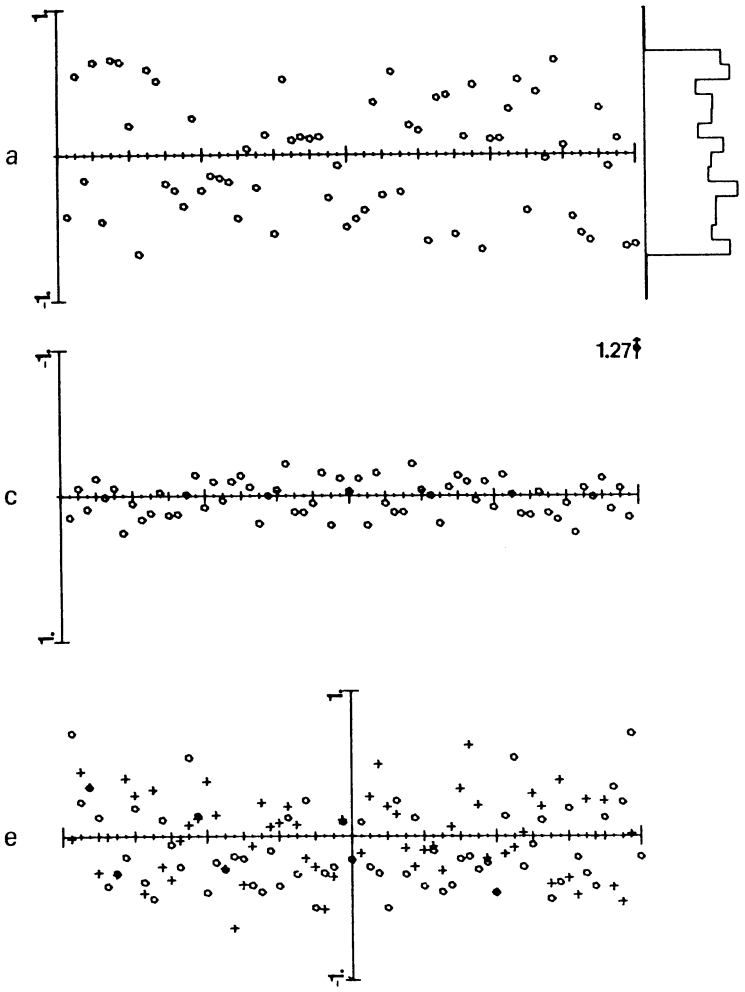
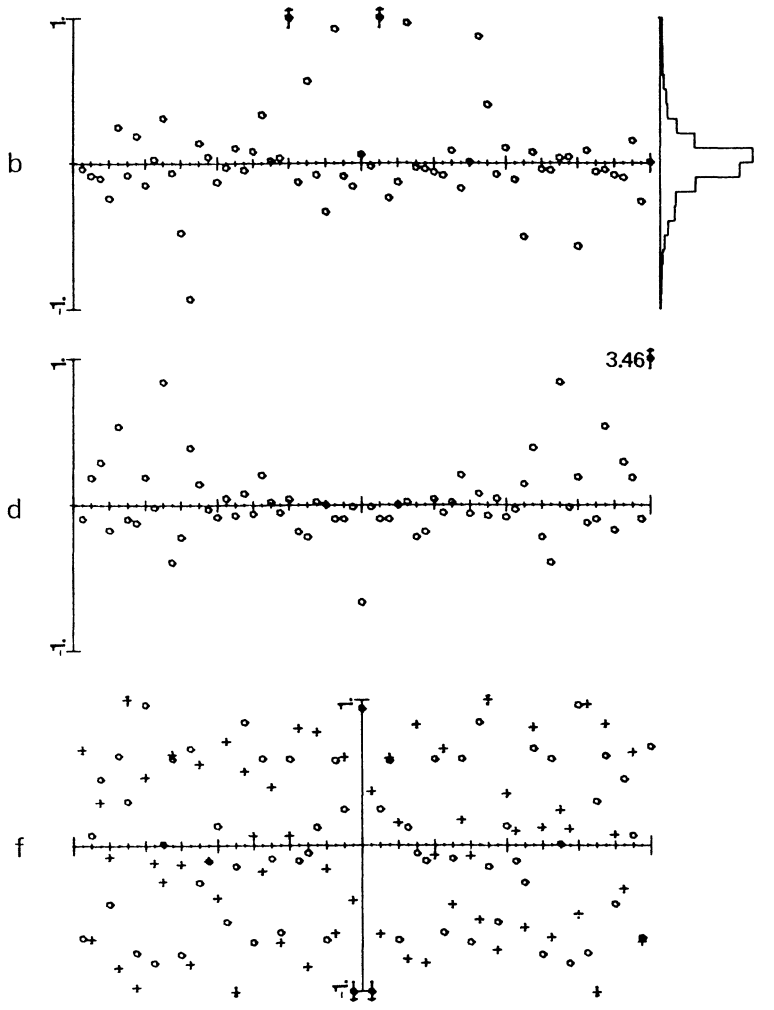


Fig. 3.9. (a) Constant-density noise and (b) Gaussian noise. The histograms to the right divide the ordinate range in 20 "bins," showing the characteristics of the distribution. (The latter were built on the basis of 1024 points rather than 64, as in the figures, in order to reduce random fluctuations.) (c) and (d) are

by n units. Suppose now we construct a "signal" $\boldsymbol{\nu}$ whose values ν_m, $m = 1, 2, \ldots, N$, are extracted from a random-number table or computer generator. Since no two values of the list are causally related, we can expect the autocorrelation function to have only a large k_0 value, but all other k_n's to fluctuate randomly. In Fig. 3.9(a) this is shown for a vector $\boldsymbol{\nu}$ constructed by a computer intrinsic "function" which produces a random sequence of real



the autocorrelations of (a) and (b), respectively. Notice the peak at the $N \equiv 0$ component of the correlation vector and the otherwise uneventful noise-like appearance of all other components. (e) and (f), Fourier transforms of (a) and (b), also have a noise-like character, showing comparable contributions from each frequency range.

numbers between -1 and 1 with constant *probability density*. This means that as the list of generated numbers tends to infinity, the proportion of those which fall in any interval $(v - \Delta v/2, v + \Delta v/2) \subset (-1, 1)$ is indepenent of the value of v. A histogram to the right of the figure shows this. The autocorrelation function in Fig. 3.9(c) is seen to exhibit only the peak at k_0. The same happens with random sequences with Gaussian probability densities [Fig.

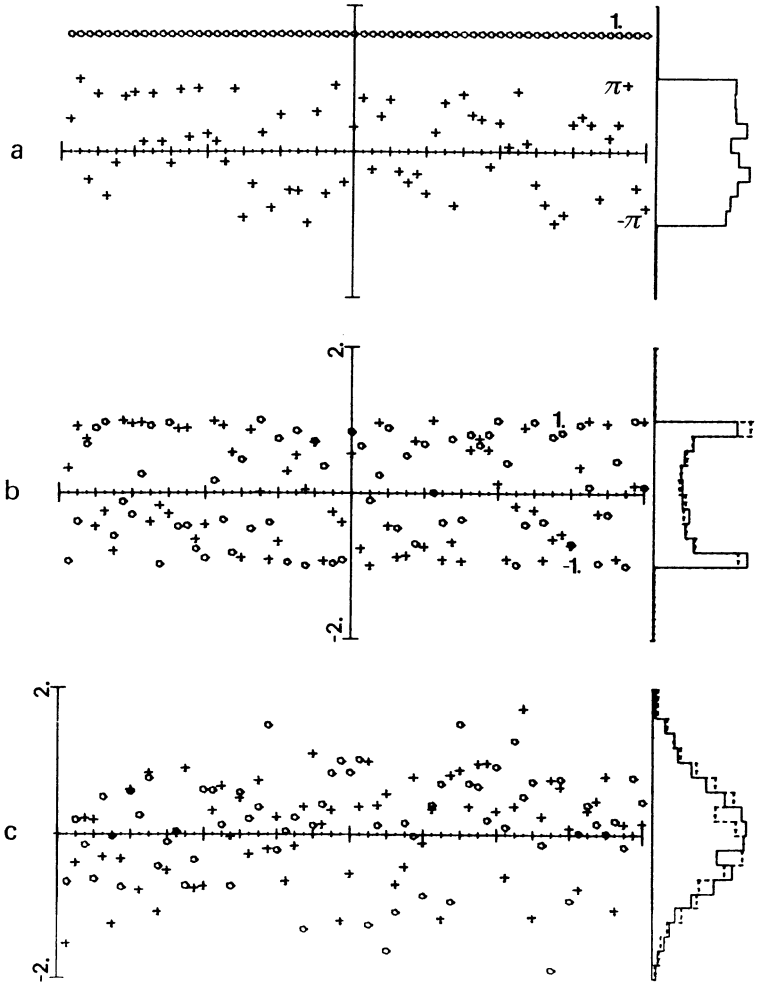


Fig. 3.10. White noise (a) built by requiring that all Fourier partial-wave coefficients have unit modulus (open circles) while their phases (crosses) be randomly distributed in $(-\pi, \pi)$ with constant density (histogram at the right). In terms of the real and imaginary parts of the Fourier coefficients (b), the probability density has a csc πx shape (see the histograms at the right—unbroken lines for the real parts and dotted lines for the imaginary parts). By inverse Fourier transformation, white noise (c) is obtained. As before, all histograms were built with 1024-component vectors, while the figures have only 64 points.

3.9(b)]. Figures 3.9(e) and (f) are the Fourier transforms of Figs. 3.9(a) and (b).

Exercise 3.12. Are there reasons to expect that as N grows without bound, $k_n \to 0$ for $n \neq 0$?

3.2.3. White Noise

Signals with random components are generically referred to as *noise*. This is a good working definition which describes the kind of background "signal" produced by the thermal agitation of electrons in radio or radar receivers and amplifiers. A broader "definition" of noise in communication is any "unwanted" part of the signal; of course this varies from case to case.

As Fig. 3.9 suggests, the definition of noise is not unique. For standardization purposes in filtering, it is common to define *white noise* as that which has *the same power spectrum at all frequencies*, i.e., such that $p_n^{\nu} = |\bar{\nu}_n|^2 =$ constant, so that only the *phase* of individual Fourier coefficients takes a random sequence of values. This is shown in Fig. 3.10.

Exercise 3.13. Note that a filter $\mathbb{Q}$ can change the characteristics of the noise input $\boldsymbol{\nu}$. Consider an averager and a differencer filter, and examine the correlation of the output. See that for these two cases $k_1^{\nu'} = \pm\frac{1}{4}k_0^{\nu} +$ random terms.

3.2.4. Signal Detection and Filtering of Noise

Noise is the part of the input signal $\mathbf{s}$ we usually want to get rid of. We consider $\mathbf{s} = \mathbf{s}_0 + \boldsymbol{\nu}$, $\mathbf{s}_0$ being the "true" signal and $\boldsymbol{\nu}$ the noise. In detecting signals $\mathbf{s}_0$ we should separate clearly two kinds of situations: first, when we have a fair idea of what $\mathbf{s}_0$ should be and we are interested in *detecting* the presence or absence of the signal, and second, when $\mathbf{s}_0$ is unknown and only its overall characteristics—as distinct from those of noise—can be used for *filtering* $\mathbf{s}$. The first situation corresponds, for instance, to radar technology, while the second was typical of early telephony.

The detection of known signals amid background noise is usually tackled by finding the correlation, in a time window, of the incoming signal. If $\mathbf{s}$ is a train of square pulses (Fig. 3.11), it has a correlation function which is quite distinct from that of $\boldsymbol{\nu}$ [Figs. 3.9(c) and (d)]. The correlation of $\mathbf{s} = \mathbf{s}_0 + \boldsymbol{\nu}$ is $\mathbf{s}_0\mathbf{c}\mathbf{s}_0 + \mathbf{s}_0\mathbf{c}\boldsymbol{\nu} + \boldsymbol{\nu}\mathbf{c}\mathbf{s}_0 + \boldsymbol{\nu}\mathbf{c}\boldsymbol{\nu}$. The shape of the first term, when present, can be recognized in Fig. 3.11. Moreover, the correlation can also be used to detect any *change* undergone by the signal. The return pulse of a radar bouncing off the surface of a planet, for instance, will yield the distance to the body by the travel-time lag; the Doppler shift due to the planet's radial velocity away or toward the observer will lengthen or shorten the pulses,

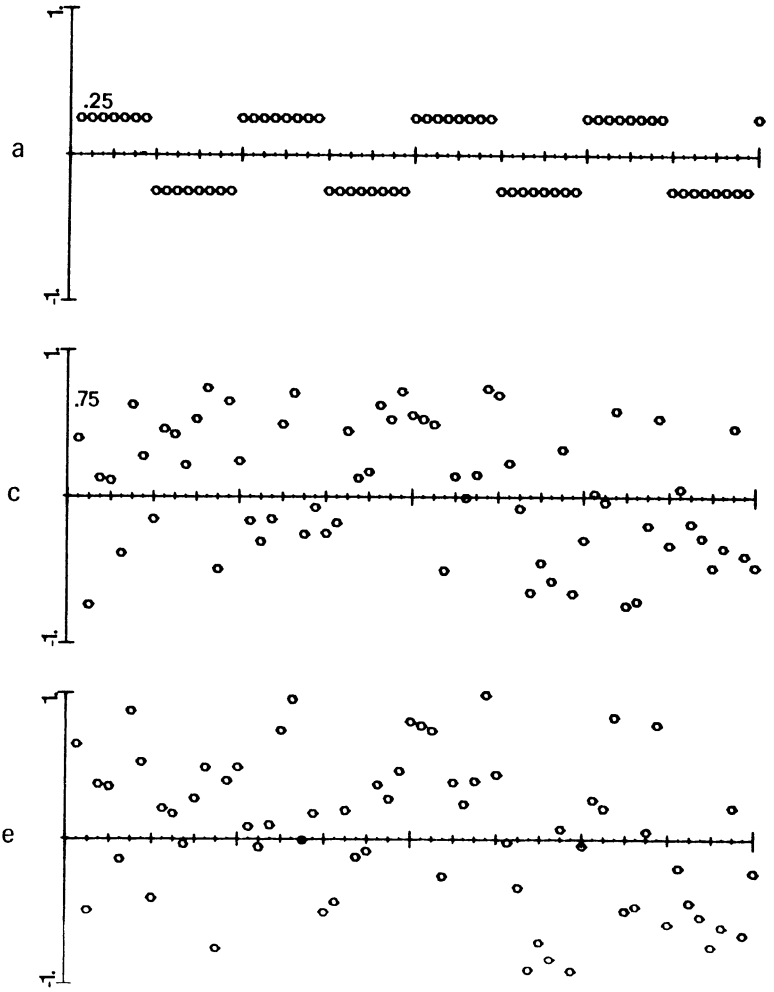
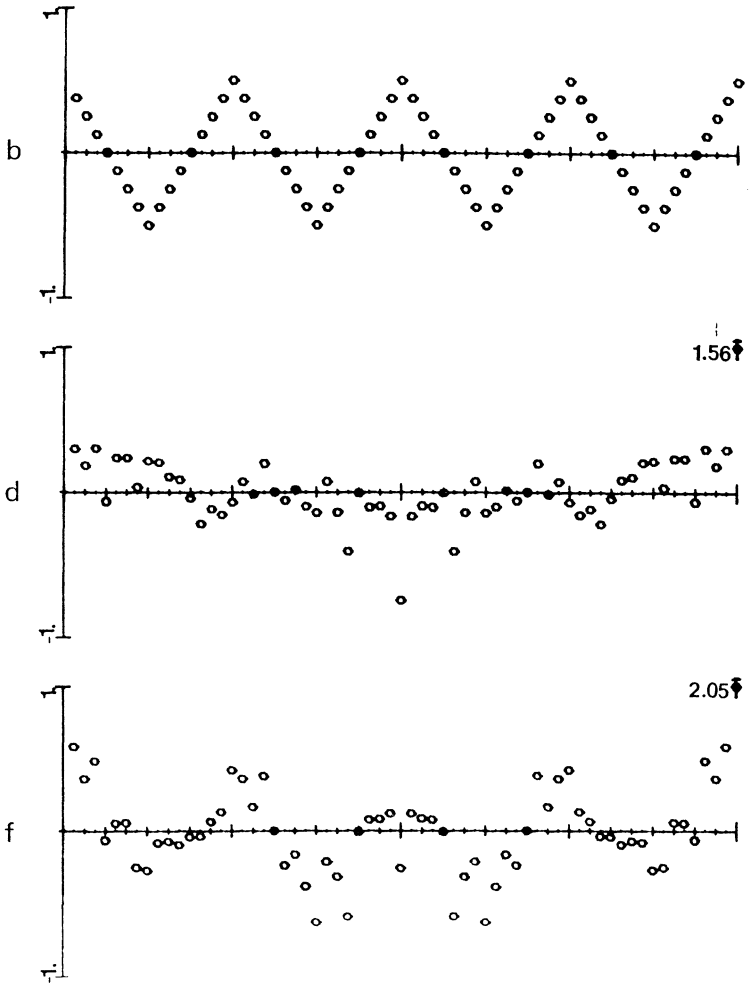


Fig. 3.11. Signal detection amid noise by correlation. (a) Periodic signal and (b) its correlation. (c) Constant-density noise and (d) its correlation. (e) Signal plus noise at a ratio of 1:3. The noise masks the signal, whose presence can

while the pulse shape will be changed by surface characteristics such as rugosity and ground reflexivity.

For the filtering of signals of which we have no *a priori* knowledge, the solution is not so clear-cut, and in fact the information of the "true" signal s_0 is never fully retrievable. An *averager* filter (see Exercise 3.5) has a transfer function which attenuates the high-frequency components. If these are suppressed in the input (Fig. 3.12), the total noise power ($\sum_n |\tilde{\nu}_n|^2$) will be



nevertheless be detected by (f) correlation. The observed peaks and their periodicity match those of the signal, so we conclude that (e) contains a signal. The more data points we have, the more effective the detection by correlation becomes.

diminished to a greater extent than the total "true" signal power ($\sum_n |\bar{s}_{0n}|^2$). The output is a "smoother" signal in which $\mathbf{s}_0$ should be recognizable. If the noise-to-signal ratio (total noise power/total "true" signal power) is large, this method—or any other filtering scheme—may not prevent loss of signal information.

A generally successful way to overcome the difficulties inherent in signal filtering is to *digitalize* the data to be transmitted, coding them into

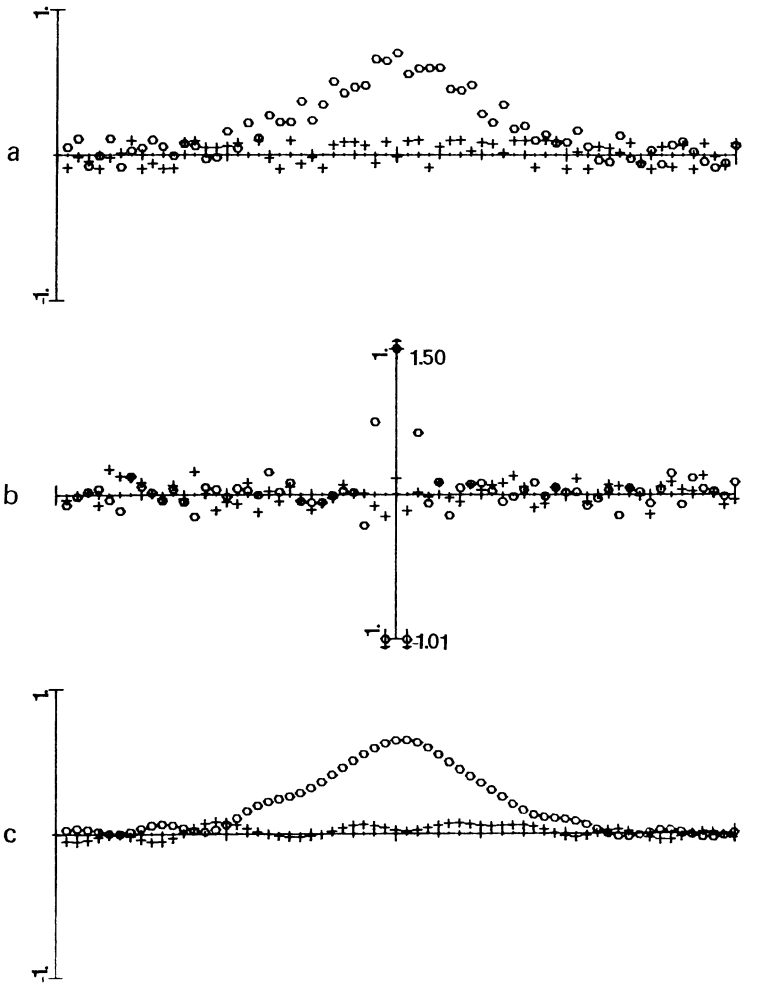


Fig. 3.12. Partial noise elimination by filtering. (a) A "smooth" signal [Fig. 3.5(a)] plus 25% white noise [Fig. 3.10(c)]. (b) The Fourier transform of the noisy signal contains large low-frequency components due to the signal [Fig. 3.5(b)] and essentially a constant high- and low-frequency noise background [Fig. 3.10(b)]. Filtering with a low-pass device whose transfer function is shown in Fig. 3.5(c) in the frequency domain, we obtain (c) the filtered signal. The small wavelets are the noise residue. Narrowing the filter's passing band would only distort the signal farther from its true shape. Broadening it would allow for more noise wavelets.

pulse sequences of "expected" shape [as in Fig. 3.11(a)] such that on arrival the message can be detected by correlation. On-the-spot planet photographs are scanned as by a TV image, but tones of gray are divided into, say, 32 values. The transmitted data will then consist of a string of numbers in this range, each in binary code whose digits, 0 or 1, are given by the absence or presence of a pulse. In this way, we trade the range of possible shades of gray (which is not too important, as 32 tones give a very accurate rendering of the picture) for protection against image degradation.

As in Section 3.1, the reader is urged to explore the source literature if he wishes to have more specialized information on the actual signal detection technology. See also the books by Papoulis (1965), Schwartz *et al.* (1966, 1970, and 1975), Gold and Rader (1969), Otnes and Enochson (1972), Stieglitz (1974), and Bloomfield (1976).

3.3. The Fast Fourier Transform Algorithm

Sections 3.1 and 3.2 point to the fact that the actual evaluation of the finite Fourier transform has a considerable range of application. Although the number of data points must in practice be finite, it can be very large, say on the order of 10^3 or 10^4, requiring a considerable amount of expensive computer time. An algorithm for the evaluation of the Fourier transform involving a drastic reduction in its computational complexity—by a factor of $N/\log_2 N$—was discovered recently by Cooley and Tukey [see Cooley and Tukey (1965); see also Cooley *et al.* (1967)].

3.3.1. Computational Complexity of the Longhand Fourier Transformation

Let us analyze the number of arithmetic operations required to calculate the Fourier transform $\{\tilde{f}_m\}_{m=1}^N$ from a given set of complex data points $\{f_n\}_{n=1}^N$. The "longhand" calculation proceeds by

$$\tilde{f}_m = N^{-1/2} \sum_{n=1}^{N} f_n \exp(2\pi imn/N) \qquad \text{for } m = 1, 2, \ldots, N. \tag{3.22}$$

First, (a) one has to calculate $\exp(2\pi i/N)$ and then its $N - 1$ powers, as these will appear as factors in (3.22). Then (b) one has to perform the $(N - 1)^2$ products of f_n's with these exponentials (for n or m equal to N the exponential factor is 1, so no product is necessary). Last, (c) there are $N(N - 1)$ sums to be performed. The overall factor $N^{-1/2}$ need not be considered, as it is usually absorbed into a redefinition of the Fourier transform in actual applications.

Typical computer times required for the operations of real, single-precision, floating-point sum and product, including memory access, are on

the order of 25 μsec for the PDP-11/40, a medium-small computer. A medium-large computer such as the Burroughs 6700 requires around 7 μsec. If we round off the complexity of (3.22) as N^2 sums and N^2 multiplications, the computer work needed for N around 1000 is comprised of some 2 million complex operations. This represents some $6\frac{1}{2}$ min on the first and 2 min on the second computer. Even if machine time were unlimited and free, the Fourier transform would not often be used for real-time data analysis unless a considerably more efficient algorithm were found. The fast Fourier transform (FFT), for $N = 2^{10} = 1024$, leads to a 100-*fold* saving factor.

3.3.2. N Divisible by 2

Suppose that N is divisible by 2. The index n can be replaced by $2r + k - 1$ and the sum (3.22) split into

$$\tilde{f}_m = N^{-1/2} \sum_{k=0}^{1} \sum_{r=1}^{N/2} f_{2r+k-1} \exp[2\pi i(2r + k - 1)m/N]$$

$$= 2^{-1/2} \sum_{k=0}^{1} \exp[2\pi i(k - 1)m/N](N/2)^{-1/2} \sum_{r=1}^{N/2} f_{2r+k-1} \exp[2\pi irm/(N/2)]. \tag{3.23}$$

The second sum,

$$\tilde{f}^1_{k,m} := (N/2)^{-1/2} \sum_{r=1}^{N/2} f_{2r+k-1} \exp(4\pi irm/N) = \tilde{f}^1_{k,N/2+m}, \tag{3.24}$$

is the $N/2$-dimensional Fourier transform, for $k = 0$, of the odd-numbered f_n's and of the even-numbered f_n's for $k = 1$. The determination of all the $\tilde{f}^1_{k,m}$'s in (3.24) involves $2(N/2)^2$ multiplications since we have two values of k and we need perform the Fourier transform only for $m = 1, 2, \ldots, N/2$. Once these have been calculated, we can *merge* the $\tilde{f}^1$'s as

$$\tilde{f}_m = 2^{-1/2}[\exp(-2\pi im/N)\tilde{f}^1_{0,m} + \tilde{f}^1_{1,m}], \qquad m = 1, 2, \ldots, N. \tag{3.25}$$

This process involves N products. The total number of multiplications in the algorithm (3.24)–(3.25) is thus $N^2/2 + N$ and about the same for sums. For large N this represents roughly a halving of the computation time.

3.3.3. N Divisible by 2^p

The reduction in computation complexity need not stop here: the $N/2$-dimensional Fourier transform (3.24) may be subject to the same process when $N/2$ is even. We need only replace r by $2s + k_2 - 1$, $s = 1, 2, \ldots, N/4$, defining a $\tilde{f}^2_{k_2k_1}$ as the $N/4$-dimensional transform of the f_n's with $n \equiv 0, 1, 2, 3 \bmod 4$ and the merging (3.25) between the $\tilde{f}^2$'s and $\tilde{f}^1$'s. The general

recursion for N divisible by 2^p involves, first, the $(2^{-p}N)$-dimensional Fourier transform [which we write without the constant $(2^{-p}N)^{-1/2}$, which should go in front],

$$\tilde{f}^p_{k_p\cdots k_2k_1,m} := \sum_{r=1}^{2^{-p}N} f_{n_p(r,k)} \exp(2^{p+1}\pi irm/N) = \tilde{f}^p_{k_p\cdots k_2k_1,2^{-p}N+m}, \tag{3.26a}$$

where

$$n_p(r, k) := 2^p r + 2^{p-1}(k_p - 1) + \cdots + 2(k_2 - 1) + (k_1 - 1). \tag{3.26b}$$

The following p steps are the mergings (again, eliminating the factor $2^{-1/2}$),

$$\tilde{f}^{q-1}_{k_{q-1}\cdots k_1,m} = [\exp(-2^q\pi im/N)\tilde{f}^q_{0k_{q-1}\cdots k_1,m} + \tilde{f}^q_{1k_{q-1}\cdots k_1,m}],$$
$$m = 1, 2, \ldots, 2^{-q+1}N, q = p, p - 1, \ldots, 1, \tag{3.27a}$$

where the last step is

$$\tilde{f}_m{}^0 := N^{-1/2}\tilde{f}_m, \qquad m = 1, 2, \ldots, N. \tag{3.27b}$$

The number of multiplications in the algorithm (3.26)–(3.27) is $(2^{-p}N)^2$ for the Fourier transform (3.26) and N for each merging.

3.3.4. $N = 2^\nu$

The regression in the dimension of the Fourier transform ends when it reaches 1, since then we have no sums or multiplications at all. Thus consider N to be the νth power of 2, i.e., $N = 2^\nu$. Then, for $p = \nu$,

$$\tilde{f}^\nu_{k_\nu\cdots k_2k_1} = f_{n_\nu(1,k)}, \tag{3.28a}$$

as r and m can only take the value 1, and

$$n_\nu(1, k) = 2^{\nu+1} + 2^\nu(k_\nu - 1) + \cdots + 2(k_2 - 1) + (k_1 - 1)$$
$$= 2^\nu k_\nu + 2^{\nu-1}k_{\nu-1} + \cdots + 2k_2 + k_1 + 1. \tag{3.28b}$$

It is only left for us to perform the ν mergings (3.27) for $q = \nu, \nu - 1, \ldots, 1$. As each merging involves N products and N sums, the total number of operations of each type is νN or

$$N \log_2 N. \tag{3.29}$$

The computational complexity of the *fast Fourier transform* algorithm (3.27)–(3.28) is thus significantly smaller than that of the direct formula (3.22).

3.3.5. Regression and Binary Digit Inversion

In Fig. 3.13 we have displayed graphically the regression and merging for the fast Fourier transform for $N = 8 = 2^3$. We started in the leftmost

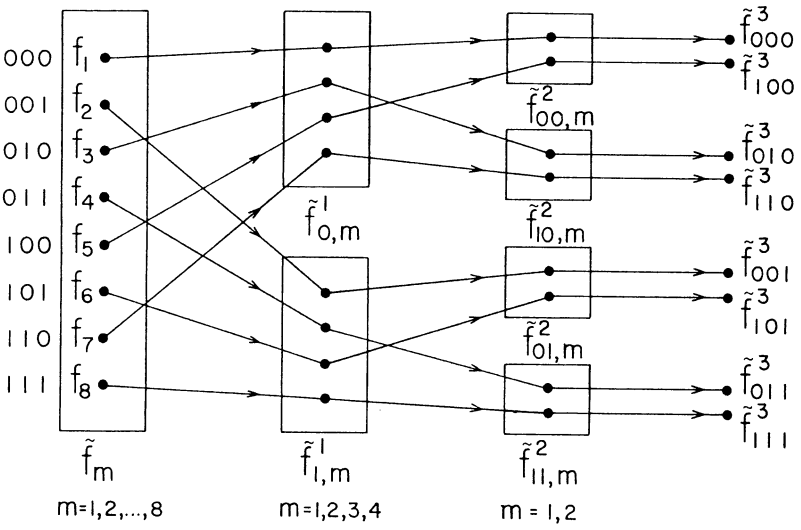


Fig. 3.13. Regression and merging of the fast Fourier transform algorithm.

column where all the $\tilde{f}_m$ depended on all the f_n. From there we proceeded to the second column having two parts, the four $\tilde{f}^1_{0,m}$'s depending on the even f_n's and the four $\tilde{f}^1_{1,m}$'s on the odd ones. From here we passed to the third column which has four pairs of $\tilde{f}^2_{k_2k_1,m}$'s, each depending on two f_n's. Last, we have eight $\tilde{f}^3_{k_3k_2k_1}$ which *are* f_n's. Note particularly that the *string of binary digits* $k_3k_2k_1$ *is the binary number representation of* $n-1$, which is written to the left of the first column. This is a general property which can be seen from (3.28b). It should also be noted that the overall shuffling of the entries in the first and last columns is such that it *inverts the digit order* of the binary representation of the row label. The merging procedure can be followed in Fig. 3.13 from right to left: each of the pair of $\tilde{f}^2_{k_2k_1,m}$'s, $m = 1, 2$, is constructed from the rightmost column entries to which it is connected, the upper link being multiplied by the phase in (3.27). Following suit, each of the $\tilde{f}^1_{k_1,m}$'s is obtained through the merging of the $\tilde{f}^2_{k_2k_1,m}$'s to which its block is linked and similarly for the $\tilde{f}_m$'s.

3.3.6. A Short Survey of the Literature

Figure 3.14 shows a FORTRAN program which calculates the direct and inverse Fourier transforms using the FFT algorithm. This program is not the ultimate in computation efficiency but should be easy to implement by the interested reader on his local computer. The software in most computing centers includes more than one version of the FFT. These are variants which follow either the *Cooley–Tukey* or the *Sande–Tukey* algorithms (Cooley and Tukey, 1965; Gentleman and Sande, 1966). Other fast algorithms

```
      SUBROUTINE FFT(X,N,NU,IT)
      COMPLEX X(N),E,T
      M=N/2
      NU1=NU-1
      K=0
      Z=IT
      U=1./SQRT(FLOAT(N))
      DO 3 I=1,NU
    1 DO 2 J=1,M
      A=INV(K/2**NU1,NU)*6.283185/N
      E=CMPLX(COS(A),Z*SIN(A))
      L=K+1
      LM=L+M
      T=X(LM)*E
      X(LM)=X(L)-T
      X(L)=X(L)+T
    2 K=K+1
      K=K+M
      IF(K.LT.N) GO TO 1
      K=0
      NU1=NU1-1
    3 M=M/2
      DO 4 K=1,N
      J=INV(K-1,NU)+1
      IF(J.LE.K) GO TO 4
      T=X(K)
      X(K)=X(J)
      X(J)=T
    4 CONTINUE
      DO 5 K=1,N
    5 X(K)=X(K)*U
      RETURN
      END
      FUNCTION INV(J,NU)
      J1=J
      INV=0
      DO 1 I=1,NU
      J2=J1/2
      INV=INV*2+J1-2*J2
    1 J1=J2
      RETURN
      END
```

Fig. 3.14. A FORTRAN IV subroutine which performs Fourier transformation through the FFT algorithm. It converts the input complex vector X of dimension N and NU = $\log_2$ N into its Fourier transform if IT = 1; if IT = −1, the vector X is converted into its inverse Fourier transform. The function INV effects the binary bit inversion. Note that the output component X(1) stands for the Nth ≡ 0th Fourier coefficient and that all other components are correspondingly shifted to one higher value.

have been developed for arbitrary N which work on similar principles (Bergland, 1967, 1968, 1969; Rader, 1968; Singleton, 1968). When the data arrays are very large and exceed the machine memory storage capacity, the use of auxiliary memory devices such as disk or tape has to be integrated properly into the algorithm. These problems have been tackled (Buijs, 1969; Singleton, 1967). Convolution and correlation of finite signals can also be profitably handled through the FFT in their many applications. The calculation of the convolution (3.8) or correlation (3.18) of two vectors involves N^2 complex products. As the FFT takes only $N \log_2 N$ operations, we may proceed to use the Fourier transform first for the two coordinate sets, multiply them in the φ-basis [Eqs. (3.7b) or (3.16)], and then Fourier-transform back. The number of operations in this roundabout way is $3N \log_2 N + N$, which is less than N^2 for $N > 16$.

The actual applications of the fast Fourier transform algorithm cover a very wide range. Some examples of what can be found in the literature are the

articles by Stockham (1966), Singleton and Poulter (1967), Welch (1967), Glisson and Black (1969), Liu and Fagel (1971), and Becker and Farrar (1972). For the reader interested in a more detailed exposition and bibliography of this rapidly growing field and its applications, we suggest the book by Brigham (1974) as well as the special issues of the *IEEE Transactions on Audio and Electroacoustics* **AU-15** (June 1967) and **AU-17** (June 1969).

3.4. The "Limit" $N \to \infty$: Fourier Series and Integral Transforms

Up to now we have dealt with complex vector spaces $\mathscr{V}^N$ with N arbitrary but finite. We shall now let N grow without bound and examine the behavior of the Fourier transform. The "limit" $N \to \infty$ is not meant to imply that $\mathscr{V}^N$ *tends* toward a "$\mathscr{V}^\infty$" since insofar as vector spaces are concerned, no convergence of the kinds familiar to the reader is defined. Yet for coordinates, inner products, and norms such a limit makes sense if focused properly. Moreover, it provides a reliable intuitive grasp of the properties of infinite-dimensional vector spaces.

3.4.1. $(2N + 1)$-Dimensional Spaces

For the following, it will prove convenient to consider $(2N + 1)$-dimensional spaces $\mathscr{V}^{2N+1}$ where basis vectors are numbered by indices with the range $-N, -N + 1, \ldots, -1, 0, 1, \ldots, N - 1, N$. The Fourier transforms between the coordinates of a vector in the $\boldsymbol{\varepsilon}$- and $\boldsymbol{\varphi}$-bases [Eqs. (1.51)] become

$$\tilde{f}_m = (2N + 1)^{-1/2} \sum_{n=-N}^{N} f_n \exp[2\pi inm/(2N + 1)], \tag{3.30a}$$

$$f_n = (2N + 1)^{-1/2} \sum_{m=-N}^{N} \tilde{f}_m \exp[-2\pi inm/(2N + 1)]. \tag{3.30b}$$

Recall that, to start with, Eqs. (1.51) defined the range of the indices as congruent modulo the dimension of the space. We shall now introduce a new indexing system for the vectors in the $\boldsymbol{\varphi}$-basis, defining

$$x \coloneqq \pi(2m + 1)/(2N + 1), \tag{3.31}$$

so that, for $m = -N, \ldots, N$, x will range in steps of

$$\Delta x = 2\pi/(2N + 1) \tag{3.32}$$

from $-\pi + \Delta x$ to π, and while the numbers m are considered modulo $2N + 1$, the numbers x are considered modulo 2π. We shall also define the set of quantities related to the $\boldsymbol{\varphi}$-basis coordinates of $\mathbf{f}$ as

$$f(x) \coloneqq [(2N + 1)/2\pi]^{1/2} \tilde{f}_m, \tag{3.33}$$

which can be seen as a function f of $2N + 1$ equidistant points on a circle. When N grows without bound these points will become *dense* on the interval $(-\pi, \pi]$; the point $-\pi$ is excluded from the interval as it is congruent with π. Changing dummy indices, Eqs. (3.30) appear as

$$f(x) = (2\pi)^{-1/2} \sum_{n=-N}^{N} f_n \exp(inx) \exp[-in\pi/(2N + 1)], \tag{3.34a}$$

$$f_n = (2\pi)^{-1/2} \sum_{x=-\pi+\Delta x}^{\pi} \Delta x f(x) \exp(-inx) \exp[in\pi/(2N + 1)]. \tag{3.34b}$$

The substitutions (3.31)–(3.33) can also be made for the Parseval identity, Eq. (1.43), which now reads

$$(\mathbf{f}, \mathbf{g}) = \sum_{n=-N}^{N} f_n^* g_n = \sum_{x=-\pi+\Delta x}^{\pi} \Delta x f(x)^* g(x). \tag{3.35}$$

3.4.2. Fourier Series

The reader can see that Eqs. (3.34) and (3.35) lend themselves quite naturally to the limit $N \to \infty$: the sums over x have the right form to be turned into Riemann integrals. Some precautions must be taken, though. We introduce first, for every function $h(x)$ of the (discrete) variable x, a *step function* $h_{(N)}(x')$ over the *continuous* variable x' by

$$h_{(N)}(x') = h(x), \qquad x' \in (x - \Delta x/2, x + \Delta x/2]. \tag{3.36}$$

See Fig. 3.15. By this device, the $\sum_x \Delta x \cdots$ can be turned into $\int_{-\pi}^{\pi} dx' \cdots$. We can assume (at this stage) that the limit of $h_{(N)}(x')$ as $N \to \infty$ is a "proper" function $h(x')$ of x', e.g., a continuous function with a finite number of discontinuities so that it is Riemann-integrable. Next, Eq. (3.35) for $\mathbf{f} = \mathbf{g}$ states that the sum of the now-infinite series in the middle term must equal

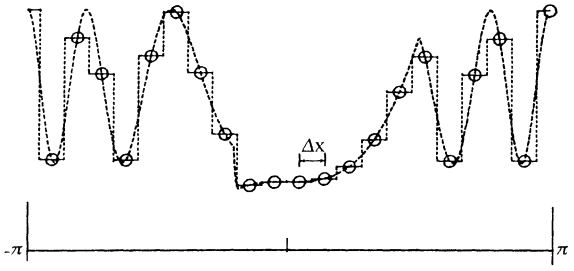


Fig. 3.15. An N-step function in $(-\pi, \pi]$ approximating a continuous function in the limit $N \to \infty$.

the assumed definite value of the integral. The coefficients $\{f_n\}_{n=-\infty}^{\infty}$ must satisfy some summability condition. They cannot all be equal, for instance. A finite number may be nonzero, or we may ask for appropriate decrease conditions for f_n as $n \to \infty$. In particular, we shall agree *not* to allow any f_n "near to" N to keep a finite value as $N \to \infty$. If these (admittedly vague) conditions are met, the sum in (3.34a) becomes a series where the exponential factor $\exp[\pi in/(2N+1)] \to 1$ as $N \to \infty$, and the same happens in (3.34b). The pair of equations then becomes

$$f(x) = (2\pi)^{-1/2} \sum_{n=-\infty}^{\infty} f_n \exp(inx), \tag{3.37a}$$

$$f_n = (2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f(x) \exp(-inx), \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{3.37b}$$

The first of these is the *Fourier expansion* of $f(x)$ in terms of the functions $\exp(inx)$, $n \in \mathscr{Z}$ (the set of integers), with *Fourier partial-wave coefficients* $\{f_n\}_{n\in\mathscr{Z}}$. These coefficients can be obtained from the original function by the second equation. Equations (3.37a) and (3.37b) are also referred to as the Fourier *synthesis* and *analysis* of the function $f(x)$. Finally, the Parseval identity (3.35) becomes

$$(\mathbf{f}, \mathbf{g}) = \sum_{n=-\infty}^{\infty} f_n^* g_n = \int_{-\pi}^{\pi} dx f(x)^* g(x). \tag{3.38}$$

The precise range of validity of the Fourier series pair (3.37) and Eq. (3.38) is given by the *Dirichlet conditions*, which will be proven independently of this construction in Section 4.2. We would only remark here that when $f(x)$ is a *trigonometric polynomial* of degree M, i.e., when the sum in (3.37a) is finite and n bounded,

$$f_M(x) = (2\pi)^{-1/2} \sum_{|n|\leq M} f_n \exp(inx), \tag{3.39}$$

then (3.37b) can be immediately verified by multiplying by $(2\pi)^{-1/2} \exp(-imx)$ and integrating x over $(-\pi, \pi)$, using

$$\int_{-\pi}^{\pi} dx \exp[i(n-m)x] = \begin{cases} [i(n-m)]^{-1} \exp[i(n-m)x]\big|_{-\pi}^{\pi} = 0, & n \neq m, \\ \int_{-\pi}^{\pi} dx = 2\pi, & n = m. \end{cases} \tag{3.40}$$

Indeed,

$$(2\pi)^{-1/2} \int_{-\pi}^{\pi} dx f_M(x) \exp(-imx)$$

$$= (2\pi)^{-1} \sum_{|n|\leq M} f_n \int_{-\pi}^{\pi} dx \exp[i(n-m)x] = f_m, \tag{3.41}$$

and (3.38) can be similarly proven using (3.37b) and (3.40). In restricting the degree of the polynomial to finite M, we have avoided the question of whether the infinite series (3.37a) converges to $f(x)$ for all x and what to do if the series diverges.

3.4.3. Basis Vectors

Since in Part II we shall tackle these questions using elements of functional analysis, let us have a closer look here at the vector space aspects of $\mathscr{V}^{2N+1}$ as N grows without bound. Parallel to the redefinition of the coordinates (3.33) of a vector $\mathbf{f}$, we define the basis vectors

$$\boldsymbol{\delta}_x := [(2N + 1)/2\pi]^{1/2}\boldsymbol{\varphi}_m, \tag{3.42}$$

where x and m are related by (3.31). These also constitute a *basis* for $\mathscr{V}^{2N+1}$, with coordinates

$$(\boldsymbol{\varepsilon}_n, \boldsymbol{\delta}_x) = (2\pi)^{-1/2} \exp(-inx) \exp[in\pi/(2N + 1)] = (\boldsymbol{\delta}_x, \boldsymbol{\varepsilon}_n)^*. \tag{3.43}$$

They are a set which is orthogonal, but not orthonormal, as

$$(\boldsymbol{\delta}_x, \boldsymbol{\delta}_y) = \delta_{x,y}(2N + 1)/2\pi = \delta_{x,y}/\Delta x, \tag{3.44}$$

where $\delta_{x,y}$ is the Kronecker δ in the indices x and y. The coordinates of a vector $\mathbf{f}$ in the $\boldsymbol{\delta}$-basis are thus

$$f(x) = (\boldsymbol{\delta}_x, \mathbf{f}) = \left(\boldsymbol{\delta}_x, \sum_y \Delta y f(y)\boldsymbol{\delta}_y\right) = \sum_{y=-\pi+\Delta y}^{\pi} \Delta y f(y)(\boldsymbol{\delta}_x, \boldsymbol{\delta}_y). \tag{3.45}$$

3.4.4. The Dirac δ

Whereas all expressions before (3.42) had a clear meaning as $N \to \infty$, step functions (3.36) being used and assumed to converge to Riemann-integrable functions, the step function of y corresponding to $(\boldsymbol{\delta}_x, \boldsymbol{\delta}_y)$ for fixed x is a rectangle of width $\Delta y = 2\pi/(2N + 1)$ and height $1/\Delta y$ (thus of *unit area*) centered in x. As $N \to \infty$, $\Delta y \to 0$. If we take Eq. (3.45) seriously, it tells us that such a "function" in the "limit" $N \to \infty$ has the properties

$$\delta(x - y) := (\boldsymbol{\delta}_x, \boldsymbol{\delta}_y) = \delta(y - x), \tag{3.46a}$$

$$\delta(x - y) = 0 \qquad \text{for } x \neq y, \tag{3.46b}$$

$$\int_{-\pi}^{\pi} dy\delta(x - y)f(y) = f(x) = (\boldsymbol{\delta}_x, \mathbf{f}). \tag{3.46c}$$

The symbol $\delta(x - y)$ *defined* by (3.46b) and (3.46c) is the *Dirac* δ. (The definition can be made slightly weaker.) It is not a true function. In the

rigorous framework of distribution theory, the second equality in (3.46c) is the definition of $\boldsymbol{\delta}_x$ as a *functional* or distribution, i.e., a mapping which assigns, to every function $\mathbf{f}$ in some class, a number $f(x)$. The intuitive development we have followed here is one of the standard approaches in mathematical physics, which views the Dirac δ as the symbol indicating the limit of a sequence of integrals containing the continuous function $f(x)$ and a rectangle function $\delta_N(x - y)$ of unit area centered on x whose width vanishes as $N \to \infty$. This is equivalent to the first equality in (3.46c); that is, it "punches out" the value of the *test function* $f(y)$ at the point x.

From the point of view of vector analysis, the function $f(x)$, $x \in (-\pi, \pi]$, can here be seen as the *coordinates* of a vector $\mathbf{f}$ in the $\boldsymbol{\delta}$-basis [second equality in (3.46c)], while its Fourier partial-wave coefficients $\{f_n\}_{n \in \mathscr{Z}}$ are the coordinates of the same $\mathbf{f}$ in the $\boldsymbol{\varepsilon}$-basis.

3.4.5. Fourier Integral Transforms

Another way in which the $N \to \infty$ "limit" of the finite Fourier transform leads to *integral* transforms is the following. Consider again the pair of equations (3.30) in $\mathscr{V}^{2N+1}$ for growing N and introduce new indexing variables in both the $\boldsymbol{\varepsilon}$- and $\boldsymbol{\varphi}$-bases as

$$q \coloneqq [2\pi/(2N + 1)]^{1/2}m, \qquad p \coloneqq [2\pi/(2N + 1)]^{1/2}n. \tag{3.47}$$

For $n, m = -N, \ldots, N$, q and p will correspondingly range over $2N + 1$ points spaced by decreasing intervals

$$\Delta q = [2\pi/(2N + 1)]^{1/2} = \Delta p \tag{3.48}$$

between, approximately, $\pm(\pi N)^{1/2}$. Now define the functions

$$f(q) = [(2N + 1)/2\pi]^{1/4}\tilde{f}_m, \qquad \tilde{f}(p) = [(2N + 1)/2\pi]^{1/4}f_n \tag{3.49}$$

on these points. Substituting these expressions into (3.30) and following the same procedure as before in defining step functions $f_{(N)}(q)$ and $\tilde{f}_{(N)}(p)$ for the continuous variables q and p (Fig. 3.15), assuming that as $N \to \infty$ these step functions converge to Riemann-integrable functions in the expanding integration interval and substituting $\int dq$ for $\sum \Delta q$, etc., we arrive at

$$f(q) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp\tilde{f}(p) \exp(ipq), \tag{3.50a}$$

$$\tilde{f}(p) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dqf(q) \exp(-ipq), \qquad q, p \in \mathscr{R}. \tag{3.50b}$$

From the Parseval identity (1.43) we find similarly

$$(\mathbf{f}, \mathbf{g}) = \int_{-\infty}^{\infty} dqf(q)^*g(q) = \int_{-\infty}^{\infty} dp\tilde{f}(p)^*\tilde{g}(p). \tag{3.51}$$

These equations are the analogues of (3.37) and (3.38). The function $\tilde{f}(p)$ is the *Fourier integral transform* of $f(q)$, and the latter the *inverse* Fourier transform of the former. A closer examination of the validity of (3.50)–(3.51) for different classes of functions, not necessarily integrable in the sense of Riemann, will be undertaken in Part III. Again, orthogonal bases $\{\boldsymbol{\delta}_q\}$ and $\{\tilde{\boldsymbol{\delta}}_p\}$ can be defined so that $f(q) = (\boldsymbol{\delta}_q, \mathbf{f})$ and $\tilde{f}(p) = (\tilde{\boldsymbol{\delta}}_p, \mathbf{f})$, leading to Dirac δ's with properties (3.46b) and (3.46c) on the full real line $\mathscr{R}$.

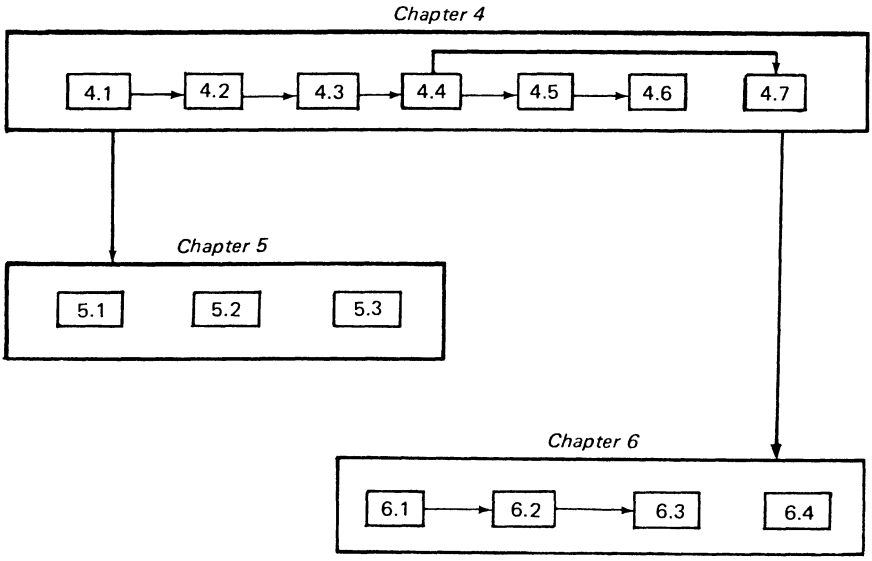
The description of infinite-dimensional spaces as "limits" of finite-dimensional ones has been made here with the purpose of giving an intuitive grasp of the subject. In Parts II and III a physicist's à la Dirac approach will be given. We shall not embark here on a mathematically complete survey of this topic in part because of space and time but mainly because once the overall picture is drawn and the relevant pitfalls are pointed out, the tools of infinite-dimensional vector analysis can be used with the same operational facility as in the finite-dimensional case.

Part II

Fourier and Bessel Series

This part presents the expansion of functions on finite intervals in series of oscillating exponentials or in Bessel functions. Applications include the description of diffusion and elastic media with periodic or fixed boundary conditions.

Chapter 4 reviews the relevant aspects of function vector spaces and covers Fourier series. The first four sections present the basic Dirichlet theorem on existence and convergence of the Fourier series and their main properties with a stress on transformation operators. The Dirac δ and its derivatives, their divergent series representations, as well as a physicist's guide to operators and infinite matrix representatives, are given in the last two sections. These methods are then applied in Chapter 5 to heat diffusion in a ring, the vibrating string, and the infinite lattice. For each, we find its Green's functions, fundamental solutions, and normal modes. The last are particularly useful when describing, in Chapter 6, the vibrations of two- and higher-dimensional elastic membranes or cavities. Normal mode expansions for regions with circular boundaries give rise to Bessel and related series. The last section of this chapter gives a sketch of other series which appear in mathematical physics. The two chapters with applications, 5 and 6, are independent. The first serves to illustrate the uses of the Dirac δ (Section 4.5) and the second those of eigenbasis expansions (Section 4.6).



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 $f(x), g(x), \ldots \in \mathscr{F}_{\mathscr{J}}$ denote functions whose domain $\mathscr{J}$ is an interval in the real line $\mathscr{R}$ and whose range is the field of complex numbers $\mathscr{C}$ (i.e., $f: \mathscr{J} \to \mathscr{C}$, $\mathscr{J} \subseteq \mathscr{R}$). Then $af(x) + bg(x)$, where $a, b \in \mathscr{C}$ is another such function, an element of $\mathscr{F}_{\mathscr{J}}$. The defining properties of vector spaces (Section 1.1) are satisfied, and $\mathscr{F}_{\mathscr{J}}$ 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 $\{f_n(x)\}_{n=1}^N := \{f_1(x), f_2(x), \ldots, f_N(x)\}$, $f_k(x) \in \mathscr{F}_{\mathscr{J}}$, 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 $\mathscr{F}_{\mathscr{J}}$:

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

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 deter-

minant 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 $\mathscr{J}$, 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 $\mathscr{J}$. 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 $\mathscr{F}_{\mathscr{J}}$. 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 $\mathscr{F}_{\mathscr{J}}$. For $\mathbf{f}$ and $\mathbf{g} \in \mathscr{F}_{\mathscr{J}}$ representing the functions $f(x)$ and $g(x)$, respectively, we define this (in analogy to Section 1.2) as

$$(\mathbf{f}, \mathbf{g}) \coloneqq \int_{\mathscr{J}} dx f(x)^* g(x). \tag{4.7}$$

In the process of introducing such an inner product, we shall be losing those functions in $\mathscr{F}_{\mathscr{J}}$ 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

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

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 $\mathscr{J}$,

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 $\mathscr{L}^2(\mathscr{J})$.

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 $\mathscr{J}$ is a *finite* interval within $\mathscr{R}$. By translations and changes of scale in x we can always transform $\mathscr{J}$ 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

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

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

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

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

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

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

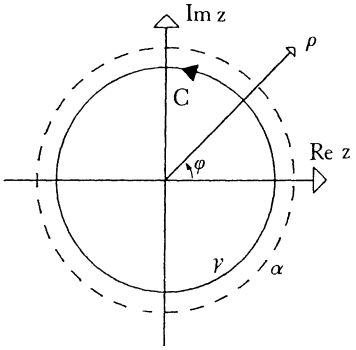


Fig. 4.1. Integration contour for Eq. (4.15b).

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

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

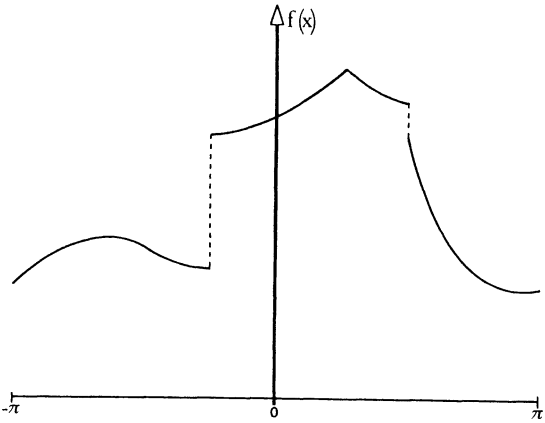


Fig. 4.2. A piecewise differentiable function has bounded derivatives everywhere, except at most at a finite number of points, where it may have bounded discontinuities. Even at these points, however, the limits of the derivatives are defined and bounded as we approach the discontinuity points from the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

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

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, $f'(x^\pm) \coloneqq \lim_{\varepsilon\to 0} df(y)/dy|_{y=x\pm\varepsilon}$, $\varepsilon > 0$, 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)].

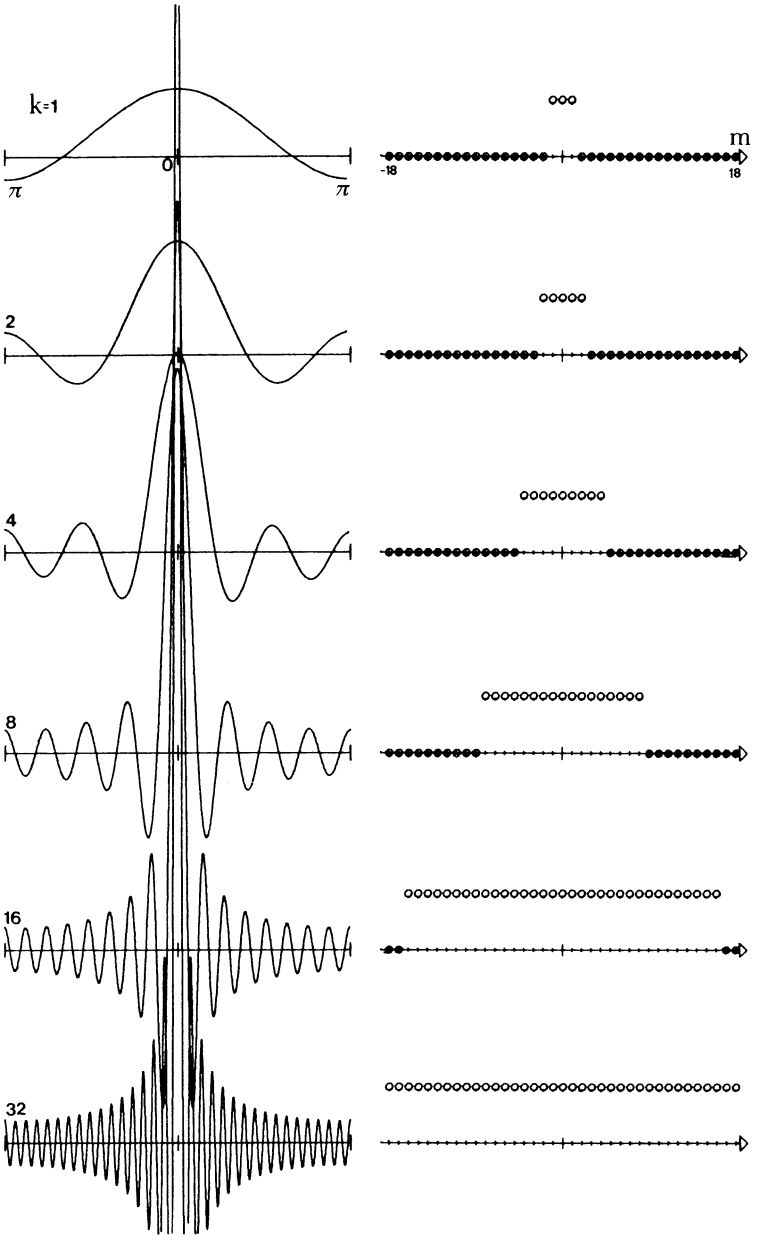


Fig. 4.3. Dirichlet kernel functions $D_k(x)$ for increasing values of k (left). These functions have constant partial-wave coefficients $(2\pi)^{-1/2}$ for $|m| \leqslant k$ (right). For increasing k, the central peak grows without bound.

Consider now the difference between the kth truncated sum $f_k(x)$ and $\frac{1}{2}[f(x^+) + f(x^-)]$, where $f(x^\pm) \coloneqq \lim_{\varepsilon \to 0} f(x \pm \varepsilon)$, $\varepsilon > 0$. 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,

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

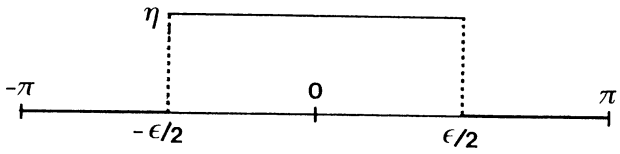


Fig. 4.4. The rectangle function.

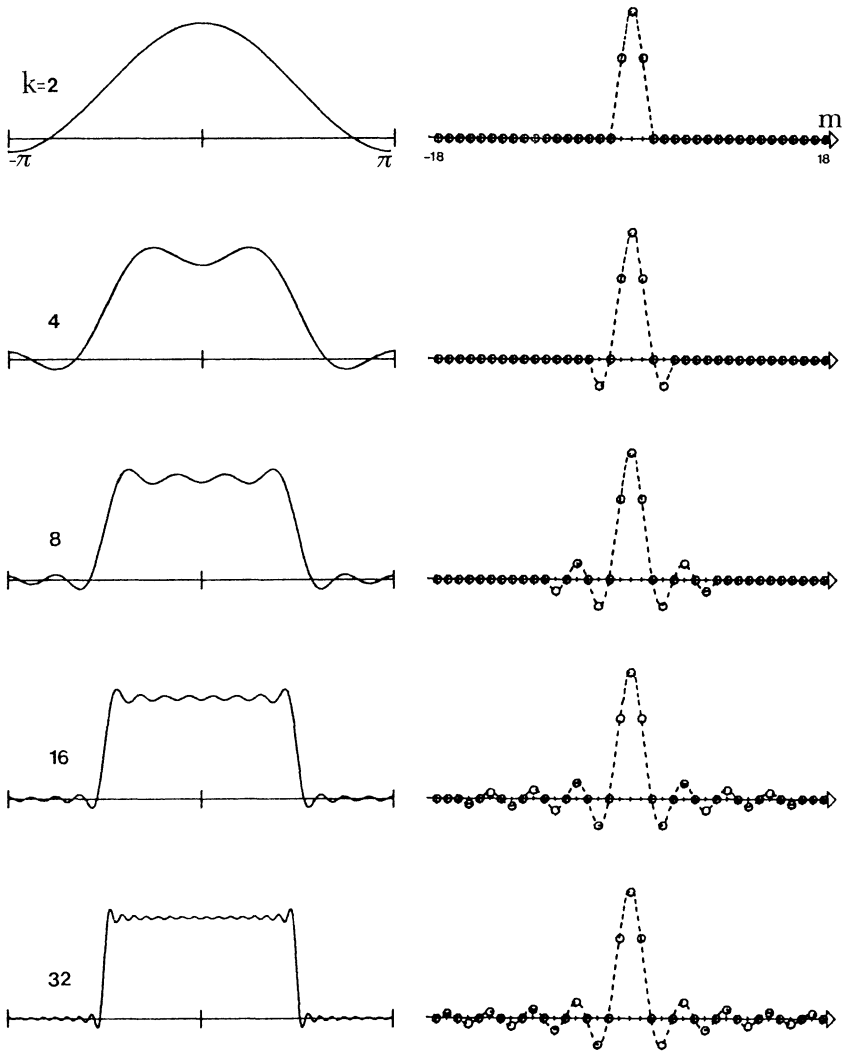


Fig. 4.5. Succession of truncated Fourier sums approximating the rectangle function (left) with k summands. The Fourier coefficients (right) are zero for $|m| > k$.

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

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

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

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 $g(x) \in \mathscr{L}^2(-\pi, \pi)$,

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

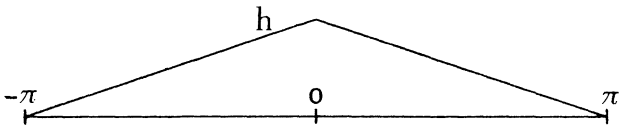


Fig. 4.6. The triangle function.

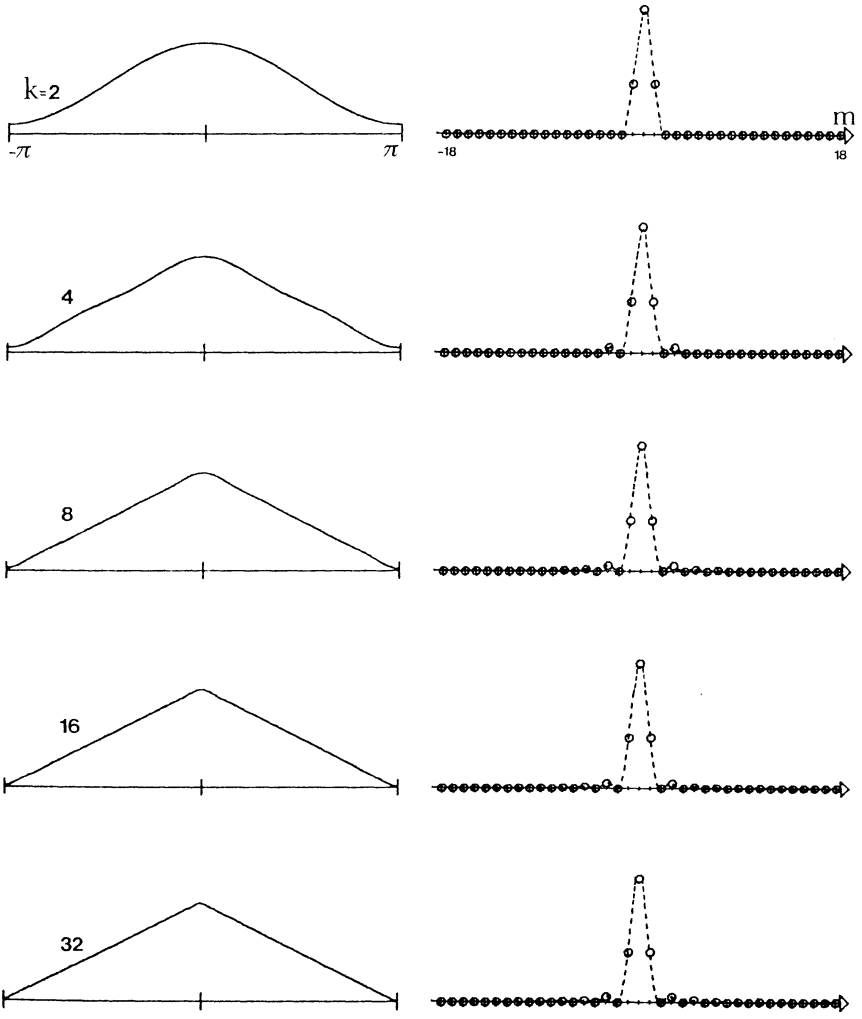


Fig. 4.7. Succession of truncated sums approximating the triangle function (left) and Fourier coefficients (right). The latter are zero for $|m| > k$.

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

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

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

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

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

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

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

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

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

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

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

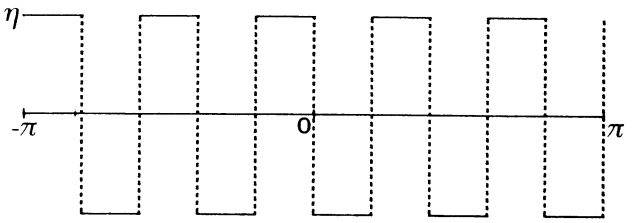


Fig. 4.8. Square wave with five pulses.

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

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

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

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

Operation	Function	Fourier Partial-Wave Coefficients		
		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 $\exp(2\pi i l/k)$	$f_n = 0$ 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

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

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

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

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

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

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

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

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

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

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).

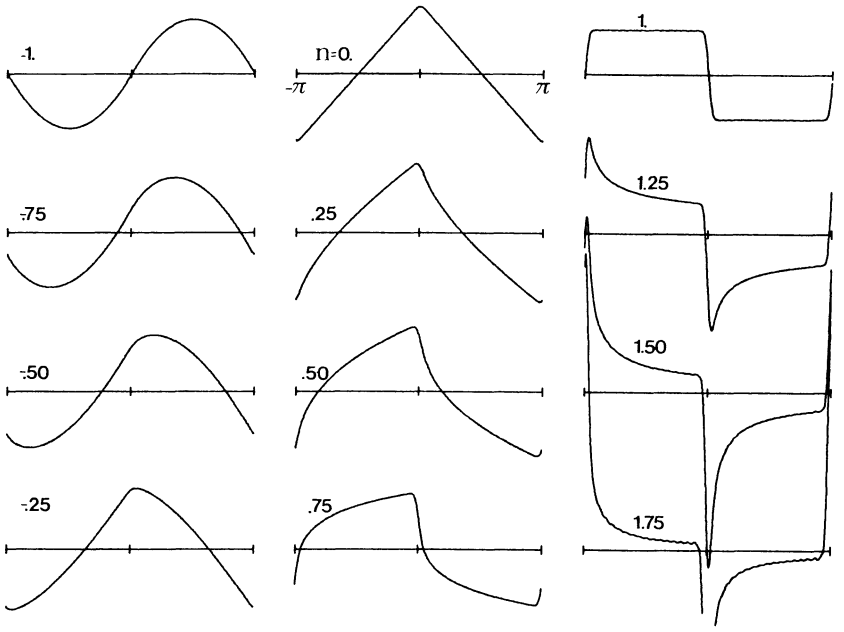


Fig. 4.9. Fractional derivatives of order n of the triangle function. The latter has been slightly smoothed so as to avoid the appearance of the Gibbs phenomenon for positive derivatives in the finite computed series; still, spurious oscillations appear in the highest derivatives.

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

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

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

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

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

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

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

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

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

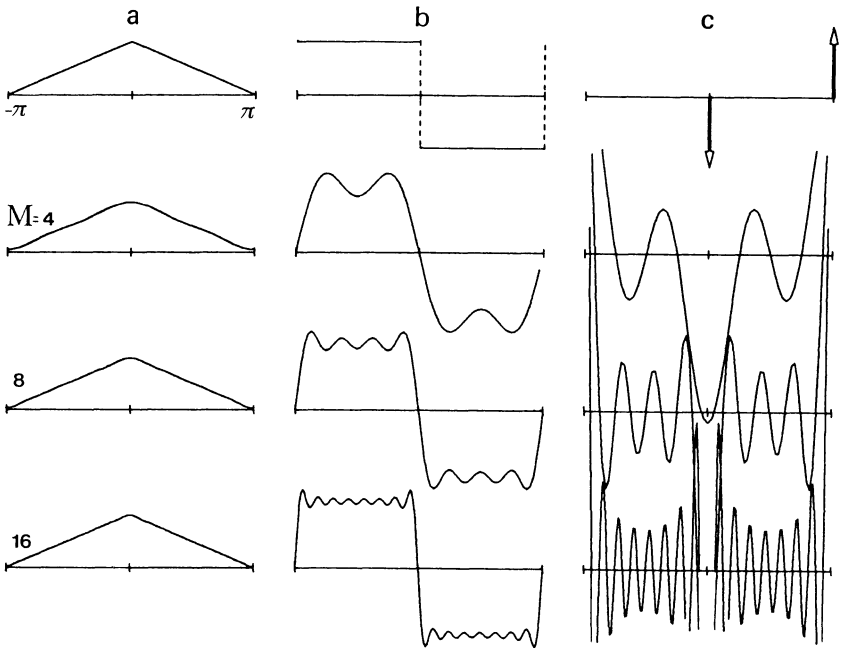


Fig. 4.10. Relation between differentiability and convergence. (a) The triangle function and its first few truncated Fourier sums; (b) and (c) are their first and second derivatives.

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

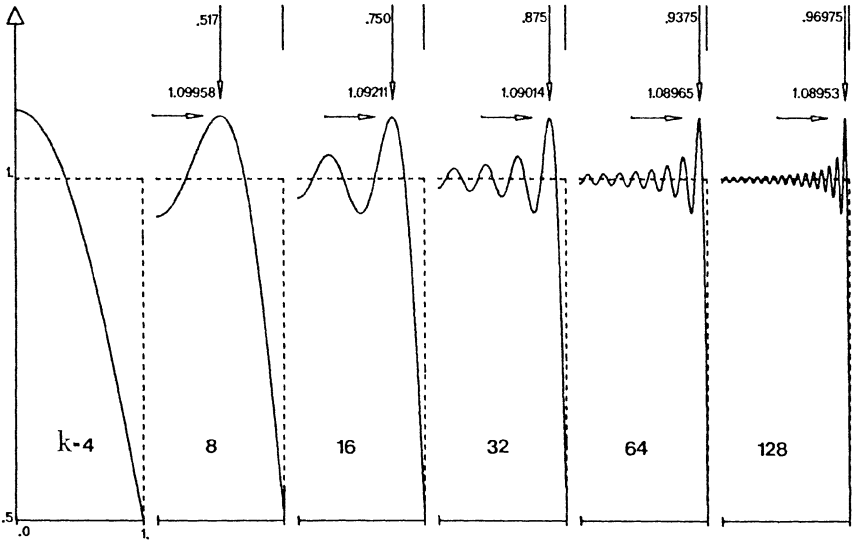


Fig. 4.11. The Gibbs phenomenon. This is an amplification of Fig. 4.5 extending from $x = \pi/4$ to $\pi/2$ over the upper half of the rectangle height. The vertical arrows indicate the position of the maxima as they approach the discontinuity edge and the horizontal ones, their values. The numbers beside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

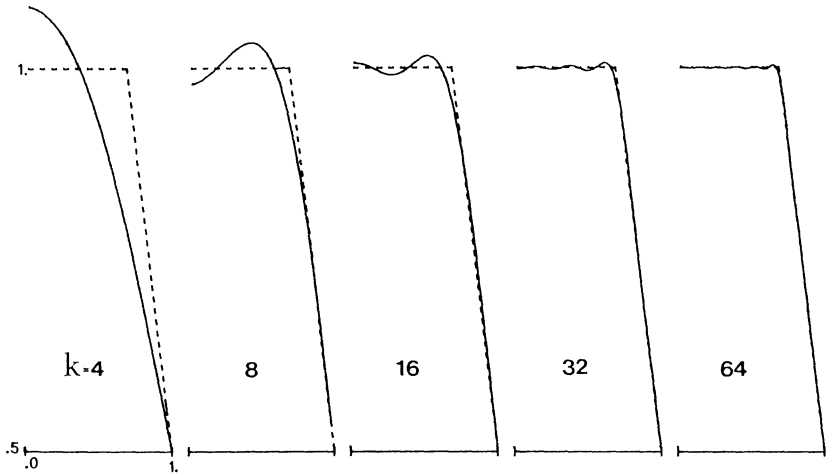


Fig. 4.12. Convergence improvement through the Lanczos σ-factors. Convoluting the function of Figure 4.11 with a rectangle function of width $\varepsilon = \pi/6$ [Eq. (4.63)], the truncated sums approach the trapezium limit with decreasing overshoot.

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

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

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),

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

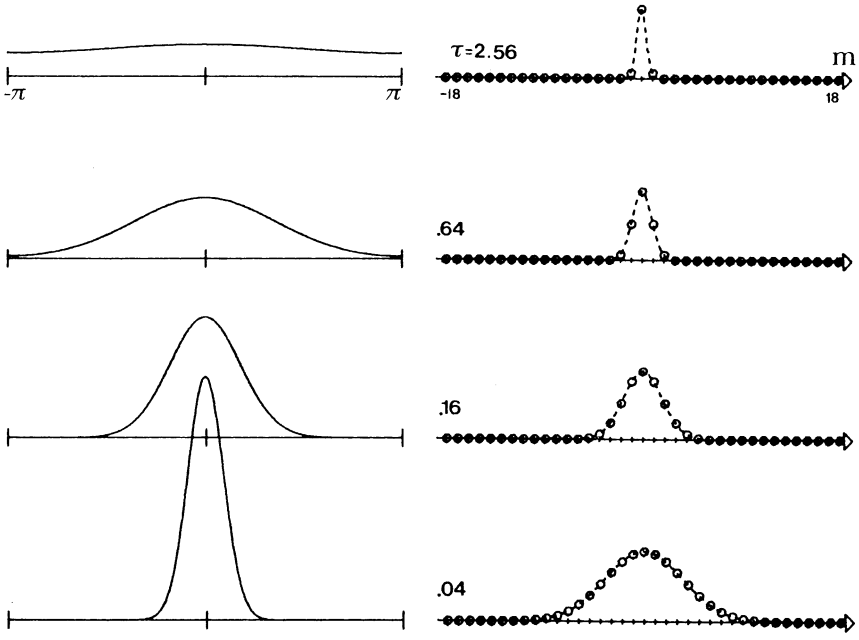


Fig. 4.13. The Jacobi theta function in Eq. (4.64) for (left) various values of the width parameter τ and (right) their Fourier coefficients.

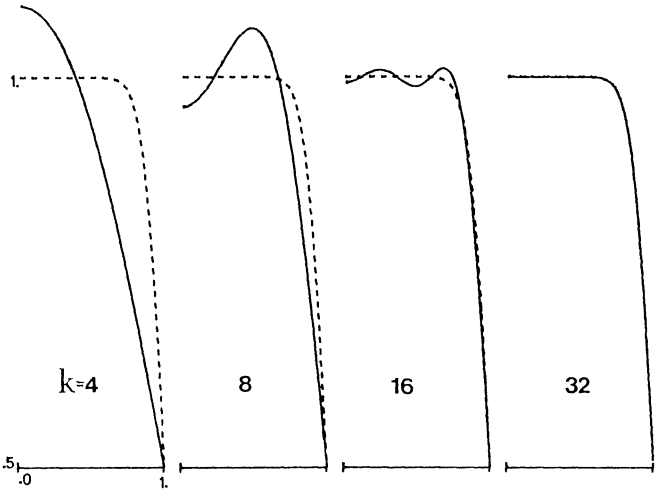


Fig. 4.14. Convergence improvement by the θ-factors of Eq. (4.65) for a value of $\tau = 0.005$.

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	$\frac{d^p}{dx^p} f(x)$	$(in)^p f_n$
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),

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

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

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

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

$$(\mathbf{S}^{(1,D/2)'}, \mathbf{g}) = (D(-\boldsymbol{\delta} + \mathbb{T}_{-\pi}\boldsymbol{\delta}), \mathbf{g}) \tag{4.87}$$

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

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

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

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

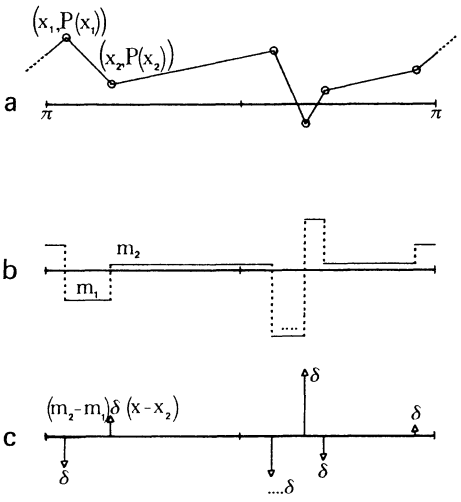


Fig. 4.15. (a) The polygonal function joining the points $[x_k, P(x_k)]$, $k = 1, 2, \ldots, N$, by straight lines; (b) and (c) are its first and second derivatives.

and we identify

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

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.,

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

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

$$(\boldsymbol{\delta}^{(p)}, \mathbb{T}_y \mathbf{g}) = \int_{-\pi}^{\pi} dx[d^p\delta(x)/dx^p]g(x+y)$$

$$= (-1)^p \int_{-\pi}^{\pi} dx\delta(x)[d^p g(x+y)/dx^p]$$

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

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

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

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 $\mathscr{L}^2(\mathscr{J})$ is a Hilbert space. Another Hilbert space one can construct is l^2, the space of all infinite-dimensional vectors $\tilde{\mathbf{f}} \coloneqq \{f_n\}_{n\in\mathscr{Z}}$ with inner product $(\tilde{\mathbf{f}}, \tilde{\mathbf{g}})_{l^2} \coloneqq \sum_{n\in\mathscr{Z}} f_n^* g_n$. 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 $\mathscr{L}^2(\mathscr{J})$ *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* $\{\boldsymbol{\delta}_y\}$, $\boldsymbol{\delta}_y \coloneqq \mathbb{T}_{-y}\boldsymbol{\delta} \in \mathscr{S}'$, 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: $\mathbf{f}^{(p)} = \mathbb{\nabla}^p\mathbf{f}$. 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

$$A = \Phi \mathbf{A} \Phi^{\dagger}, \qquad \mathbf{A} = \Phi^{\dagger} A \Phi, \qquad \Phi := \|(\delta_x, \varphi_n)\|, \tag{4.120c}$$

where Φ is the "rectangular" matrix suggested in the discussion at the end of Section 4.5.

Exercise 4.49. Prove

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

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

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 $-i\nabla$ 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

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

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:

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

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

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

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

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: $f^L{}_{-n} = -f_n^L$ (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

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

Eqs. (4.132) can be written again as

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

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

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

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

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

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

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

where $\tilde{f}(p)$ now stands for the function of $p \in \pi\mathscr{L}/L$ 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.

5

Fourier Series in Diffusion and Wave Phenomena

One of the main fields of application of Fourier series is in finding the solution of processes governed by linear partial differential equations where the space derivative is the Laplacian. In such processes, it is the *local curvature* of the disturbance which is subject to the time development as determined by the time derivatives. If the latter is a first-order derivative, we have the diffusion equation [Eq. (5.1)], where the *rate* of change in temperature is proportional to its local curvature. In the wave equation [Eq. (5.15)], it is the *acceleration*, the second time derivative, which responds linearly to the disturbance curvature. If the boundary conditions are *periodic* with some period $2L$, Fourier series will provide an expansion of the solution in terms of a basis of Laplacian eigenfunctions with exactly these periodicity conditions.

The diffusion equation is analyzed in Section 5.1, and in Section 5.2 the wave equation is presented. The boundary conditions proposed in the latter are those of a fixed-end string rather than those of a vibrating ring, say. This is done partly because of the general interest of *constrained* elastic media and partly for the opportunity it provides to illustrate the use of the Fourier sine series. In both cases we present several approaches: (a) the Green's function treatment, (b) normal modes, (c) hyperdifferential time-evolution operators, and (d) for the wave equation, traveling waves. In Section 5.3 we apply Fourier series to describe a mechanical lattice composed of an infinity of masses and springs.

5.1. Heat Diffusion in a Ring

In this section we derive the diffusion equation from physical considerations about heat conduction. This partial differential equation is easily

solved by Fourier series, the theta function of Section 4.4 being the Green's function for the system. Operator methods, introduced later, will be seen to abbreviate the derivation.

5.1.1. The Heat Equation

A homogeneous conducting medium whose temperature $f(\mathbf{x}, t)$ is a function of the point $\mathbf{x}$ at time t will satisfy the *heat equation*

$$\frac{\partial}{\partial t} f(\mathbf{x}, t) = a^2 \nabla^2 f(\mathbf{x}, t), \qquad a^2 = \kappa/\mu s, \tag{5.1}$$

where a is the diffusion constant given in terms of the conductivity κ, mass density μ, and the specific heat s of the medium. Equation (5.1) states that the rate of change of temperature with time at a point is proportional to the local curvature of the function in the direction of concavity ("nature hates vacua"). The constant a^2 describes the time scale of the diffusion process.

We shall sketch how Eq. (5.1) arises in a one-dimensional ("thin rod") medium. See Fig. 5.1. The *heat flux* $\Phi(x, t)$ across a point x (in calories per unit time) is observed to be proportional to the *temperature gradient* at x (in °K per unit length), i.e., $\Phi(x, t) = -\kappa\, \partial f(x, t)/\partial x$, the proportionality constant κ being the conductivity of the medium and the minus sign indicating that heat flows from warmer to colder regions. The *net flux* of heat into the segment extending from x to $x + \Delta x$ is $\Phi_{\text{net}}(x, t) = \Phi(x, t) - \Phi(x + \Delta x, t)$ and results in a change of temperature. The number of calories needed to raise the rod element mean temperature by 1°K is given by the specific heat s of the material times the linear mass density μ times the length Δx. Thus $\Phi_{\text{net}}(x, t) = \mu s\, \Delta x\, \partial f(x, t)/\partial t$. Equating the expressions involving the temperature, dividing by Δx, and letting $\Delta x \to 0$, one obtains Eq. (5.1) in one dimension. The basic arguments outlined here can be repeated for heat diffusion in two, three, or more dimensions.

The differential equation (of *parabolic* type) in Eq. (5.1) still has to be complemented by boundary conditions in time and space in a manner which

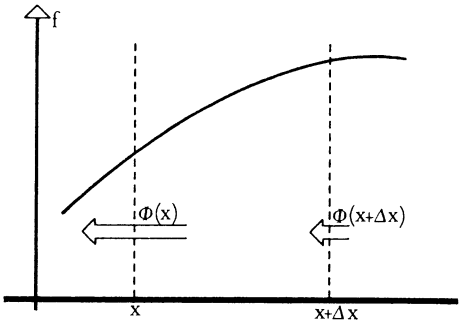


Fig. 5.1. Temperature and heat flux in a thin rod.

will be brought out below. In what follows, we shall absorb the constant a^2 into rescaling the time units. In the resulting formulas, the diffusion constant a can be regained by replacing t by a^2t.

Equation (5.1) for the temperature $f(\mathbf{x}, t)$ can be multiplied on both sides by the *heat capacity* C (in calories per °K per unit volume), giving an identical equation for $\rho(\mathbf{x}, t) \coloneqq Cf(\mathbf{x}, t)$; the amount of heat per unit volume Equation (5.1) then describes a compressible but nonevanescent fluid which can represent such diverse processes as the interpenetration of one liquid by another or the diffusion of neutrons through matter.

5.1.2. Solution by Fourier Series

The boundary conditions we use here to illustrate the use of Fourier series describe a conducting *ring* of unit radius, where x represents the arc length. A ring with arbitrary radius does not introduce any novel features: it can be easily treated using the form (4.132) for the series. The boundary conditions in space are thus $f(x, t) = f(x + 2\pi, t)$, and the temperature function can be taken to represent a vector $\mathbf{f}(t)$ in the function space described in Chapter 4. Equation (5.1) thus becomes the vector equation (with rescaled time)

$$\frac{d}{dt}\mathbf{f}(t) = \nabla^2\mathbf{f}(t). \tag{5.2}$$

In the $\boldsymbol{\varphi}$-basis, (5.2) implies the equality of the corresponding column-vector coefficients. Those on the left-hand side are $\dot{f}_n(t) \coloneqq df_n(t)/dt$, while those on the right can be found from (4.51). Hence (5.1) plus the periodic boundary conditions are equivalent to the set of equations

$$\dot{f}_n(t) = -n^2 f_n(t), \qquad n \in \mathscr{Z}. \tag{5.3}$$

[The process of finding (5.3) from (5.1) is analogous to the uncoupling of the lattice equations of motion in Chapter 2. From the second-order *partial* differential equation (5.1) we thus find an (infinite) set of first-order *ordinary* differential equations. The x and t derivatives are now uncoupled. The interaction operator is the Laplacian ∇^2, in correspondence with the second-difference operator which appeared in Chapter 2.]

The general solution of (5.3) is of the type $c_n \exp(-n^2t)$, with arbitrary constants c_n which are fixed when the initial conditions in time are specified. For $t = t_0$, let the temperature be $\mathbf{f}(t_0)$ with Fourier components $f_n(t_0)$. The constants c_n can then be uniquely evaluated in terms of the initial condition yielding

$$f_n(t) = f_n(t_0) \exp[-n^2(t - t_0)], \qquad n \in \mathscr{Z}, \tag{5.4}$$

as the general solution of (5.3). The original temperature function $f(x, t)$ can finally be regained as the Fourier synthesis of (5.4), i.e., by Eq. (4.32a),

$$f(x, t) = (2\pi)^{-1/2} \sum_{n \in \mathscr{Z}} f_n(t) \exp(inx). \tag{5.5}$$

5.1.3. The Green's Function and Fundamental Solutions

We note that the Fourier coefficients (5.4) of $f(x, t)$ are the product of the Fourier coefficients of $f(x, t_0)$ times $\exp[-n^2(t - t_0)]$, which are the Fourier coefficients of the theta function $\theta(x, t - t_0)$ in Eq. (4.64), times $(2\pi)^{1/2}$. The temperature function (5.5) will thus be the *convolution* of the two, i.e.,

$$\begin{aligned} f(x, t) &= [\theta(\cdot, t - t_0) * f(\cdot, t_0)](x) \\ &= \int_{-\pi}^{\pi} dx' \theta(x - x', t - t_0) f(x', t_0). \end{aligned} \tag{5.6}$$

This expression has a very transparent physical meaning. To bring this out, consider the special (unphysical) case where the initial conditions are $f(x', t_0) = \delta(x' - x_0)$, i.e., an infinitely hot spot at x_0. The temperature thereafter is then given by (5.6) as the *fundamental solution*

$$f(x, t) = \theta(x - x_0, t - t_0), \qquad t \geqslant t_0, \tag{5.7}$$

which is a theta function centered at x_0. See Fig. 4.13.

If the initial temperature distribution were a finite collection of hot points at x_i, that is, $\sum_i f_i \delta(x - x_i)$, the resulting solution would be a sum of θ's centered at x_i with coefficients f_i. An arbitrary initial condition $f(x, t_0)$ can be seen as a sum—à la Riemann, gone to the limit—of δ's distributed over $x' \in (-\pi, \pi]$ with coefficients $f(x', t_0)\, dx'$. The resulting temperature distribution is then (5.6). The theta function is thus the *Green's function* for diffusive processes; it appears as an integral kernel in (5.6) and relates the initial condition at (x', t_0) and its effect at (x, t). It has the properties:

(a) It is an *even* function of space: $\theta(x, t) = \theta(-x, t)$, which means that, preserving their time ordering, the points of cause x' and the points of effect x can be *exchanged*. This is the principle of *reciprocity*.

(b) The effect of x' on x depends only on their *relative* separation $x' - x$, as can be seen in the corresponding functional dependence of the Green's function: the system is *translationally invariant*.

(c) The system is *invariant under inversions* since the Green's function depends only on the absolute value $|x' - x|$. (Compare with Section 2.2.)

The theta function $\theta(x, t - t_0)$ is infinitely differentiable in x and in $t > t_0$ as its Fourier series shows. Since the solution $f(x, t)$ is a convolution

of the initial condition with $\theta(x, t - t_0)$, it follows that $f(x, t)$ itself will also be infinitely differentiable in the half-plane (x, t), $t > t_0$.

5.1.4. The Time-Evolution Operator

From the above discussion it follows that the integral kernel given by the Green's function $\theta(x, t)$ acts as a linear operator,

$$\mathbf{f}(t) = \mathbb{G}(t - t_0)\mathbf{f}(t_0), \tag{5.8}$$

mapping the space of generalized functions which are the initial conditions $\mathbf{f}(t_0)$ of the system on the space of infinitely differentiable functions for $t > t_0$.

Since any linear combination of solutions of (5.1) is also a solution to this equation, *the set of all solutions of the diffusion equation constitutes a linear vector space.*

Further properties of the Green's function are that *total heat is preserved* and that the set of Green's functions for all $t > t_0$ constitutes a *semigroup of integral kernels.* This we leave to the reader to verify in Exercises 5.1 and 5.2.

Exercise 5.1. Show that the *total heat* of the system

$$Q \coloneqq \int_{-\pi}^{\pi} dx f(x, t) \tag{5.9}$$

is a constant, independent of time. This can be proven (a) by substitution of (5.6) into (5.9), exchange of integrals, and the property (4.68) of the theta function, or (b) by calculating the time derivative of (5.9), using the governing equation (5.1) and showing that the evaluated integral is zero due to the periodic boundary conditions in x. Another proof is suggested in Exercise 5.5.

Exercise 5.2. Let the temperature function at time t be due to initial conditions at t_1 and these in turn a consequence of an earlier t_0 temperature distribution. Show that time evolution is a *transitive* process in the sense that

$$\begin{aligned} f(\cdot, t) &= \theta(\cdot, t - t_1) * f(\cdot, t_1) = \theta(\cdot, t - t_1) * \theta(\cdot, t_1 - t_0) * f(\cdot, t_0) \\ &= \theta(\cdot, t - t_0) * f(\cdot, t_0), \end{aligned} \tag{5.10}$$

which is satisfied since

$$\int_{-\pi}^{\pi} dx' \theta(x - x', t_1)\theta(x' - x'', t_2) = \theta(x - x'', t_1 + t_2). \tag{5.11}$$

Equation (5.11) can be proven either directly or by the product of the Fourier coefficients of the θ's in convolution. This associates to every time $t \geqslant 0$ an integral kernel with (a) the composition law (5.11), (b) identity given by the Dirac δ, and (c) associativity. For negative time t the θ-function series is strongly divergent, so the general inverse for the set of integral kernels does not exist. We have thus a *semigroup* of time-evolution operators.

Exercise 5.3. Can a temperature distribution of the form of a rectangle or a triangle function be regressed in time at all? Find a condition so that a temperature distribution allows time regression to $-\tau$. Can any temperature distribution be regressed in time indefinitely? Work in the Fourier basis only.

Exercise 5.4. As Eq. (5.1) manifestly allows, search for its *separable* solutions $f_n(x, t) = X_n(x)T_n(t)$, n specifying the separation constant. By introducing this form into (5.1) and recalling the space boundary conditions, the solutions found will be of the form $\exp(-n^2t + inx)$ for $n \in \mathscr{Z}$. These are the "normal modes" for heat diffusion in the ring. The most general solution will be a sum over n of these solutions with coefficients determined from the initial conditions. Show that one regains the form (5.6) with the series development of the theta function.

5.1.5. Hyperdifferential Form of the Evolution Operator

The solutions of the diffusion equation lend themselves to a general presentation by *hyperdifferential* operators. One can formally expand the solution of (5.1) using the Taylor series in t around t_0 as

$$f(x, t) = \sum_{n=0}^{\infty} \frac{(t - t_0)^n}{n!} \frac{\partial^n}{\partial t'^n} f(x, t')|_{t'=t} =: \exp\left[(t - t_0)\frac{\partial}{\partial t'}\right] f(x, t')|_{t'=t}. \tag{5.12}$$

Now, on the space of solutions of (5.1), the operator $\partial/\partial t$ is equivalent to ∇^2, and hence (5.12) can be expressed as

$$f(x, t) = \exp[(t - t_0)\nabla^2] f(x, t_0), \tag{5.13}$$

which should then be equivalent to the time evolution (5.6) in terms of an integral kernel. [Compare with Eq. (2.38b).] It would appear that (5.13) can hold only when the initial temperature distribution is infinitely differentiable. Actually, (5.13) holds *weakly* for any generalized function $f(x, t_0)$ as can be seen when $f(x, t_0) = \delta(x - x_0)$ so that $f(x, t)$ is the fundamental solution (5.7). The weak equality between the integral convolution (5.6) and the *hyperdifferential* operator in (5.13) was established in (4.100).

We can state quite generally that *the exponentiation of a second-order differential operator is weakly equivalent to the action of an integral kernel*, both representing here the time-evolution operator $\mathbb{G}(t - t_0)$ in Eq. (5.8). In Eq. (4.129) we characterized operators represented by diagonal matrices in the φ-basis as *convolution* operators. Since any powers or sums thereof are diagonal in this basis, $\mathbb{G}(\tau) = \exp(\tau\nabla^2)$ is clearly such an operator.

Exercise 5.5. Prove total heat conservation using the hyperdifferential form of the solution. Note that (5.9) can be written as $Q = (\mathbf{1}, \mathbf{f}(\cdot, t))$, where $\mathbf{1}$ is the unit constant function in $(-\pi, \pi]$. The Parseval identity then allows us to write Q as an inner product in the φ-basis, which is manifestly time independent.

Exercise 5.6. Prove the semigroup property (5.11) from the corresponding time-evolution operator product

$$\mathbb{G}(t_1)\mathbb{G}(t_2) = \mathbb{G}(t_1 + t_2), \qquad \mathbb{G}(0) = \mathbb{1}, \tag{5.14}$$

which in turn is an immediate consequence of the hyperdifferential form (5.13).

Lest the solution of the diffusion equation appear trivial, let us remark that the greater practical difficulties in solving Eq. (5.1) appear when realistic boundary conditions are imposed as curves in the (x, t)-plane and when *sources* of heat or fluid are present. The latter case will be taken up in Part III in studying applications of the Fourier and Laplace transforms. The study of *some* boundary conditions will be taken up in the context of separating coordinates for the diffusion equation as an application of canonical transforms in Chapter 10. Meanwhile, two simple boundary conditions which can be reduced to the periodic case are suggested in Exercises 5.7 and 5.8.

Exercise 5.7. Assume one has a conducting rod extending between two "*cold walls*" at $x = 0$ and $x = \pi$ which maintain the conditions $f(0, t) = 0 = f(\pi, t)$ for all t. Since $\exp(t\nabla^2)$ commutes with $\mathbb{I}_0$ [see Eqs. (4.121)], the "*method of images*" is applicable. It consists of choosing a rod to extend between $x = -\pi$ and π, the segment $(-\pi, 0)$ being the negative mirror image of the temperature function in $(0, \pi)$, i.e., $f(-x, t_0) = -f(x, t_0)$. This relation is preserved for all t. The description can be made using the *sine* Fourier series, Eqs. (4.134).

Exercise 5.8. Assume now that the conducting rod has *insulated* ends at $x = 0$ and π. As there the heat flux is zero, $\partial f(x, t)/\partial x|_{x=0,\pi} = 0$ are the space boundary conditions. The "method of images" with functions symmetric under inversions will use the *cosine* Fourier series (4.135). The reader may find it worthwhile before solving Exercises 5.7 and 5.8 to browse through Section 5.2 where the method of images is used for the wave equation with similar boundary conditions.

5.2. The Vibrating String

Fourier series are well suited for the description of wave phenomena in elastic media with Cartesian boundaries. The disturbance or characteristic $f(\mathbf{x}, t)$ of the medium we want to analyze will be governed by the *wave equation*

$$c^{-2}\frac{\partial^2}{\partial t^2}f(\mathbf{x}, t) = \nabla^2 f(\mathbf{x}, t), \tag{5.15}$$

where c is a constant which will turn out to be the propagation velocity. Equation (5.15) has to be complemented by *boundary conditions* in space and time, typically

$$f(\mathbf{x}, t) = 0 \text{ for } \mathbf{x} \in B, f(\mathbf{x}, t_0) = u(\mathbf{x}), \dot{f}(\mathbf{x}, t_0) = v(\mathbf{x}), \tag{5.16}$$

where B is a fixed boundary enclosing a finite region in **x**-space. Here we shall concentrate on finding the solutions of (5.15)–(5.16) describing a finite string with fixed ends. Various other boundary conditions and regions will be presented in Chapter 6.

5.2.1. The Wave Equation

Consider a thin string of linear mass density μ stretched with tension τ between two points and allowed to undergo longitudinal or small transverse vibrations. Let $f(x, t)$ be the elongation from equilibrium of the point x of the string at time t. Isolating the string element which extends from x to $x + \Delta x$ (Fig. 5.2, where the elongation is represented as transversal), we see that it is subject only to a net restitution force in the direction of the displacement. At x the force is $-\tau\, \partial f(x, t)/\partial x$, while at $x + \Delta x$ it is $\tau\, \partial f(x', t)/\partial x'|_{x'=x+\Delta x}$. The net force is the sum of these two and will produce an acceleration $-\partial^2 f(x, t)/\partial t^2$ on the mass $\mu \Delta x$ of the element. Using Newton's laws, dividing by Δx, and letting $\Delta x \to 0$, we obtain the wave equation (5.15) with $c^2 := \tau/\mu$. Dimensional analysis shows that c has units of velocity. We could absorb this constant into a redefinition of time units, but we prefer here to leave it appearing explicitly in the ensuing developments.

The boundary conditions which describe a string of length L with fixed endpoints are

$$f(0, t) = 0, \qquad f(L, t) = 0 \qquad \text{for all } t. \tag{5.17}$$

5.2.2. Eigenfunctions of the Laplacian

Since this chapter deals with applications of Fourier series, we can expect that the use of this series will solve the problem posed by (5.15)–(5.17). In fact it does: if we follow the approach used in Section 5.1, we will find that the partial differential wave equation is reduced to a set of ordinary (second-order) differential equations. We would like to present here a line

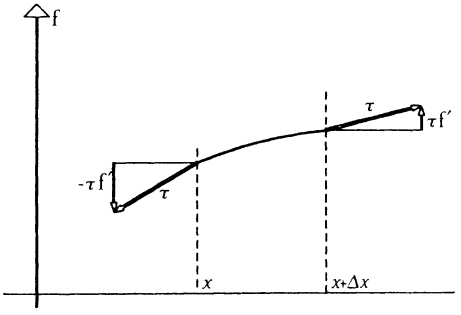


Fig. 5.2. Elongation and tension of an elastic string element.

of reasoning which is somewhat different and which, although leading to the same results, will generalize more easily to the solution of the systems posed in Chapter 6, where the boundary conditions are those of a two-dimensional rectangular, circular, annular, or sectorial membrane.

It is readily verified that in the Hilbert space of functions $\mathscr{L}_0^2(0, L)$ with the inner product (4.134c) on $(0, L)$ and boundary conditions (5.17), the operator ∇^2 is hermitian. For twice-differentiable $\mathbf{g}$, $\mathbf{f}$, integrating by parts,

$$\begin{aligned}(\mathbf{g}, \nabla^2\mathbf{f})_L^\circ &= \int_0^L dx g(x)^* \frac{\partial^2 f(x)}{\partial x^2} \\ &= g(x)^* \frac{\partial f(x)}{\partial x}\bigg|_0^L - \int_0^L dx \left[\frac{\partial g(x)}{\partial x}\right]^* \frac{\partial f(x)}{\partial x} \\ &= \left\{g(x)^* \frac{\partial f(x)}{\partial x} - \left[\frac{\partial g(x)}{\partial x}\right]^* f(x)\right\}\bigg|_0^L + \int_0^L dx \left[\frac{\partial^2 g(x)}{\partial x^2}\right]^* f(x) \\ &= 0 + (\nabla^2\mathbf{g}, \mathbf{f})_L^\circ. \end{aligned} \tag{5.18}$$

Moreover, ∇^2 can be shown to be *self-adjoint*. The set of all its eigenvectors

$$\nabla^2 f_\lambda(x) = \lambda f_\lambda(x) \tag{5.19}$$

will constitute a complete orthogonal basis for that space (Section 4.7).

The solutions of the differential equation (5.19) have the general form

$$a \sin[(-\lambda)^{1/2}x] + b \cos[(-\lambda)^{1/2}x], \qquad a, b, \lambda \in \mathscr{C}. \tag{5.20}$$

If we impose the boundary conditions (5.17) at $x = 0$, we obtain the restriction $b = 0$, while the condition at $x = L$ requires $(-\lambda)^{1/2}L \equiv 0 \bmod \pi$, i.e., $(-\lambda)^{1/2}L = n\pi$, $n \in \mathscr{Z}$, or $\lambda = -(n\pi/L)^2$. The eigenfunctions of ∇^2 are thus $\sin(n\pi x/L)$ in $\mathscr{L}_0^2(0, L)$, and we can use n to label the eigenfunctions. The values $+|n|$ and $-|n|$ yield the same function, while for $n = 0$ we obtain the zero function. Hence we let $n = 1, 2, 3, \ldots$. The constant a in (5.20) may depend on n and t, so we let $a = a_n(t)$.

We can thus expand any function $f(x, t) \in \mathscr{L}_0^2(0, L)$ satisfying (5.15) in terms of eigenfunctions of ∇^2 with these boundary conditions as

$$f(x, t) = (2/L)^{1/2} \sum_{n \in \mathscr{Z}^+} a_n(t) \sin(n\pi x/L), \tag{5.21a}$$

introducing the constant $(2/L)^{1/2}$ in order to match exactly Eqs. (4.134). These allow us to solve for the $a_n(t)$:

$$a_n(t) = (2/L)^{1/2} \int_0^L dx f(x, t) \sin(n\pi x/L) = f_n^\circ(t). \tag{5.21b}$$

Equations (5.21) do not yet describe solutions of the wave equation (5.15); they are only an expansion tailored for this equation plus boundary condi-

tions. Now, upon requiring that (5.21a) be a solution to (5.15), we find a set of uncoupled ordinary differential equations for $a_n(t)$ to satisfy, viz.,

$$0 = \left(c^{-2}\frac{\partial^2}{\partial t^2} - \mathbb{V}^2\right) f(x, t)$$

$$= (2/L)^{1/2} \sum_{n\in\mathscr{Z}^+} \left(c^{-2}\frac{\partial^2}{\partial t^2} + \lambda_n\right) f_n^{\circ}(t) \sin(n\pi x/L). \tag{5.22}$$

Linear independence of the eigenvectors of $\mathbb{V}^2$ now implies that each of the coefficients of the series (5.22) is zero. The $f_n^{\circ}(t)$ are thus determined up to two arbitrary constants, which we write, introducing for later use an "initial time" t_0, as

$$f_n^{\circ}(t) = b_n \sin[\omega_n(t - t_0)] + c_n \cos[\omega_n(t - t_0)], \qquad b_n, c_n \in \mathscr{C}, \tag{5.23a}$$

$$\omega_n := n\pi c/L, \qquad n \in \mathscr{Z}^+. \tag{5.23b}$$

5.2.3. Initial Conditions and Green's Function

The series (5.21a) with coefficients (5.23) is the most general solution of the problem. It remains now to fix the constants b_n and c_n in terms of boundary conditions in time. Any pair of initial conditions on $f(x, t)$ or its time derivatives for fixed t will be suitable. The most common pair is the initial elongation $f(x, t_0)$ and velocity $\dot{f}(x, t_0)$ for t_0. By (5.21b) and (5.23) this determines the b_n and c_n in terms of the sine Fourier coefficients of the two initial conditions. We find

$$b_n = \dot{f}_n^{\circ}(t_0)/\omega_n, \qquad c_n = f_n^{\circ}(t_0), \tag{5.24}$$

so that upon substitution of (5.24) into (5.23) and (5.23) into (5.21a), the solution can be expressed as

$$\begin{aligned} f(x, t) &= (2/L)^{1/2} \sum_{n\in\mathscr{Z}^+} \omega_n^{-1} \sin[\omega_n(t - t_0)] \sin(n\pi x/L) \dot{f}_n^{\circ}(t_0) \\ &\quad + (2/L)^{1/2} \sum_{n\in\mathscr{Z}^+} \cos[\omega_n(t - t_0)] \sin(n\pi x/L) f_n^{\circ}(t_0) \\ &=: \sum_{n\in\mathscr{Z}^+} G_n^{\circ}(x, t - t_0) \dot{f}_n^{\circ}(t_0) + \sum_{n\in\mathscr{Z}^+} \dot{G}_n^{\circ}(x, t - t_0) f_n^{\circ}(t_0) \\ &= (\mathbb{T}_{-x}\mathbf{G}(t - t_0), \dot{\mathbf{f}}(t_0))_L^{\circ} + (\mathbb{T}_{-x}\dot{\mathbf{G}}(t - t_0), \mathbf{f}(t_0))_L^{\circ} \\ &= \int_0^L dx' G(x - x', t - t_0) \dot{f}(x', t_0) + \int_0^L dx' \dot{G}(x - x', t - t_0) f(x', t_0). \end{aligned} \tag{5.25}$$

The last two equalities deserve comment. The second term in (5.25) contains

two sums, each of which gives rise to an inner product (4.134c). The first one involves $\mathbf{f}(t_0)$ with a vector with sine Fourier components

$$G_n^{\circ}(x, t - t_0) \coloneqq (2/L)^{1/2}\omega_n^{-1} \sin[\omega_n(t - t_0)] \sin(n\pi x/L)$$
$$= (\mathbb{T}_{-x}\mathbf{R}^{[2c(t-t_0),1/2c]})_n^{\circ} = G_n^{\circ}(x, t - t_0)^*. \quad (5.26a)$$

We recognize in the expression (5.26a) the sine Fourier coefficients of the rectangle function of width $2c(t - t_0)$, height $1/2c$, and centered at x as obtained in Eq. (4.135). [Recall the remark about the negative "phantom" function in $(-L, 0)$.] The second sum in (5.25) involves the time derivative of (5.26a),

$$\dot{G}_n^{\circ}(t - t_0) = (2/L)^{1/2} \cos[\omega_n(t - t_0)] \sin(n\pi x/L)$$
$$= \tfrac{1}{2}(\mathbb{T}_{x+c(t-t_0)}\boldsymbol{\delta} + \mathbb{T}_{x-c(t-t_0)}\boldsymbol{\delta})_n^{\circ}, \quad (5.26b)$$

which we recognize as the coefficients of two δ's sitting at $x + ct$ and $x - ct$. The last equality in (5.25) expresses the convolution of the vector $\dot{\mathbf{f}}(t_0)$, represented by the function $\dot{f}(x', t_0)$, initial velocity, and (5.26a), which is the *Green's function* for the system at hand,

$$G(x - x', \tau) = R^{(2c\tau,1/2c)}(x - x'), \quad (5.27a)$$

and that of the initial condition $f(x', t_0)$ and (5.26b),

$$\dot{G}(x - x', \tau) = \tfrac{1}{2}[\delta(x' - (x + c\tau)) + \delta(x' - (x - c\tau))], \quad (5.27b)$$

integrated over x'.

5.2.4. Fundamental Solutions

To bring out the meaning and properties of Green's function we shall consider the *fundamental solutions* below. [Compare these results with those in Section 2.3.] Assume that initially the string starts from *rest* with a δ-*like* "shape" at some point x_0, i.e., $\dot{f}(x', t_0) = 0$, $f(x', t_0) = \delta(x' - x_0)$. The ensuing development of the string shape is then $\dot{G}(x - x_0, t - t_0)$. Equation (5.27b) tells us that the δ-pulse splits into two pulses traveling along $x = x_0 \pm c(t - t_0)$, i.e., they keep their δ-shape at all times and propagate with velocity $\pm c$. Such a pulse is shown in Fig. 5.3(a). Assume next that the string starts from zero elongation, $f(x, t_0) = 0$, but with a δ-pulse in velocity at some x_0, $\dot{f}(x, t_0) = \delta(x - x_0)$, as if impelled by a sharp, localized blow. The string shape will then develop as $G(x - x_0, t - t_0)$, shown in Fig. 5.3(b); it is a rectangle function which broadens with velocity c. The most general solution with initial conditions given by $f(x, t_0)$ and $\dot{f}(x, t_0)$ will be an integral—a generalized linear combination—of these fundamental solutions.

Exercise 5.9. Verify that (5.27b) is the time derivative of (5.27a). You can write $R^{(2ct,1)}(x) = \Theta(ct - x)\Theta(ct + x)$, where Θ is the Heaviside step function [$\Theta(y) = 1$ for $y > 0$, $\Theta(0) = \frac{1}{2}$, $\Theta(y) = 0$ otherwise for $y \in (0,L)$], and use the fact that the derivative of a discontinuous function is a Dirac δ.

We recognize the following properties of the Green's function, which hold for the lattice of Section 2.2 or the diffusive systems in Section 5.1: (a) reciprocity, (b) translational, and (c) inversion invariance. In addition, the system exhibits (d) *causality*: a disturbance at (x_0, t_0) can affect only those points x at future times t which are inside the *cone* $|x - x_0| \leqslant c|t - t_0|$. Both the Green's function and its derivative are zero outside this region.

Exercise 5.10. Let the string elongation at time t depend on conditions at time t_1 and these in turn on still earlier initial conditions at time t_0. Express this transitive property in terms of an integral relation between the Green's function and its derivative for times t, t_1, and t_0. Refer to Exercises 2.13 and 5.2 and ahead to Exercise 5.17.

5.2.5. Traveling Waves and Reflection Phenomena

As Figs. 5.3(a) and (b) suggest, something rather dramatic happens when the disturbance traveling with velocity $\pm c$ hits the endpoints of the string. These are kept fixed, and the pulse undergoes a *reflection*, propagating backwards after the collision. Rather than unearth this phenomenon from the Green's function, we can show rather easily what the mechanism is. For this it is sufficient to note that if $g^{\rightarrow}(y)$ and $g^{\leftarrow}(y)$ are two arbitrary functions,

$$f(x, t) = g^{\rightarrow}(x - ct) + g^{\leftarrow}(x + ct) \tag{5.28}$$

will be a solution of the wave equation (5.15). In fact, the most general solution can be built in this way: a right-moving disturbance plus a left-moving one. The boundary conditions (5.17) impose $g^{\rightarrow}(-ct) = -g^{\leftarrow}(ct)$ and $g^{\rightarrow}(L - ct) = -g^{\leftarrow}(L + ct)$, which can be combined as

$$g^{\rightarrow}(y) = -g^{\leftarrow}(-y) = g^{\rightarrow}(2L + y). \tag{5.29}$$

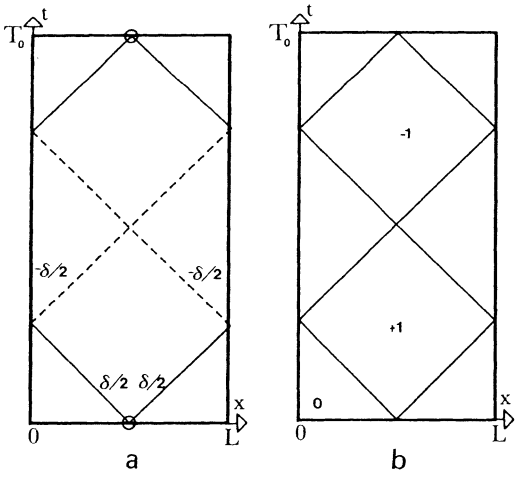


Fig. 5.3. The Green's function and its time derivative for an elastic string of fixed endpoints stretching between 0 and L. (a) $\dot{G}(x - L/2, t)$, (b) $G(x - L/2, t)$. The first consists of traveling Dirac δ's, while the second has values 0, $+1$, and -1 in the regions shown.

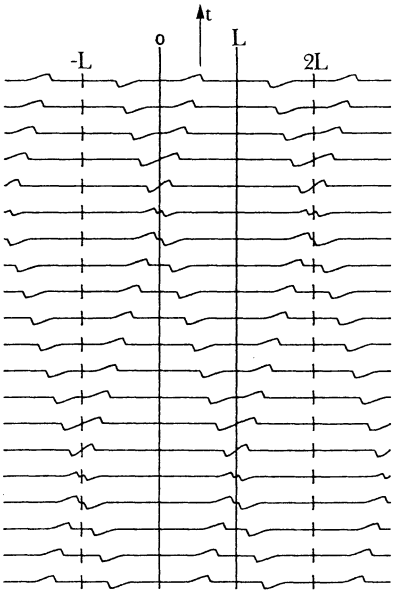


Fig. 5.4. A "lone" traveling pulse in a string undergoing reflection at the endpoints (heavy lines). It is mathematically accompanied by mirror pulses beyond the string ends 0, L. Reflection thus appears as the entrance of a "mirror" pulse in the "real" string.

This means that the right-moving disturbance must be equal to the negative of the inverted left-moving disturbance, and both must be periodic with period $2L$. Any string movement will be a superposition of two such opposing *traveling waves*. A pulse moving "alone" along the string (Fig. 5.4) is mathematically accompanied by an infinity of companion pulses spaced by $2L$ moving in the same direction and by a second infinity of negative mirror pulses traveling in the opposite direction. When the pulse "hits" the wall, it superimposes with its mirror counterpart. As the pulse proceeds into the mirror region, the mirror pulse becomes real and travels through the string. Reflection has taken place. In Fig. 5.5 we show in detail the reflection process undergone by a moving square pulse.

Exercise 5.11. Show that the above description of companion and mirror images of any string shape is contained in the Green's function formalism from Eq. (5.25) onward. Note that Eq. (5.25) can be rewritten as

$$f(x, t) = (2L)^{-1/2}\Big[\sum_{n\in\mathscr{Z}^+} (f_n^{\circ} s_n^{+} - \dot{f}_n^{\circ}\omega_n^{-1} c_n^{+}) - \sum_{n\in\mathscr{Z}^+} (f_n^{\circ} s_n^{-} - \dot{f}_n^{\circ}\omega_n^{-} c_n^{-})\Big], \tag{5.30a}$$

$$f_n^{\circ} = f_n^{\circ}(t_0), \qquad \dot{f}_n^{\circ} = \dot{f}_n^{\circ}(t_0), \tag{5.30b}$$

$$s_n^{\pm} := \sin\{n\pi[c(t - t_0) \pm x]/L\}, \qquad c_n^{\pm} := \cos\{n\pi[c(t - t_0) \pm x]/L\}. \tag{5.30c}$$

Note that for $t = t_0$ this is the sine and cosine Fourier series for functions of period $2L$ and that as $x \leftrightarrow -x$, $s^+ \leftrightarrow s^-$ and $c^+ \leftrightarrow c^-$; hence $f(-x, t) = -f(x, t)$.

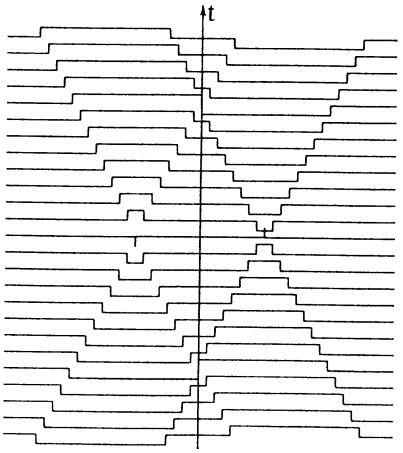


Fig. 5.5. Reflection of a square pulse at a string endpoint. Either half of the figure may represent the "real" string; the other will represent its image.

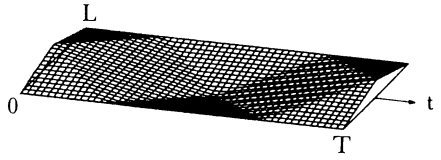


Fig. 5.6. String which starts from rest with a triangle shape.

Exercise 5.12. Explain the development of a string shape which starts from rest in terms of superpositions of right- and left-traveling waves. You can guide yourself with Fig. 5.3(a). Do the same with a string the shape of that in Fig. 5.3(b).

Exercise 5.13. Consider a string which starts from rest with a triangular shape as in Fig. 5.6 as a superposition of right- and left-traveling shapes. Show that the string motion is indeed the one depicted in the figure. At what time does the string recover its initial shape? Did such a "fundamental period" exist for the finite lattice (Chapter 2)?

5.2.6. Normal Modes

The description of the fundamental solutions following Eq. (5.25) was made assuming that the initial displacements and velocities were Dirac δ's. As in Section 2.3, we can now investigate the string motion when the initial conditions are given by the ∇^2 eigenvectors, $(2/L)^{1/2} \sin(n\pi x/L)$, $n \in \mathscr{Z}^+$, in $\mathscr{L}_0^2(0, L)$. The solutions thus obtained are the *normal modes* of the string and can be read from the second member of (5.25), letting the $f_n^{\circ}(t_0)$ and $\dot{f}_n^{\circ}(t_0)$ be different from zero one at a time. Setting $t_0 = 0$ for simplicity, we define

$$\dot{\varphi}_n(x, t) \coloneqq (2/L)^{1/2} \sin(n\pi x/L) \cos \omega_n t, \qquad \omega_n \coloneqq n\pi c/L \quad (5.31a)$$

$$\varphi_n(x, t) \coloneqq (2/L)^{1/2} \sin(n\pi x/L)\omega_n^{-1} \sin \omega_n t, \qquad n \in \mathscr{Z}^+. \quad (5.31b)$$

The most general solution to the string problem is a linear combination of these, as (5.25) can be rewritten in the form

$$f(x, t) = \sum_{n \in \mathscr{Z}^+} f_n^{\circ} \dot{\varphi}_n(x, t) + \sum_{n \in \mathscr{Z}^+} \dot{f}_n^{\circ} \varphi_n(x, t). \tag{5.32}$$

[Note the perfect analogy with (2.48) and (2.50).] A few normal modes (5.31a) have been drawn in Fig. 5.7. Some of their relevant properties are the following: (a) The $\dot{\varphi}_n(x, t)$ represent waveforms which start from rest and maximum elongation, while the $\varphi_n(x, t)$ start from the equilibrium shape with maximum velocity. (b) The nth normal mode presents $n - 1$ *nodes* (i.e., zeros) within the interval $(0, L)$, not counting the endpoints. (c) They oscillate with angular velocities ω_n, Eq. (5.23b), which are *discrete* and directly proportional to n. [In terms of the finite lattice Brillouin diagram of Section 2.3, they are all in the "linear" (low-frequency) region, where $\sin z \sim z$.] (d) The period of oscillation of the nth fundamental mode is

$$T_n = 2\pi/\omega_n = 2L/nc = T_0/n, \qquad T_0 := 2L/c \tag{5.33}$$

and is a submultiple of the *fundamental period* T_0. The original form of *any* string disturbance is thus reproduced after a time T_0, the nth component mode having completed n full oscillations. See again Fig. 5.6. (e) Each normal mode is a sinusoidal string shape modulated by an oscillating function of time: they are the *separated* solutions of the wave equation [i.e., of the form $X_n(x)\tau_n(t)$]. In fact, we would have found precisely these had we set out proposing separated solutions for this equation, the separation constant being proportional to n^2. (f) The odd-n modes are *even* under inversions

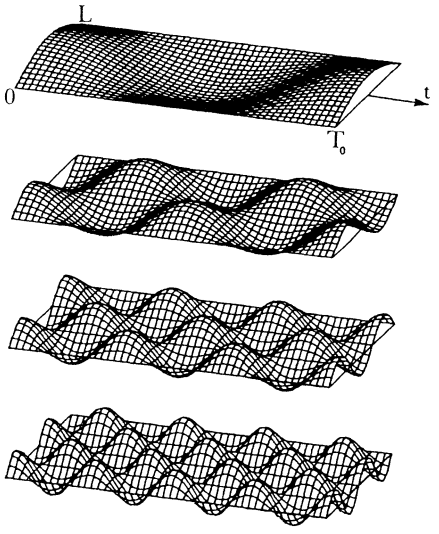


Fig. 5.7. The first four normal modes for a vibrating string that starts from rest [Eq. (5.31a) for $n = 1, 2, 3,$ and 4].

through the string midpoint $x = L/2$. Even-n modes are odd. (g) Under time inversion, the $\dot{\varphi}_n(x, t)$ are even, while the $\varphi_n(x, t)$ are odd.

Exercise 5.14. Analyze the string motion in Fig. 5.6 in terms of the constituent normal modes. Show that only the *odd* modes appear. This can be predicted on the basis of the symmetry of the initial conditions with respect to the string midpoint.

Exercise 5.15. Analyze the translation and inversion symmetries of Fig. 5.6: (a) periodicity in time under translations T_0 and $T_0/2$, and in space under translations by L and $2L$; (b) inversions in time through $t = 0$, $T_0/4$,and $T_0/2$, and in space through $x = 0$, $L/4$, and $L/2$.

5.2.7. Two-Component First-Order Differential Form of the Wave Equation

The solutions of the wave equation on the finite string can also be expressed in terms of hyperdifferential operators acting on the initial conditions. This follows a similar treatment of the diffusion problem in Eq. (5.13) but with the introduction of a space of velocity functions $\dot{f}(x, t)$ in addition to the functions $f(x, t)$ which describe the string elongation. [This is analogous to the phase space in Section 2.6.] We consider $\mathbf{f}$ and $\dot{\mathbf{f}}$ as the components of a two-vector $\boldsymbol{\zeta}(x, t)$ so that the wave equation (5.15) appears as a two-component equation:

$$\mathbb{H}\boldsymbol{\zeta}(x, t) = \frac{\partial}{\partial t}\boldsymbol{\zeta}(x, t), \tag{5.34a}$$

$$\boldsymbol{\zeta}(x, t) \coloneqq \begin{pmatrix} f(x, t) \\ \dot{f}(x, t) \end{pmatrix}, \qquad \mathbb{H} \coloneqq \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ c^2\nabla^2 & \mathbb{0} \end{pmatrix}. \tag{5.34b}$$

The first component of (5.34a) states that $\dot{f}(x, t) = \partial f(x, t)/\partial t$, while the second component rewrites (5.15) in terms of f and $\dot{f}$.

5.2.8. Hyperdifferential Form of the Evolution Operator

Following step by step the formal development (2.108)–(2.113) (with $M \to 1$, $k \to c^2$, $\mathbb{\Delta} \to \nabla^2$), we can expand the time development of the elongation and velocity functions as

$$\begin{aligned}
\boldsymbol{\zeta}(x, t) &= \exp\left[(t - t_0)\frac{\partial}{\partial t'}\right]\boldsymbol{\zeta}(x, t')|_{t'=t_0} \\
&= \exp[(t - t_0)\mathbb{H}]\boldsymbol{\zeta}(x, t_0) \\
&= \left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cosh[c(t - t_0)\nabla]\right. \\
&\quad \left. + \begin{pmatrix} 0 & 1 \\ c^2\nabla^2 & 0 \end{pmatrix}(c\nabla)^{-1}\sinh[c(t - t_0)\nabla]\right\}\boldsymbol{\zeta}(x, t_0) \\
&\coloneqq \mathbb{G}(t - t_0)\boldsymbol{\zeta}(x, t_0).
\end{aligned} \tag{5.35}$$

(Note that only positive powers of ∇ actually appear in this equation.) This defines *Green's* (i.e., the time-evolution) *operator* for the wave equation. Note that the operator entries of the 2×2 matrix $\mathbb{G}(t - t_0)$ involve only *even* powers of ∇, so that the symmetry properties of $f(x, t)$ and $\dot{f}(x, t)$ under inversions or translations in x are not affected [Eq. (4.121)]. Hence the boundary conditions (5.17) for the string of length L are unchanged, as we should expect, under time evolution.

For $f(x, t)$, the first component, Eq. (5.35) tells us that

$$f(x, t) = \{(c\nabla)^{-1} \sinh[c(t - t_0)\nabla]\}\dot{f}(x, t_0) + \cosh[c(t - t_0)\nabla]f(x, t_0), \tag{5.36}$$

while the second component is only the time derivative of this. Comparison of the hyperdifferential form (5.36) with the corresponding integral kernel form (5.25) of the time-evolution operator implies the (weak) equivalence

$$\cosh(\tau\nabla)f(x) = \tfrac{1}{2}[f(x + \tau) + f(x - \tau)]. \tag{5.37}$$

This is obvious by now due to (4.124) and $\cosh z = (e^z + e^{-z})/2$. The second equivalence implied is

$$\nabla^{-1} \sinh(\tau\nabla)f(x) = \tfrac{1}{2}\int_{x-\tau}^{x+\tau} dx' f(x'), \tag{5.38}$$

which is the antiderivative in τ of the first.

Exercise 5.16. Verify (5.38) in more detail (a) in comparison with (5.25)–(5.27a), (b) as the antiderivative in τ of (5.37), and (c) as the antiderivative in x of $\sinh \tau\nabla$ using $\sinh z = (e^z - e^{-z})/2$. Note that due to the absence of an $n = 0$ mode in the string, ∇^{-1} exists as an operator on the space of vibrating string solutions. Compare this to the Lanczos smoothing (4.62).

Exercise 5.17. Verify the *composition* of the time-translation operators

$$\mathbb{G}(t - t_1)\mathbb{G}(t_1 - t_0) = \mathbb{G}(t - t_0) \tag{5.39}$$

(a) formally as the exponential of $\mathbb{H}$, (b) as the 2×2 matrix with operator entries involving hyperbolic functions of ∇, (c) by the matrix representatives of $\mathbb{G}$ in the Fourier basis [Eqs. (5.26)], and (d) by the integral kernels (5.27). Recall Exercise 5.10.

5.2.9. Kinetic and Potential Energy in the Vibrating String

The last aspect we want to present of the vibrating string system is that of the energy present in the motion. This bears considerable resemblance to the energy in a vibrating finite lattice (Section 2.5) and some differences as well. In deriving the relation between $f(x, t)$ and the energy, we deal again with string elements Δx and then let $\Delta x \to 0$ and integrate over x. All quantities describing observables are assumed real.

The kinetic energy of the string element is one-half the mass $\mu\Delta x$ multiplied by the square of the velocity $\dot{f}(x, t)$. The whole string therefore has kinetic energy

$$\begin{aligned} E^k(t) &:= \tfrac{1}{2}\mu \int_0^L dx|\dot{f}(x, t)|^2 \\ &= \tfrac{1}{2}\mu(\dot{\mathbf{f}}(t), \dot{\mathbf{f}}(t))_L^0 \\ &= \tfrac{1}{2}\mu \sum_{n\in\mathscr{Z}^+} \omega_n^2|\omega_n^{-1}\cos(\omega_n t)\dot{f}_n^0 - \sin(\omega_n t)f_n^0|^2. \end{aligned} \tag{5.40}$$

In the second step we have used the inner product (4.134c) and in the third the corresponding Parseval identity, the sine Fourier coefficients being given by the time derivative of (5.25). For simplicity we have set $t_0 = 0, f_n^0 := f_n^0(0)$ and $\dot{f}_n^0 := \dot{f}_n^0(0)$.

The potential energy of the same string element is found by multiplying the net force acting on it, $-c^2\nabla^2 f(x, t)$, times the position $\alpha f(x, t)$ integrated from $\alpha = 0$ (equilibrium) to $\alpha = 1$ (actual position),

$$\begin{aligned} E^p(t) &:= -\mu c \int_0^L dx f(x, t)\nabla^2 f(x, t) \int_0^1 \alpha\, d\alpha \\ &= -\tfrac{1}{2}\mu c^2(\mathbf{f}(t), \nabla^2\mathbf{f}(t))_L^0 \\ &= \tfrac{1}{2}\mu c^2 \sum_{n\in\mathscr{Z}^+} (n\pi/L)^2|\omega_n^{-1}\sin(\omega_n t)\dot{f}_n^0 + \cos(\omega_n t)f_n^0|^2, \end{aligned} \tag{5.41}$$

where we have followed steps analogous to the derivation of (5.40).

5.2.10. Total and Partial Energy Conservation

The total energy in the string can be found after some algebra as

$$E := E^k(t) + E^p(t) = (\mu c^2\pi^2/2L^2) \sum_{n\in\mathscr{Z}^+} n^2(|f_n^0|^2 + \omega_n^{-2}|\dot{f}_n^0|^2) =: \sum_{n\in\mathscr{Z}^+} E_n. \tag{5.42}$$

The end result is only a function of the initial condition coefficients, and hence E is a constant of motion. Note in particular that the partial energies corresponding to the constituent normal modes [the sum of one term in (5.40) and the same-n term in (5.41)], denoted by E_n in (5.42), are *separately* conserved as well. Thus *there is no energy exchange between the normal modes.* (All these features have their exact counterpart in the finite lattice whose energy characteristics occupies Section 2.5.)

An interesting point to notice is the factor n^2 inside the sum in (5.42). If the total energy is to be finite, f_n^0 has to decrease faster than $n^{-3/2}$ with growing n (while $\dot{f}_n^0$ only faster than $n^{-1/2}$). This means that if $f(x, 0)$ has a discontinuity, the total energy of the string is unbounded. This is due to the

fact that the normal mode energies are proportional to n^2, turning a converging partial-wave sum into a diverging energy sum. Discontinuities in velocity are allowed, however, as they produce only trapezoid-like string shapes.

Exercise 5.18. Follow Section 2.5 in showing that the normal mode and total energies are constant without the explicit calculation undertaken in (5.40)–(5.42).

Exercise 5.19. Follow Section 2.6 in finding other constants of motion for the vibrating string.

Exercise 5.20. Pick up the idea mentioned in Exercise 2.61 of defining a sesquilinear inner product in the string elongation–velocity space (5.34):

$$E(\zeta_1, \zeta_2) := (\dot{\mathbf{f}}_1, \dot{\mathbf{f}}_2)_{\mathfrak{L}}^{\circ} - c^2(\mathbf{f}_1, \nabla^2 \mathbf{f}_2)_{\mathfrak{L}}^{\circ}. \tag{5.43}$$

As the spectrum of ∇^2 is strictly negative, the inner product (5.43) is positive. With respect to this product, the operator in (5.34b) is self-adjoint, and the time-evolution operator $\mathbb{G}$ in (5.35) is *unitary*.

Exercise 5.21. Consider the string to be immersed in a viscous fluid so that a velocity-dependent damping term is present. The governing equation is then

$$c^{-2} \frac{\partial^2}{\partial t^2} f(x, t) + \Gamma \frac{\partial}{\partial t} f(x, t) = \nabla^2 f(x, t). \tag{5.44}$$

In finding the solutions of this equation with the boundary conditions (5.17), note that the ∇^2-eigenfunction methods developed in this section apply with the difference that the angular frequencies (5.23b) will have a constant imaginary part, damping the oscillation, and a real part that is an "effective" oscillation frequency. The tools for this analysis have been given in Section 2.1. Lower frequencies become overdamped, while higher ones remain oscillatory. They are no longer multiples of a fundamental frequency, and hence the medium becomes dispersive, i.e., signals lose their shape during propagation as long waves lag behind short ones. This provides a rough model for the propagation of electromagnetic waves in an ionized medium.

Exercise 5.22. The boundary conditions (5.17) could be done away with as in analyzing a vibrating metal ring. The ∇^2 eigenfunctions are then $\exp(in\pi x/L)$, $n \in \mathscr{Z}$; the different approaches to the string can be applied to the ring with little conceptual difference.

Exercise 5.23. Assume the boundary conditions in space are that $\partial f(x, t)/\partial x$ be zero at $x = 0$ and L. Show that the spectrum and eigenvalues of ∇^2 are the set of nonnegative integers and that the eigenfunctions are cosines. The relevant expansion is thus the cosine Fourier series (4.136). Find the Green's function. Describe disturbances in terms of traveling waves: the mirror image disturbance is now equal in sign to the "real" one.

Exercise 5.24. Let the boundary conditions be "mixed": $f(0, t) = 0$ and $\partial f(x, t)/\partial x|_{x=L} = 0$. The problem is equivalent to that of an ordinary string with disturbances which are even with respect to reflections across $x = L/2$, the "real" string extending from zero to $L/2$. The freedom one has in choosing boundary conditions in the eigenvector procedure is that the constant term in the integration by parts (5.18) vanishes.

5.3. The Infinite Lattice

The study of finite N-point coupled lattices occupied Chapter 2 and was solved by the use of finite-dimensional vector space and transform methods. Since then, we have let $N \to \infty$ and found Fourier series. In this section we shall study the vibrations of a lattice composed of an infinity of discrete points: fundamental solutions, normal modes, and traveling waves. They are all $N \to \infty$ counterparts of the finite case. An "effective" propagation velocity for disturbances will be defined.

5.3.1. Equations of Motion

By infinite *lattice* we mean a system with a countable infinity of masses coupled by harmonic oscillator two-body interactions or their electric circuit analogues (Fig. 2.5). The equations governing such systems were found in Section 2.2. In the *simple* lattice, i.e., the case when all masses M and springs k are equal, when viscous and external forces are absent and only first-neighbor interactions are taken to exist, the governing system of equations for the disturbances $f_n(t)$ of the nth mass point is (2.26), i.e.,

$$M\ddot{f}_n = k(f_{n+1} - 2f_n + f_{n-1}) =: k(\Delta \mathbf{f})_n. \tag{5.45}$$

The only difference between (5.45) and (2.26) is that here the number N of masses is unbounded and n can take any integer value ($n \in \mathscr{Z}$). We expect that the coupled set of equations (5.45) will uncouple if we consider $\{f_n\}_{n\in\mathscr{Z}}$ to be the Fourier coefficients of a function $f(x)$ and perform Fourier synthesis on (5.45). The second-difference operator Δ becomes multiplication by $-4 \sin^2 x$ [see Eqs. (4.72)], turning Eq. (5.45) into

$$M\ddot{f}(x, t) = -4k \sin^2(x/2) f(x, t). \tag{5.46}$$

This is one ordinary differential equation in t for every value of $x \in (-\pi, \pi]$. Once $f(x, t)$ is found as determined by (5.46) with the usual initial conditions, the f_n's can be found by Fourier analysis (4.17b). The important point is that the "original function" and "partial-wave coefficients" are here, respectively, $\{f_n(t)\}_{n\in\mathscr{Z}}$ and $\{f(x, t)\}_{x\in(-\pi,\pi]}$. Their roles are reversed with respect to the ones they had in the last two sections.

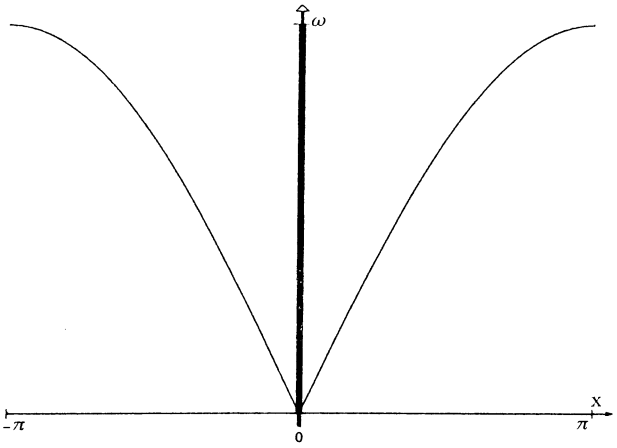


Fig. 5.8. Brillouin diagram for the oscillation angular frequencies of an infinite lattice: The allowed ω's extend from zero to $2(k/M)^{1/2}$ and are doubly degenerate for all $0 < \omega < 2(k/M)^{1/2}$.

5.3.2. Solution

If at time t_0 we state that the lattice has elongations and velocities $\{f_n(t_0), \dot{f}_n(t_0)\}_{n\in\mathscr{Z}}$, the solution to (5.46) will be determined, by the usual arguments, as

$$f(x, t) = f(x, t_0)\cos[\omega(x)(t - t_0)] + \dot{f}(x, t_0)\sin[\omega(x)(t - t_0)]/\omega(x), \quad (5.47a)$$

$$\omega(x) := 2(k/M)^{1/2}|\sin(x/2)| = \omega(2\pi - x), \quad (5.47b)$$

where $f(x, t_0)$ and $\dot{f}(x, t_0)$ are the Fourier syntheses of the initial conditions. These solutions are directly comparable with their finite-lattice counterparts (2.28), except for having a continuum of partial waves labeled by x. As x is periodic with period 2π, its range and "center" conform to Brillouin's convention. The angular frequencies $\omega(x)$ can be plotted in a Brillouin diagram (Fig. 5.8), which is the continuous counterpart of Fig. 2.10. The oscillation frequency $\omega(x)$, note, is *not* simply proportional to x, as it was for the vibrating string. This, we shall see, implies that the medium is *dispersive*: signals lose their shape as they propagate along the lattice.

5.3.3. Green's Function

The general solution to the lattice equations (5.45) can now be found as the Fourier analysis of (5.47), which is a sum of *products* of functions. As before, its structure will be that of a *convolution* between the initial conditions and the Green's function for the system and its time derivative, the latter ones

being the Fourier analyses of the factors $\sin[\omega(x)(t - t_0)]/\omega(x)$ and $\cos[\omega(x)(t - t_0)]$ in (5.47), viz.,

$$f_n(t) = \sum_{m \in \mathscr{Z}} \dot{G}_{nm}(t - t_0) f_m(t_0) + \sum_{m \in \mathscr{Z}} G_{nm}(t - t_0) \dot{f}_m(t_0), \tag{5.48a}$$

$$G_{n,m}(\tau) := (2\pi)^{-1} \int_{-\pi}^{\pi} dx [\omega(x)]^{-1} \sin[\omega(x)\tau] \exp[-i(n - m)x], \tag{5.48b}$$

$$\dot{G}_{n,m}(\tau) := (2\pi)^{-1} \int_{-\pi}^{\pi} dx \cos[\omega(x)\tau] \exp[-i(n - m)x]. \tag{5.48c}$$

We have defined $G_{n,m}(\tau)$ using matrix notation, as this leads to the vector equation

$$\mathbf{f}(t) = \dot{\mathbb{G}}(t - t_0)\mathbf{f}(t_0) + \mathbb{G}(t - t_0)\dot{\mathbf{f}}(t_0), \tag{5.49}$$

in complete analogy with the expressions (2.29) for finite lattices, (5.8) for heat diffusion, and (5.35) for the vibrating string. It has in common with these systems the properties of (a) reciprocity, (b) translational invariance, and (c) invariance under inversions, as follows from noting that $G_{n,m}(\tau)$ is exclusively a function of $|n - m|$, m and n being the sites of cause and effect along the lattice. Indeed, as $[\omega(x)]^{-1} \sin \omega(x)$ is an *even, real* function of x, it follows that its Fourier synthesis is an even, real function of the index. As we shall see, causality, valid for a continuous medium with a definite propagation velocity, does not strictly hold here.

5.3.4. "Effective" Propagation Velocity

We now turn to the explicit calculation of the Green's functions and its time derivative, Eqs. (5.48b) and (5.48c). The integral gives rise to a transcendental function, *Bessel's* function, which is studied in Appendix B. The result can be written as

$$\dot{G}_{n,m}(\tau) = J_{2(n-m)}(2(k/M)^{1/2}\tau), \tag{5.50}$$

while $G_{n,m}(\tau)$ itself can be written as the τ-integral of (5.50) and explicitly computed by its Taylor series. In Fig. 5.9 we have plotted (5.50) for $n = 0$, integer m, and τ in a positive range. A lattice which starts from rest ($\dot{\mathbf{f}} = \mathbf{0}$) with one mass out of line with unit elongation will progress in time as shown in the figure. The disturbance propagates symmetrically on both sides of the initial elongated mass point as $J_{2k}(z) = J_{-2k}(z)$ for $k \in \mathscr{Z}$. (Fig. 5.9 should be compared with Fig. B.1, where *real* values of the index are plotted.) At time $\tau = 0$ $J_k(0) = 0$ for all k except $J_0(0) = 1$, so at $t = t_0$ (5.49) is identically satisfied. Fig. 5.9 can be seen to resemble—in a neighborhood of $\tau = 0$—the corresponding Green's function derivative for a finite lattice in

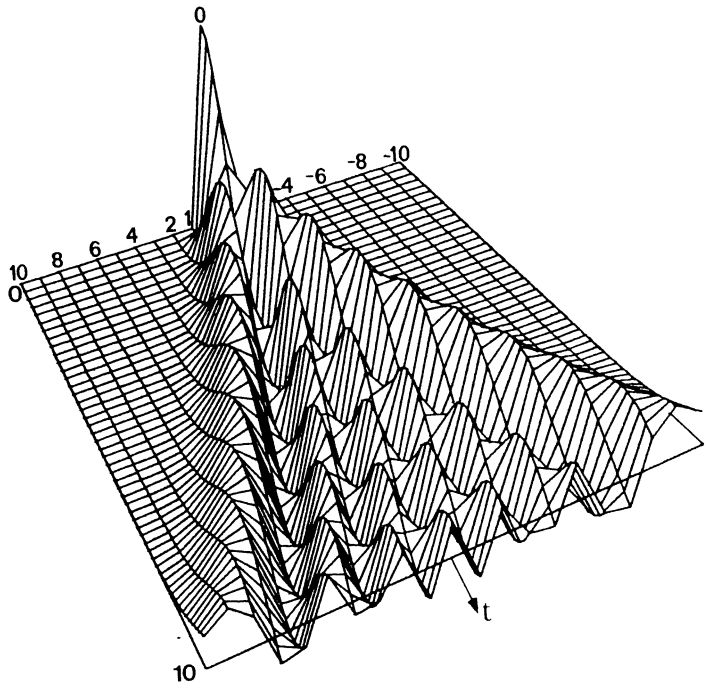


Fig. 5.9. The Green's function time derivative $\dot{G}_{n,m}(\tau)$. This represents the motion of the mass points in a lattice which starts from rest with the zeroth mass displaced. Time is given in units of $(M/4k)^{-1/2}$.

Fig. 2.8(a). The resemblance ends when the finite lattice points antipodal to the initial disturbance start to have a significant elongation, as then the motion propagates around the finite lattice but extends indefinitely along the infinite one.

It may seem paradoxical that there is actually an infinite propagation velocity for signals in the lattice. For small z, $J_{2k}(z) \simeq (z/2)^{2k}/(2k)! \neq 0$, as can be seen from the Taylor expansion in (B.7). Hence every mass point in the lattice feels the disturbance instantaneously. A "physical" lattice of masses joined by springs, of course, *does* exhibit a finite propagation velocity due to the necessarily massive springs. The nature of the Bessel function, however, allows for a working definition of a propagation velocity. As Fig. 5.9 suggests, at points far from the disturbance focus, the elongation increases slowly up to a point where it starts oscillating. This change of response happens at a time given approximately by the first zero of the Bessel function. In Chapter 6, Fig. 6.6, we have plotted the zeros of the Bessel function. For large orders it can be shown [e.g., Watson (1922, Section 15-81) and Abramowitz and Stegun (1964, Eq. 9.5.14 and the references therein)] that

the first root of $J_k(x)$ has the asymptotic value $k + 1.8557571k^{1/3} + 1.033150k^{-1/3} + \cdots$, $k \to \infty$. A given mass point at n units on either side of the disturbance (for n large) crosses this equilibrium point at a time $\tau = n(k/M)^{-1/2}$, as given by (5.50) and defines thus an "*effective*" propagation velocity of $(k/M)^{1/2}$ in units of interparticle separation per unit time. [A different justification of this estimate and the treatment of dispersion is given by Weinstock (1970), Merchant and Brill (1973), and Jones (1974).]

Exercise 5.25. Consider pth-neighbor interactions through spring constants k_p along the lines of the first part of Section 2.4. Show that the only change in the formulas in this section involves the angular frequency $\omega(x)$, which instead of (5.47b) becomes

$$\omega(x) = 2\left[k_0/4M + \sum_{p=1}^{\infty} (k_p/M) \sin^2(px/2)\right]^{1/2}, \tag{5.51}$$

in complete analogy to (2.64). The Green's function now becomes rather complicated to calculate.

Exercise 5.26. Out of (5.51) we can contrive a lattice where $\omega(x) = cx$. This will lead to a *nondispersive* lattice which can be used to propagate signals without shape loss. Replacing $2\sin^2(\alpha/2)$ by $1 - \cos\alpha$, the problem is to find the appropriate k_p's. Cosine Fourier analysis of c^2x^2 provides the answer.

5.3.5. Normal Modes

The *normal modes* for the infinite lattice can be defined, as before, as the time development of the eigenfunctions of the second-difference operator Δ in (5.45) or (5.46). These are the vectors of the Dirac δ-basis [recall Eq. (4.127)]. If we let the initial conditions be $\boldsymbol{\delta}_y$ first for the elongation and then for the velocity, the corresponding normal mode solutions will be given by (5.47) for $\delta(x - y)$ and Fourier analysis, namely,

$$\dot{\varphi}_n^{y+}(t) = (2\pi)^{-1/2} \cos ny \cos[\omega(y)(t - t_0)], \tag{5.52a}$$

$$\dot{\varphi}_n^{y-}(t) = (2\pi)^{-1/2} \sin ny \cos[\omega(y)(t - t_0)], \tag{5.52b}$$

$$\varphi_n^{y+}(t) = (2\pi)^{-1/2} \cos ny \sin[\omega(y)(t - t_0)]/\omega(y), \tag{5.52c}$$

$$\varphi_n^{y-}(t) = (2\pi)^{-1/2} \sin ny \sin[\omega(y)(t - t_0)]/\omega(y), \tag{5.52d}$$

where we have taken real and imaginary parts following the nomenclature of the finite lattice case (2.48). The only difference, clearly, is that the normal modes now form a continuous set labeled by $y \in (-\pi, \pi]$. Equations (5.52) represent standing waves of wavelength $\lambda_y = 2\pi/y$ in units of interparticle separation [compare with (2.53)] and oscillation angular frequency $\omega(y)$. The shortest wavelength which can be carried by the lattice happens at the edge of the first Brillouin zone, $y = \pi$, and is $\lambda_\pi = 2$ interparticle separa-

tions. In this mode, two neighboring particles oscillate in opposite directions. Beyond the first zone ($|y| > \pi$) we have no effectively shorter wavelengths for the same reason as for the finite lattice in Fig. 2.13.

Exercise 5.27. Find the normal mode solutions (5.52) proposing *separable* solutions for the equation of motion (5.45), i.e., solutions of the form $f_n(t) = \nu(n)\tau(t)$.

Exercise 5.28. The initial condition $(2\pi)^{-1/2}\exp(-imy)$ substituted into (5.48) should yield the normal mode solutions. Perform this derivation by the Bessel generating function Eq. (B4). As only *even*-order Bessel functions will appear in the sum, use $G_B(z, t) + G_B(-z, t)$. The real and imaginary parts of the result will match Eqs. (5.52).

5.3.6. Traveling Waves

The last family of vibration modes examined for finite lattices were *traveling waves* [Eqs. (2.54)]. Here, they appear as

$$\varphi_n^{y\rightleftarrows}(t) = (2\pi)^{-1/2}\sin[ny \mp \omega(y)(t - t_0)]/\omega(y), \tag{5.53a}$$

$$\dot{\varphi}_n^{y\rightleftarrows}(t) = \mp(2\pi)^{-1/2}\cos[ny \mp \omega(y)(t - t_0)], \tag{5.53b}$$

exhibiting a propagation velocity

$$v_y^{\rightleftarrows} = \pm\omega(y)/y = \pm 2(k/M)^{1/2}|\sin(y/2)|/y \tag{5.54}$$

in units of interparticle separation per unit time. (See Fig. 2.15.) Again, as for finite lattices, the main features are that longer wavelengths have higher propagation velocities (in spite of having lower oscillation frequencies; see Fig. 2.14 to dispel this apparent paradox). Shorter wavelengths propagate slower—hence signal *dispersion* occurs. The lower limit for velocities is $2(k/M)^{1/2}/\pi$ for $y = \pi$, while the upper one is $(k/M)^{1/2}$ for $y = 0$. Not surprisingly, $(k/M)^{1/2}$ was found to be the "effective" propagation velocity from the Green's function. The instantaneous response of the whole lattice to any localized disturbance stems mathematically from the expansion of a localized function in terms of "frozen" traveling waves for $t = t_0$. Each component extends over the whole lattice, and, as time is allowed to flow, the sum—initially zero everywhere except at the disturbed site—becomes non-vanishing as the different constituent waves move at their own pace.

The production of a continuous elastic medium out of a discrete, infinite lattice proceeds as in Section 3.4: we view the lattice from an increasing distance so that only the correspondingly longer partial waves are significant. All of them have, with increasing accuracy, the same propagation velocity, as we are in the "linear" region of the Brillouin diagram near $y = 0$. In the limit, we regain the characteristics of causality common to wave phenomena in one dimension.

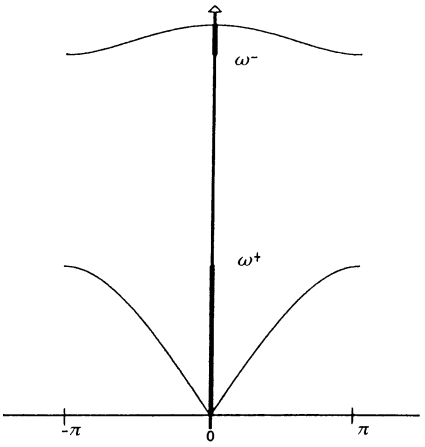


Fig. 5.10. Brillouin diagram for the oscillation angular frequencies of the molecular–diatomic infinite lattice with a spring/mass ratio of 1:2.

Exercise 5.29. Consider molecular and diatomic infinite lattices following Section 2.4 and the present description. Show that the oscillation frequency Brillouin diagram appears as in Fig. 5.10.

Exercise 5.30. Show in greater detail how Eq. (5.45), for decreasing interparticle separation, becomes the wave equation of Section 5.2. Would a molecular or diatomic lattice behave differently (exhibiting birefringence, for example)?

Exercise 5.31. Examine the *energy* in the vibration of a lattice along the lines of Section 2.5. There are no significant differences except normal modes and traveling waves have infinite energy.

6

Normal Mode Expansion and Bessel Series

The eigenfunctions of the Laplacian operator in function spaces with certain sets of boundary conditions constitute orthogonal sets of functions on the region enclosed by the boundaries. This is developed in Section 6.1 for rectangular boundaries and in Sections 6.2 and 6.3 for circular, sectorial, and annular boundaries in the plane. These are a few of the systems which appear in physics and engineering, where a great variety of operators and boundaries occur. The Laplacian applies mainly to wave and diffusion phenomena, which makes it specially relevant. As for boundary value problems, the above have been chosen for simplicity and because Fourier and *Bessel* series appear. Bessel series are a family of expansions in terms of orthonormal sets of functions which include those of Fourier as a particular case. In Section 6.4 we give a broad survey of the variants of eigenfunction expansions and some references.

6.1. Eigenfunctions of the Laplacian on Finite Regions: The Rectangular Membrane

Chapter 5 dealt with one-dimensional problems of diffusion and vibration where the key element was the expansion of the solution in series of eigenfunctions of the Laplacian with boundary conditions which restricted the "physical" space to a region of finite (*compact*) extent: 2π for the conducting ring and L for the fixed-end vibrating string. Here we shall see some general features of these expansions in more than one dimension. If the boundary conditions are given on certain coordinate lines or surfaces, the

solutions can be obtained exactly in terms of known functions. In this section we shall refer mostly to Cartesian coordinates, while in the rest of this chapter polar coordinates in the plane will be used.

6.1.1. Vector Spaces of Functions on $\mathscr{R}^N$

In working with the space of functions of N variables

$$\mathbf{x} = (x_1, x_2, \ldots, x_N) \in \mathscr{R}^N$$

we can endow it with a sesquilinear inner product which is the natural extension of the one-variable function space inner product (4.7), namely

$$(\mathbf{f}, \mathbf{g})_R := \int_R d^N\mathbf{x} f(\mathbf{x})^* g(\mathbf{x}), \tag{6.1}$$

where R is a region in N-dimensional space which for simplicity we consider to be a connected subset of Euclidean space with finite volume. The set of functions with finite norm [i.e., $\|\mathbf{f}\| := (\mathbf{f}, \mathbf{f})_R^{1/2} < \infty$ with (6.1) being a *Lebesgue* integral] which *vanish* on the boundary B of R can be shown to be in a Hilbert space. We denote it by $\mathscr{L}_0^2(R)$.

6.1.2. The N-Dimensional Laplacian

In $\mathscr{L}_0^2(R)$, the N-dimensional Laplace operator

$$\nabla^2 = \frac{\partial^2}{\partial {x_1}^2} + \frac{\partial^2}{\partial {x_2}^2} + \cdots + \frac{\partial^2}{\partial {x_N}^2} \tag{6.2}$$

is self-adjoint. The weaker condition of hermiticity is easy to prove—without reference to Cartesian coordinates—by integration by parts using the Gauss theorem for $\mathbf{f}, \mathbf{g} \in \mathscr{C}^{(2)}$,

$$\begin{aligned}
(\mathbf{f}, \nabla^2\mathbf{g})_R &= \int_R d^N\mathbf{x} f(\mathbf{x})^* \nabla \cdot \nabla g(\mathbf{x}) \\
&= \oint_B d^{N-1}\mathbf{s} \cdot f(\mathbf{x})^* \nabla g(\mathbf{x}) - \int_R d^N\mathbf{x} [\nabla f(\mathbf{x})]^* \cdot \nabla g(\mathbf{x}) \\
&= \oint_B d^{N-1}\mathbf{s} \cdot \{f(\mathbf{x})^* \nabla g(\mathbf{x}) - [\nabla f(\mathbf{x})]^* g(\mathbf{x})\} + \int_R d^N x [\nabla^2 f(\mathbf{x})]^* g(\mathbf{x}) \\
&= (\nabla^2\mathbf{f}, \mathbf{g})_R,
\end{aligned} \tag{6.3}$$

where as usual $d^{N-1}\mathbf{s}$ is the directed surface element of B. The vanishing of the boundary term is due to the restriction $f(\mathbf{x}), g(\mathbf{x}) = 0$ at $\mathbf{x} \in B$ which has been assumed in defining $\mathscr{L}_0^2(R)$.

6.1.3. The Laplacian Eigenbasis

The hermiticity property (6.3) is sufficient to guarantee that if we find the eigenvectors of ∇^2 in $\mathscr{L}_0^2(R)$,

$$\nabla^2\varphi_{\mathbf{n}}(\mathbf{x}) = \lambda_{\mathbf{n}}\varphi_{\mathbf{n}}(\mathbf{x}), \tag{6.4}$$

their eigenvalues $\lambda_{\mathbf{n}}$ will be *real*, and any two eigenvectors corresponding to different eigenvalues will be *orthogonal*. The proof of these facts follows (1.106). Pending its exact specification, the label $\mathbf{n}$ attached to the eigenvectors and eigenvalues in (6.4) will be assumed to belong to a denumerable set $\mathscr{N}$. Actually, one can in all cases establish a natural correspondence between $\mathscr{N}$ and $\mathscr{Z}^N$, N-dimensional vectors $\mathbf{n}$ of integer components. The set $\{\boldsymbol{\varphi}_{\mathbf{n}}\}_{\mathbf{n}\in\mathscr{N}}$ can then be chosen *orthonormal* by appropriate normalization. The fact that ∇^2 has the stronger property of being self-adjoint has the consequence of allowing the statement that $\{\boldsymbol{\varphi}_{\mathbf{n}}\}_{\mathbf{n}\in\mathscr{N}}$ is not only an orthogonal set but a *complete basis* for $\mathscr{L}_0^2(R)$, i.e., any function $f(\mathbf{x})$ in this space can be expanded as

$$f(\mathbf{x}) = \sum_{\mathbf{n}\in\mathscr{N}} f_{\mathbf{n}}\varphi_{\mathbf{n}}(\mathbf{x}), \tag{6.5a}$$

with *generalized Fourier coefficients*

$$f_{\mathbf{n}} \coloneqq (\boldsymbol{\varphi}_{\mathbf{n}}, \mathbf{f})_R = \int_R d^N\mathbf{x}\varphi_{\mathbf{n}}(\mathbf{x})^* f(\mathbf{x}), \tag{6.5b}$$

and the Parseval identity holds in the form

$$(\mathbf{f}, \mathbf{g})_R = \int_R d^N\mathbf{x} f(\mathbf{x})^* g(\mathbf{x}) = \sum_{\mathbf{n}\in\mathscr{N}} f_n^* g_n. \tag{6.5c}$$

Exercise 6.1. Note that the vanishing of the functions on the boundary B of the region R is not necessary to guarantee the *hermiticity* of the Laplacian in (6.3). It is only necessary that the surface integral over B vanish. This can be brought about if the *directional derivatives* of the functions involved along the normal to B are proportional to the functions themselves, i.e., $d^{N-1}\mathbf{s}\cdot\nabla f(\mathbf{x}) = \sigma f(\mathbf{x})\, d^{N-1}\mathbf{s}$, where σ can depend on the points of B where it is taken. We have treated the case $\sigma = \infty$. The case $\sigma = 0$ corresponds to functions whose normal derivative vanishes at B.

The reader can see that for the one-dimensional case the ordinary sine Fourier series (4.134) is described by (6.5) with $R = (0, L)$, $B = \{0, L\}$, $\varphi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$ and $n \in \mathscr{Z}^+$.

6.1.4. Boundary Conditions along Cartesian Coordinates

Our next example concerns N-dimensional space when the region R is a hyperprism $R_\square$ extending along Cartesian axes x_j from 0 to L_j, $j = 1, 2, \ldots, N$.

In Cartesian coordinates ∇^2 has the form (6.2). It is simplest to solve the eigenfunction equation (6.4) by proposing *separable* solutions of the form $\varphi(\mathbf{x}) = X_1(x_1)X_2(x_2)\cdots X_N(x_N)$, substituting them into (6.2)–(6.4), applying the Leibnitz rule, and dividing by $\varphi(\mathbf{x})$. We obtain

$$X_1^{-1}X_1'' + X_2^{-1}X_2'' + \cdots + X_N^{-1}X_N'' = \lambda, \tag{6.6}$$

where primes indicate differentiation with respect to the function's argument. Every summand $X_j^{-1}X_j''$ can depend only on x_j so its transfer to the right-hand side would leave an equality between a function of x_j and a sum of functions of all x's *but* x_j. Hence every summand $X_j^{-1}X_j''$ can only be a constant λ_j and $\lambda_{\mathbf{n}} = \sum_{j=1}^{N} \lambda_j$. The independent eigenfunction equations we are left with are $X_j''(x_j) = \lambda_j X_j(x_j)$ with the boundary conditions $X_j(0) = 0 = X_j(L_j)$, $j = 1, 2, \ldots, N$. Their solution has been given in Section 5.2, so we can write the $\varphi_{\mathbf{n}}(\mathbf{x})$ in (6.4) as

$$\varphi_{\mathbf{n}}(\mathbf{x}) = (2^N/L_1L_2\cdots L_N)^{1/2} \sin(n_1\pi x_1/L_1) \sin(n_2\pi x_2/L_2)\cdots \sin(n_N\pi x_N/L_N) \tag{6.7a}$$

and label the function by the N-tuple

$$\mathbf{n} := (n_1, n_2, \ldots, n_N), \qquad n_j \in \mathscr{Z}^+, j = 1, 2, \ldots, N. \tag{6.7b}$$

In the solution process we have found $\lambda_j = -(n_j\pi/L_j)^2$, so that the eigenvalue corresponding to (6.7) is

$$\lambda_{\mathbf{n}} = -\pi^2 \sum_{j=1}^{N} (n_j/L_j)^2. \tag{6.8}$$

The spectrum of ∇^2 in $\mathscr{L}_0^2(R_\square)$ with $R_\square$ as described here is then the set of all $\lambda_{\mathbf{n}}$ for $n_j \in \mathscr{Z}^+$. We note that all values in the spectrum in (6.4) are *negative*.

6.1.5. Mode Labeling Degeneracy

It should also be noted, however, that the numerical value of $\lambda_{\mathbf{n}}$ may not label the eigenfunction uniquely. Assume all L_j's are equal so $R_\square$ is a hypercube. Then clearly any permutation of n_j's will yield the same value of $\lambda_{\mathbf{n}}$. This situation is referred to as *degeneracy* and has been mentioned before in Section 1.7, where we pointed out that in order to *resolve* the degeneracy and provide a unique numerical labeling for the eigenfunctions, hermitian operators commuting with the first one had to be found. In the process of deriving (6.7) we have used $\partial^2/\partial x_j^2$, $j = 1, 2, \ldots, N$, as the N labeling operators. They are all self-adjoint and obviously commute with each other. Any $N - 1$

linear combinations of these and ∇^2—itself such a linear combination—thus provide a commuting set whose common eigenfunctions (6.7) are a complete and orthonormal basis for $\mathscr{L}_0^2(R_\square)$. It is the set of eigenvalues $\{\lambda_j\}_{j=1}^N$ which labels the eigenbases uniquely. This is equivalent to their specification by the N-tuple $\mathbf{n} = \{n_1, n_2, \ldots, n_N\}$, $n_j \in \mathscr{Z}^+$.

6.1.6. The Two-Dimensional Case

The use which can be made of the eigenfunctions and values of ∇^2 in $\mathscr{L}^2(R)$ has been shown in Sections 5.1 and 5.2 for the heat and wave equations. Let us now proceed along the same lines briefly to analyze the vibrations of a two-dimensional rectangular elastic membrane. The extension to a prismoidal three-dimensional cavity or higher-dimensional such systems will then be evident. Any function $f(x_1, x_2, t)$ on $R_\square$ can be expanded in the functions (6.7) with coefficients (6.5b) which are time dependent:

$$f(x_1, x_2, t) = (4/L_1L_2)^{1/2} \sum_{n_1 n_2 \in \mathscr{Z}^+} f_{n_1n_2}(t) \sin(n_1\pi x_1/L_1) \sin(n_2\pi x_2/L_2). \quad (6.9)$$

For the function (6.9) to be a solution of the two-dimensional wave equation, its Fourier coefficients must satisfy [as for (5.22)]

$$c^{-2} \frac{\partial^2}{\partial t^2} f_{n_1n_2}(t) = \lambda_{n_1n_2} f_{n_1n_2}(t), \quad (6.10)$$

i.e., they are oscillatory functions of time,

$$f_{n_1n_2}(t) = b_{n_1n_2} \sin[\omega_{n_1n_2}(t - t_0)] + c_{n_1n_2} \cos[\omega_{n_1n_2}(t - t_0)] \quad (6.11a)$$

with angular frequency

$$\omega_{n_1n_2} \coloneqq c(-\lambda_{n_1n_2})^{1/2} = \pi c[(n_1/L_1)^2 + (n_2/L_2)^2]^{1/2} \quad (6.11b)$$

and constants $b_{n_1n_2}$, $c_{n_1n_2}$ which can be fixed by the initial conditions at time t_0.

6.1.7. Nodal Lines, Frequency Lattice, and Accidental Degeneracy in the Two-Dimensional Case

Rather than analyze the Green's function (which will be discussed in Chapter 8), we shall point out some features of the normal modes

$$\dot{\varphi}_{n_1n_2}(x_1, x_2, t) \coloneqq (4/L_1L_2)^{1/2} \sin(n_1\pi x_1/L_1) \sin(n_2\pi x_2/L_2) \cos \omega_{n_1n_2}t \quad (6.12)$$

and their time antiderivatives $\varphi_{n_1n_2}(x_1, x_2, t)$: (a) They are waveforms which start from rest and maximum elongation and from equilibrium and maximum

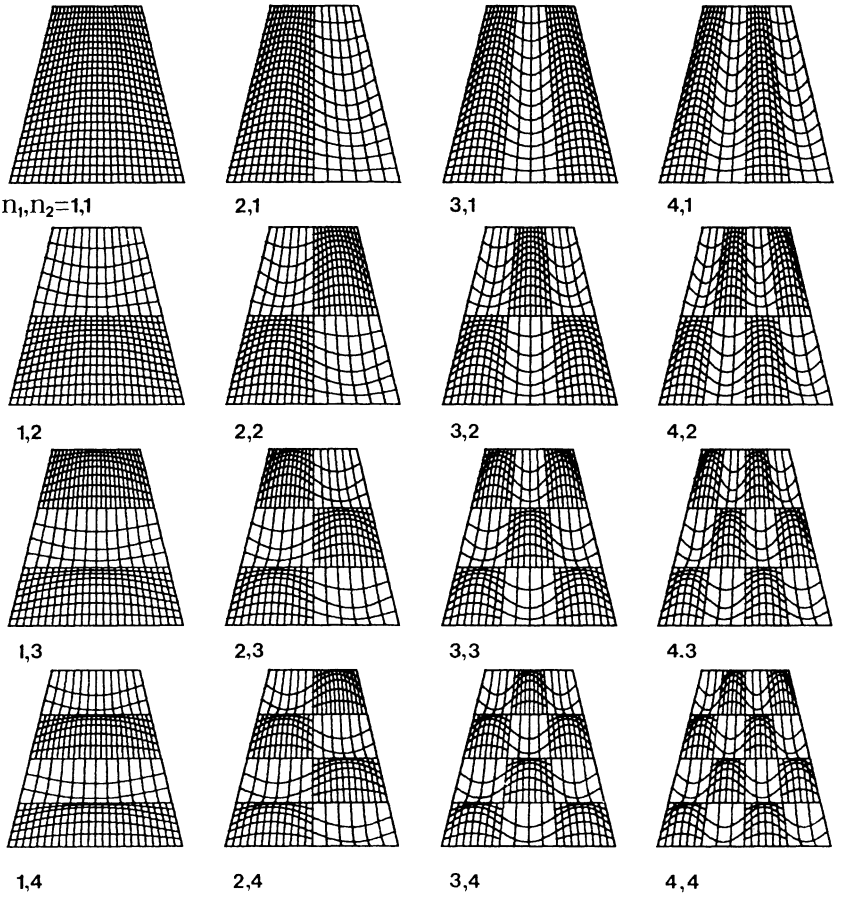


Fig. 6.1. Normal modes n_1, n_2 of the rectangular membrane and their nodal lines. The regions of the membrane with positive elongation have been shaded with a finer grid.

velocity, respectively. (b) The n_1, n_2 mode presents $n_1 - 1$ and $n_2 - 1$ *nodal lines* in the x_1 and x_2 coordinates excluding the boundaries. They are simple-zero lines within the membrane walls, across which the functions change sign (Fig. 6.1). The nodal lines are fixed in time. (c) The normal modes oscillate with angular frequencies $\omega_{n_1 n_2}$ as given by (6.11b) which are discrete and whose allowed values form a two-dimensional *lattice*. See Fig. 6.2. (d) The corresponding periods are $T_{n_1 n_2} = 2\pi/\omega_{n_1 n_2} = mT_{mn_1, mn_2}$. Thus in Fig. 6.2 the periods of modes lying on straight lines passing through the origin are multiples of a fundamental period $T_{p_1 p_2}$ with p_1 and p_2 relatively prime. (e) "Accidental" degeneracies can occur whenever L_1 and L_2 are commen-

surable. In Fig. 6.3 are some low-lying degeneracies for a 1:2 ratio of the rectangle sides. As the corresponding modes have the same angular velocity, so will any linear combination of them. These give rise to *degenerate subspaces* of modes, the elements of which have fixed nodes which are not straight lines. In Fig. 6.4 is a sequence of such linear combinations. Note that the *total number of nodal lines is conserved.* (f) The **x**-dependent factors of the normal modes (6.12) are orthonormal under the inner product

$$(\varphi_{n_1n_2}, \varphi_{n_1'n_2'})_\square := \int_{R_\square} d^2\mathbf{x}\varphi_{n_1n_2}(\mathbf{x})^*\varphi_{n_1'n_2}(\mathbf{x}) = \delta_{n_1n_1'}\delta_{n_2n_2'}. \tag{6.13}$$

Exercise 6.2. Consider a membrane in the form of a narrow annulus of radius ρ and width ω. A fair description of the vibration characteristics is to assume that the radial functions are those of a string of length ω with fixed ends and the angular functions are *periodic* with period $2\pi\rho$. What is the relevant inner product? Is ∇^2 hermitian in such a region? Show that the mode labels would be (n, m), $n \in \mathscr{Z}^+$ labeling the radial functions and $m \in \mathscr{Z}$ the angular ones.

Exercise 6.3. Analyze the modes and oscillation frequency degeneracy of a vibrating cubic cavity. Note that there is degeneracy between $\omega_{n_1n_2n_3}$ and the ω's with the same permuted indices. Relate this to the fact that the system—differential equation and boundary conditions—is *invariant* under symmetry transformations of the cube.

Exercise 6.4. Show that the degeneracies of the oscillation frequency fix uniquely the ratios of the sides of the vibrating membrane or cavity.

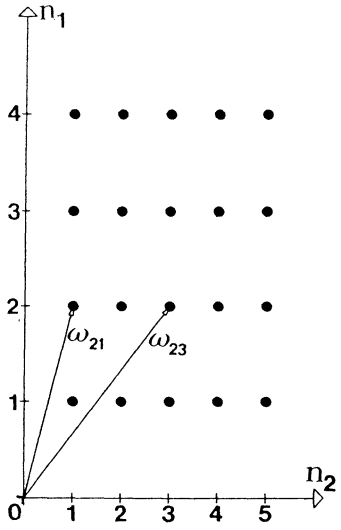


Fig. 6.2. "Reciprocal" lattice of allowed frequency values $\omega_{n_1n_2}$ for a rectangular membrane with a length ratio $L_1:L_2 :: 1:2$. The distance from the origin to each of the points gives the magnitude of $\omega_{n_1n_2}$.

The method of separation of variables in finding the eigenfunctions of the Laplacian operator in more than one variable will be applied in Section 6.2 to polar coordinates in the plane. At the end of this chapter we shall add some remarks on other coordinate systems in the plane where this is possible. In each case, when the region R is finite, the spectrum of ∇^2 is negative and the eigenfunctions are orthogonal, giving rise to a corresponding generalized Fourier series.

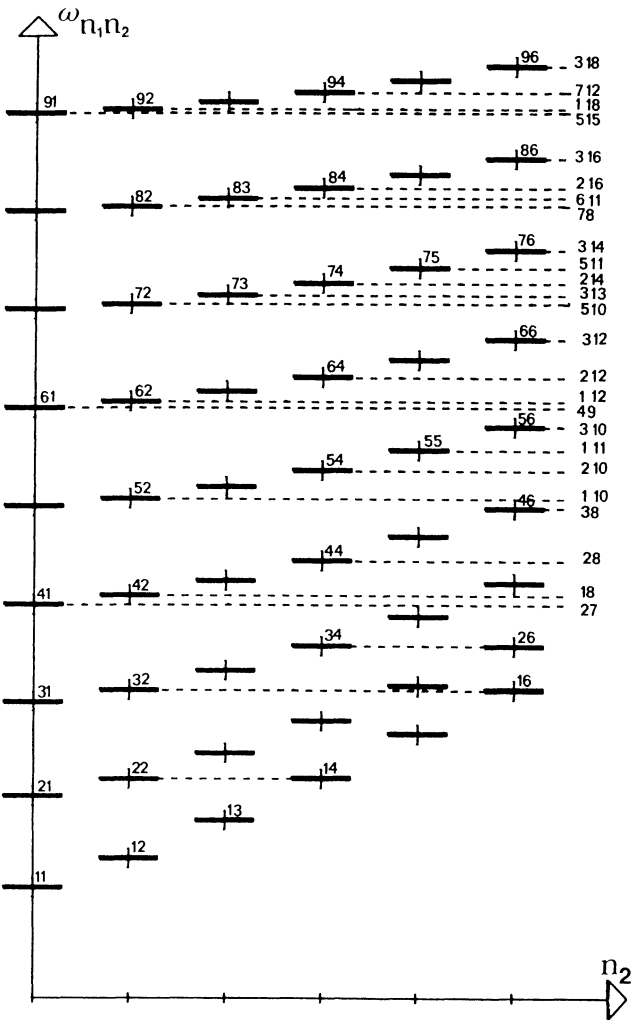


Fig. 6.3. Frequency degeneracies of a rectangular membrane with length ratio 1:2. Dashed lines join the degenerate pairs of $\omega_{n_1 n_2}$'s. If a partner lies beyond $n_2 = 6$, only the n_1, n_2 values are indicated.

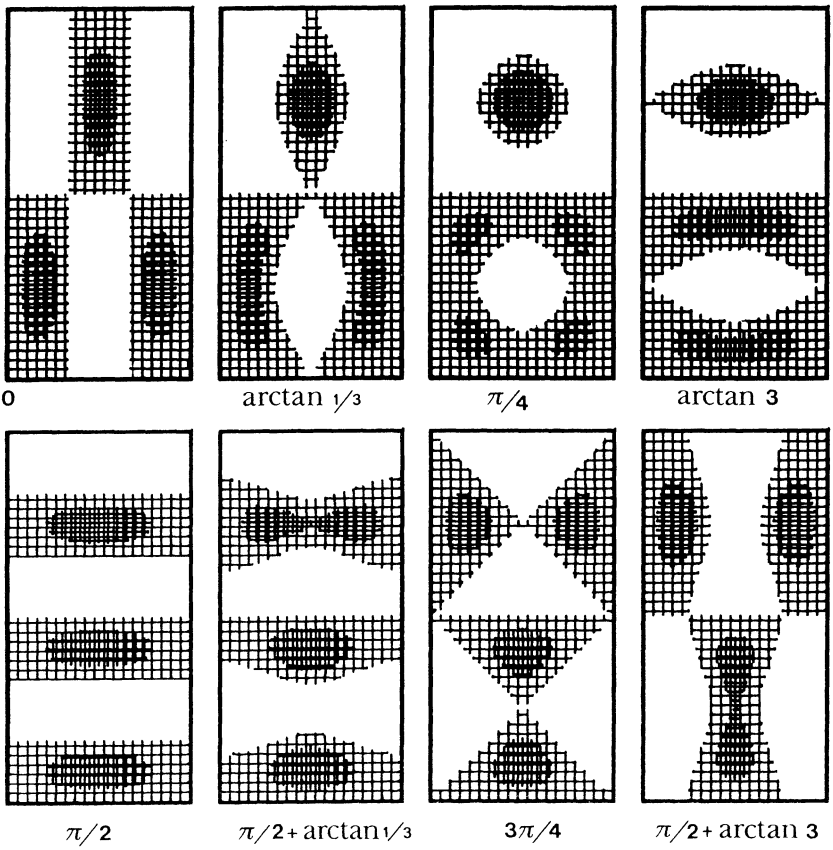


Fig. 6.4. Degenerate subspaces of normal modes. The modes $\varphi_{3,1}$ and $\varphi_{1,6}$ of a 1:2 rectangular membrane have the same angular frequency $(10)^{1/2}$. We plot here the linear combinations $\varphi_\theta = \cos\theta\varphi_{31} + \sin\theta\varphi_{16}$ for various selected values of θ indicated below each figure. Blank and lightly shaded regions indicate negative and positive values of φ_θ, the fixed nodal lines being the boundaries. Heavily shaded areas indicate values of φ_θ larger than 0.6.

6.2. Laplacian on the Unit Disk: The Circular Membrane

The eigenfunctions of the Laplacian operator will be found now when the domain is the space of square-integrable functions on the unit disk, which vanish on its boundary circle. In polar coordinates, we shall see that these consist of circular functions for the angular variable times *Bessel* functions for the radial part. The former have been treated extensively in Chapter 4 as the basis functions for the Fourier series expansion, while the

latter (a summary of whose properties can be found in Appendix B) are a basis for one of the Bessel series expansions. The product of the two functions provides the spatial part of normal modes for the description of a vibrating circular membrane.

6.2.1. Polar Coordinates

When the region R in (6.1) is the unit disk $R_\bigcirc$, it is convenient to parametrize the plane in *polar* coordinates,

$$x_1 = r\cos\phi, \qquad x_2 = r\sin\phi, \qquad r \in [0, \infty), \phi \in (-\pi, \pi], \tag{6.14a}$$

$$d^2\mathbf{x} = dx_1\, dx_2 = r\, dr\, d\phi, \tag{6.14b}$$

so that the inner product between two functions on this region can be written as

$$(\mathbf{f}, \mathbf{g})_\bigcirc = \int_0^1 r\, dr \int_{-\pi}^{\pi} d\phi f(r, \phi)^* g(r, \phi). \tag{6.15}$$

The space of functions with finite norm [induced by (6.15)] which vanish for $r = 1$ will be denoted again as $\mathscr{L}_0^2(R_\bigcirc)$. It is a Hilbert space. The functions in this space are of course periodic in ϕ with period 2π.

The expression for the Laplacian operator in polar coordinates is well known to be

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}. \tag{6.16}$$

Exercise 6.5. Verify directly that (6.16) is hermitian. This is just (6.3) in coordinate form using (6.15) and $\mathbf{f}, \mathbf{g} \in \mathscr{C}^{(2)}$.

6.2.2. Separation of Variables

To solve the eigenfunction equation for (6.16) on $\mathscr{L}_0^2(R_\bigcirc)$,

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right) f_{\mathbf{n}}(r, \phi) = -\lambda_{\mathbf{n}} f_{\mathbf{n}}(r, \phi), \tag{6.17}$$

we propose separable solutions $f(r, \phi) = R(r)\Phi(\phi)$. We have put a minus sign in front of the $\lambda_{\mathbf{n}}$ on the basis of the observation in (6.8) that the spectrum of ∇^2 there was negative. By substituting the proposed solution form in (6.17), applying the Leibnitz rule, and dividing by $r^{-2}f(r, \phi)$, the equation is transformed into

$$r^2\frac{R''(r)}{R(r)} + r\frac{R'(r)}{R(r)} - \lambda r^2 = c = -\frac{\Phi''(\phi)}{\Phi(\phi)}. \tag{6.18}$$

As before, the purpose of the separation of variables method is to be able to write Eq. (6.17) in a form (6.18) in which one side depends only on one variable and the other side only on the other, independent, variable. Both sides can only be equal to the same constant c, and we are left with two ordinary differential equations coupled by the separation constant. As the functions in $\mathscr{L}_0^2(R_\bigcirc)$ are to be periodic in ϕ, the right-hand side yields the well-known circular functions

$$\Phi_m{}^\bigcirc(\varphi) = (2\pi)^{-1/2} \exp(im\phi), \qquad m \in \mathscr{Z}, \tag{6.19}$$

fixing the separation constant as $c = m^2$ and providing one label for the Laplacian eigenfunctions. The left-hand side of (6.18) then becomes

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{m^2}{r^2}\right) R_m(r) = -\lambda R_m(r). \tag{6.20}$$

6.2.3. General Solution of the Radial Part

Upon the simple change of scale $\lambda^{1/2} r \to r$, Eq. (6.20) is *Bessel's* differential equation. (See Appendix B.) The general solution of (6.20) is then

$$R_m(r) = a_m J_m(\lambda^{1/2} r) + b_m N_m(\lambda^{1/2} r), \tag{6.21}$$

where a_m and b_m are as yet arbitrary constants, m is an integer, and J_m and N_m are the *Bessel* and *Neumann* functions of order m. [These are also called Bessel functions of the *first* and *second* kind; see the National Bureau of Standards tables edited by Abramowitz and Stegun (1964). There, the symbol Y_m is employed for the latter, for which the name *Weber* function is also occasionally used, as in Watson's classic treatise (1922). In mathematical physics, however, Neumann's name seems to be more popular. See Morse and Feshbach (1953)].

6.2.4. Boundary Conditions and Frequency Quantization

We now require the space and boundary conditions to hold for Eq. (6.21). A first observation (Figs. B.1 and B.2) is that the Neumann function becomes infinity at $r = 0$ and is in fact not square-integrable, so it cannot belong to $\mathscr{L}_0^2(R_\bigcirc)$ and therefore, *unless* $b_m = 0$, neither will $R_m(r)$. A second remark is that (6.20) is the same equation for $+m$ and $-m$. No essential features in (6.21) distinguish between the two since, for integer m, $J_{-m} = (-1)^m J_m$. The third argument, we note, is that the boundary condition of the function's vanishing at the membrane edge, $R_m(1) = 0$, fixes the allowed values of λ and thereby the spectrum of the Laplacian. Indeed, this condition implies $J_m(\lambda^{1/2}) = 0$. Now, this is clearly valid only if $\lambda^{1/2}$ is a *zero* of the Bessel

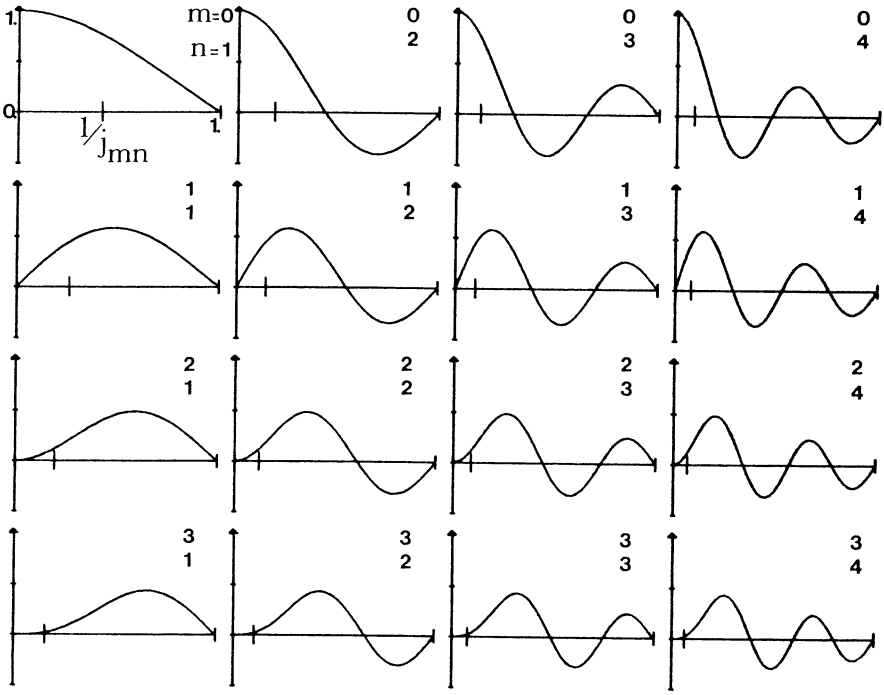


Fig. 6.5. Radial functions in the circular membrane normal modes φ°_{mn}. The left edge is the membrane center, while the right edge is the fixed boundary. All $m \neq 0$ modes are zero at the former, and all vanish at the latter, coinciding with the nth zero of the Bessel function.

function. The Bessel function of any order m has a denumerable infinity of simple zeros. [A small table of the first few is given in Appendix B. A more complete list can be found in Abramowitz and Stegun (1964, Table 9.5).] The effect of this condition is then to fix

$$\lambda_{mn} = (j_{m,n})^2, \qquad m \in \mathscr{Z}, n \in \mathscr{Z}^+, \tag{6.22}$$

where j_{mn} is the nth *zero of the Bessel function of order m* (*not* including $r = 0$). The effect of λ_{mn} when placed in the Bessel function in (6.21) is to change the scale in the argument of $R_m(r)$ so that for $n = 1, 2, \ldots$ the nth zero of the Bessel function coincides with the region's edge at $r = 1$. This is shown in Fig. 6.5. Finally the restriction (6.22) also provides a second label, n, to mark uniquely the eigenvalues and functions. The latter are thus recombined from (6.19) and (6.21) as

$$\varphi^{\bigcirc}_{mn}(r, \phi) \coloneqq c^{\bigcirc}_{mn} J_m(j_{mn} r) \exp(im\phi), \qquad m \in \mathscr{Z}, n \in \mathscr{Z}^+. \tag{6.23a}$$

The constant $c_{mn}^{\bigcirc}$ in (6.23a) is introduced in order to *normalize* the functions with respect to the inner product (6.14). It can be shown to be

$$c_{mn}^{\bigcirc} = (2\pi)^{-1/2} g_{mn}, \qquad g_{mn} := 2^{1/2} \left[\left| \frac{dJ_m(s)}{ds} \right|_{s=j_{mn}} \right]^{-1} \tag{6.23b}$$

[see Tolstov (1962, Section 8-13)].

6.2.5. Normal Modes on the Disk

Having found the expressions (6.22) and (6.23), we have completed our task of finding and classifying the Laplacian eigenvalues and functions in $\mathscr{L}_0^2(R_{\bigcirc})$. They are a complete and orthonormal set of basis functions in this space. Equations (6.5), the generalized Fourier series for $\mathscr{L}_0^2(R_{\bigcirc})$ functions on the unit disk, can thus be written using this set. We can now use this in order to expand the time-dependent function,

$$f(r, \phi, t) = \sum_{m \in \mathscr{Z}, n \in \mathscr{Z}^+} f_{mn}(t) \varphi_{mn}^{\bigcirc}(r, \phi), \tag{6.24a}$$

$$f_{mn}(t) = \int_0^1 r\, dr \int_{-\pi}^{\pi} d\phi f(r, \phi, t) \varphi_{mn}^{\bigcirc}(r, \phi)^* = (\boldsymbol{\varphi}_{mn}^{\bigcirc}, \mathbf{f})_{\bigcirc}, \tag{6.24b}$$

which will be required to be a solution of the wave equation describing the vibrations of a circular membrane of unit radius fixed along its perimeter. As in (6.9)–(6.10), for $f(r, \phi, t)$ to be a solution of the wave equation, the Fourier coefficients must satisfy

$$c^{-2} \frac{\partial^2}{\partial t^2} f_{mn}(t) = -\lambda_{mn} f_{mn}(t), \tag{6.25}$$

which are two independent sinusoidal, oscillatory functions of time with angular frequency

$$\omega_{mn}^{\bigcirc} = c\lambda_{mn}^{1/2} = c j_{mn}, \tag{6.26}$$

exactly as in (6.11a).

The *normal modes* of the circular membrane will thus be the solutions for which the Fourier coefficients (6.24b) are different from zero one at a time,

$$\dot{\varphi}_{mn}^{\bigcirc}(r, \phi, t) = c_{mn}^{\bigcirc} J_m(j_{mn} r) \exp(im\phi) \cos \omega_{mn}^{\bigcirc} t \tag{6.27}$$

and their time antiderivatives which involve sine functions of $\omega_{mn}^{\bigcirc} t$.

6.2.6. Properties of the Disk Normal Modes

The properties we noted for the rectangular membrane normal nodes have their counterparts here: (a) The modes (6.27) start from rest at $t = 0$,

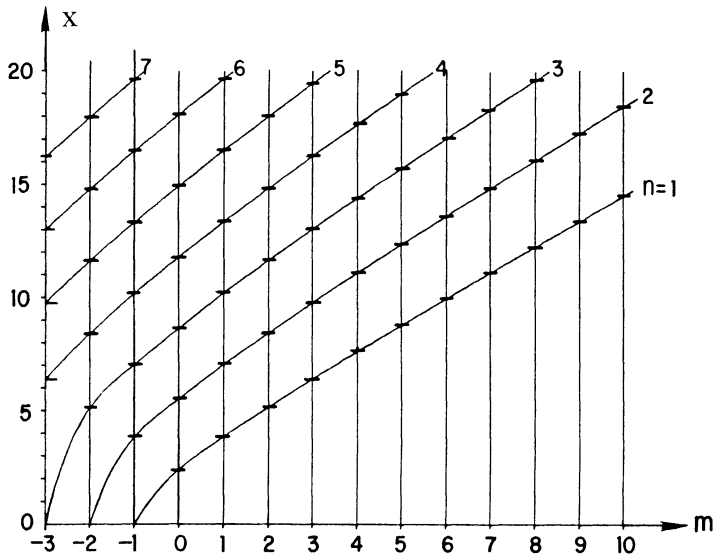


Fig. 6.6. The allowed angular frequencies of the circular membrane normal modes lie on the zeros of the Bessel function $J_m(x)$. The latter are indicated by the sloping lines corresponding to the first, second, etc., zero. For m integer (vertical lines), the position of the zero (heavier bars) gives the value of ω_{mn}.

while their antiderivatives start with maximum velocity. (b) If we consider the real or the imaginary part of (6.27), the m, n mode presents m nodal diameter lines and n nodal circles, including the boundary. They are simple-zero lines, fixed in time. (c) The angular frequencies (6.26) can be arranged in an m-n diagram as in Fig. 6.6, which is the counterpart of Fig. 6.3. They appear as points—for integer m—on the zero lines in the (m, x)-plane of the Bessel function $J_m(x)$. We can see that, quite naturally, the ω_{mn} fall into *trajectories* characterized by n. (d) The oscillation periods $T_{mn} = 2\pi/\omega_{mn}$ are all mutually incommensurable, except for $T_{mn} = T_{-mn}$. The lack of harmonic frequencies accounts for the "nonmusical" sound of a drum as compared with a guitar string, where all frequencies are multiples of a basic one. (e) The *twofold* degeneracy of all $m \neq 0$ modes is a consequence of the invariance of the system—differential equation and boundary conditions—under the group $O(2)$ of rotations and reflections across any line which passes through the origin. Clearly, as one reflection (across a line by 0°) replaces ϕ by $-\phi$, the $\varphi^{\bigcirc}_{mn}(r, \phi)$ modes are transformed into the $\varphi^{\bigcirc}_{-mn}(r, \phi)$ ones. Linear combination in these equal-frequency subspaces only rotates the position of the angular nodes.

In Fig. 6.7 we show some of the lower-lying vibrational modes of the circular membrane.

Exercise 6.6. Assume the initial conditions are invariant under rotations [i.e., $f(r, \phi, t_0) = f(r, \phi + \alpha, t_0)$ and similarly for the time derivatives, for arbitrary α]. Show that the only normal modes present in such a vibration are the $m = 0$ modes and that this invariance will hold for all time.

Exercise 6.7. Assume the initial conditions of the membrane are eigenfunctions of an element of the group $O(2)$ of rotations and reflections. Find the normal modes present in this state. Show that this symmetry will be preserved forever.

Exercise 6.8. Find the Parseval identity for (6.23).

Exercise 6.9. Consider the region R to be a *circular cylinder cavity* of unit radius and length L. The Laplacian eigenfunctions will then be

$$(2/L)^{1/2}\varphi^{\circ}_{mn}(r, \phi) \sin(k\pi z/L)$$

for $m \in \mathscr{Z}$ and $n, k \in \mathscr{Z}^+$. The system is the "direct product" of a circular membrane times a string. The normal mode oscillation angular frequencies will be the "Pythagorean sum" of those of the constituent systems, that is, $\omega_{mnk} = (\omega_{mn}^2 + \omega_k^2)^{1/2}$ in terms of (6.26) and (5.23b). Note that one needs one label for each dimension of the space.

6.2.7. Bessel Series of Integral Order

The orthogonality and completeness of the normal mode expansion (6.24) on the disk, for any fixed time, has one rather immediate consequence for functions $f(r, \phi)$ which are of the form $f(r, \phi) = f(r)\Phi^{\circ}_{m_0}(\phi)$ for a fixed m_0 [Eq. (6.19)]. Equation (6.24b), when integration over φ is performed, will yield a factor $2\pi\delta_{m,m_0}$. The generalized Fourier synthesis in (6.24a) will contain only an $m = m_0$ term so the $\Phi^{\circ}_{m_0}$'s can be canceled on both sides, turning the pair of equations (6.24) into

$$f(r) = \sum_{n \in \mathscr{Z}^+} f^J_{nm} g_{mn} J_m(j_{mn} r), \tag{6.28a}$$

$$f^J_{nm} = g_{mn} \int_0^1 r\, dr f(r) J_m(j_{mn} r). \tag{6.28b}$$

Equations (6.28) are the *order-m Bessel series* and *Bessel partial waves*: the expansion of an arbitrary $\mathscr{L}_0^2(0, 1)$ function $f(r)$ into a series of Bessel functions of order m and its corresponding order-m Bessel coefficient $f^J_{nm} = (2\pi)^{-1/2} f_{mn}$.

The Bessel series (6.28) is one example, in addition to the Fourier sine series, of expansion of an arbitrary function in $\mathscr{L}_0^2(a, b)$ in terms of a complete and orthogonal set of functions with respect to a given inner product. Note that the relevant inner product here is

$$(\mathbf{f}, \mathbf{g})_J := \int_0^1 r\, dr f(r)^* g(r) = \sum_{n \in \mathscr{Z}^+} f^J_{nm}{}^* g^J_{nm}, \tag{6.28c}$$

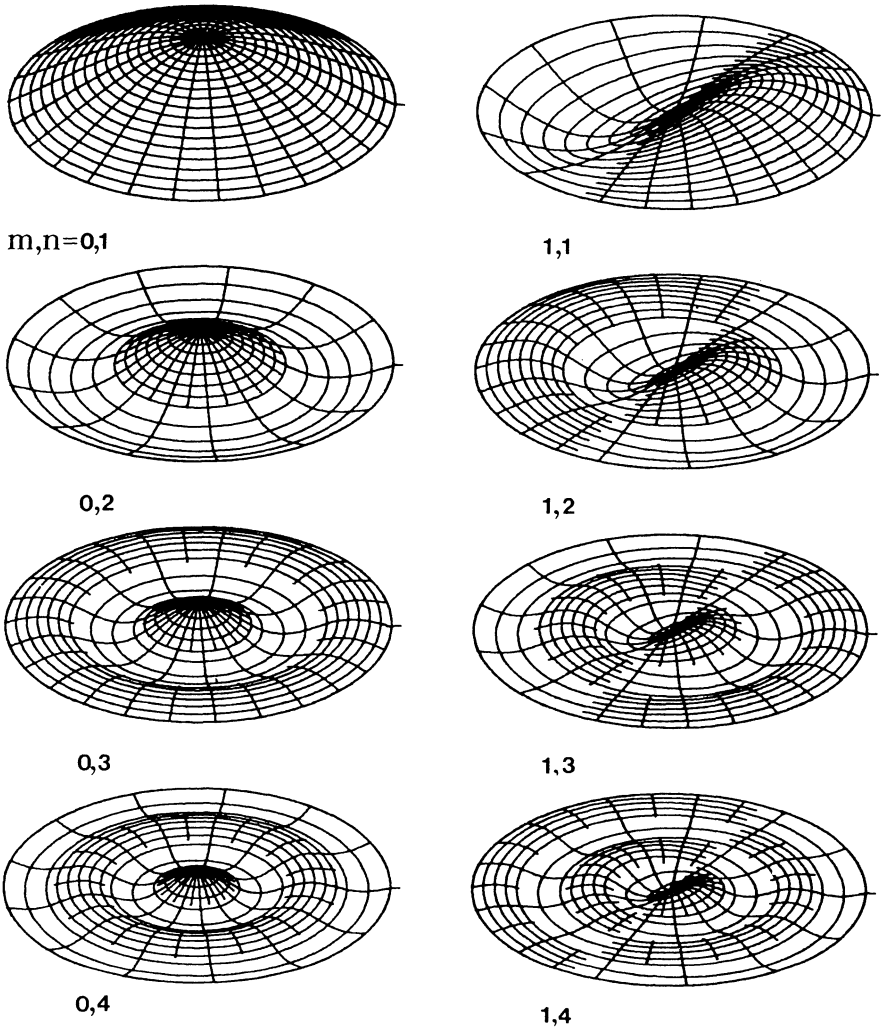
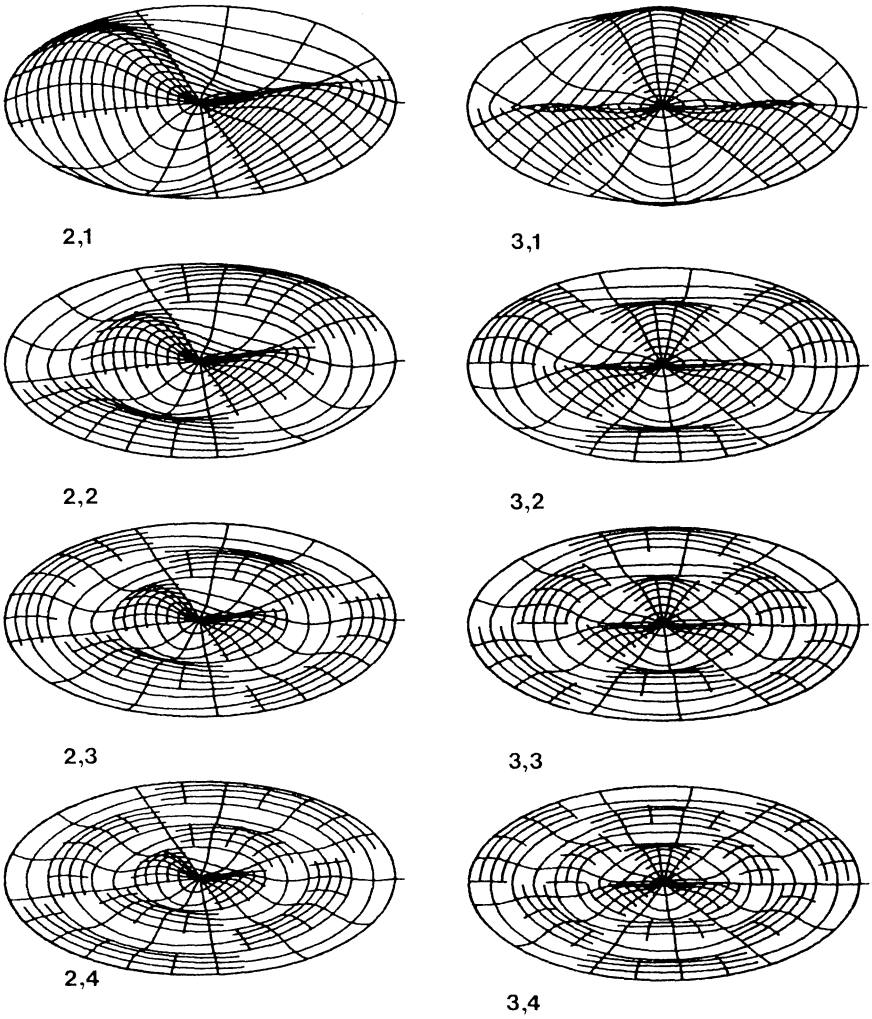


Fig. 6.7. The normal modes $\dot{\varphi}^{\circ}_{mn}$ of the circular membrane. For positive values of the function [Eq. (6.27), $t = 0$] the grid is finer. The fixed radial and angular nodes

this being the form of the Parseval identity. A trivial change of function $f(r) \to r^{-1/2}f(r)$ transforms (6.28) into an expansion of the new $f(r)$ in terms of $r^{1/2}J_m(j_{mn}r)$ having the advantage that the integral in (6.28b) and (6.28c) contains dr rather than $r\,dr$ as its differential.

Exercise 6.10. Verify the orthogonality of the Bessel functions $J_m(j_{mn}r)$ with respect to the index n under the integral (6.28). This can be done by verifying



of the membrane are the boundaries between the single- and double-gridded regions.

first that the differential operator on the left-hand side of (6.17), with $\partial^2/\partial\phi^2$ replaced by $-m^2$, is hermitian with respect to the inner product. Then apply the argument (1.106).

Exercise 6.11. Consider the $f(r)$ to be expanded in a Bessel series to be the Dirac δ, $a^{-1}\delta(r-a)$, $a \in (0, 1)$. This acts as the *reproducing kernel* in the inner product (6.28c). Find its Bessel series coefficients from (6.28b); (6.28a) then gives another divergent series representation for the Dirac δ and its derivatives.

6.2.8. Other Boundary Conditions

The series (6.28) is called, to be precise, the *Fourier–Bessel* series. The roots j_{mn} of the order-m Bessel functions appear in it due to the boundary condition that the solution to (6.20) at the membrane edge $r = 1$ be zero. This condition can be replaced by any other condition which ensures that the boundary terms in (6.3), namely $[f(r)g'(r) - f'(r)g(r)]|_{r=1}$, vanish. This is achieved if $f(1) = 0$, as we demanded from (6.21), or by the more general condition that the ratio of $f(r)$ to $f'(r)$ at the boundary be constant. In particular, if one asks for $rf'(r) + kf(r) = 0$ at $r = 1$ to be satisfied by all solutions, one finds a normal mode basis of the type (6.23a), where the roots $\{j_{mn}\}_{n=1}^{\infty}$ are replaced by the roots $\{\lambda_{mn}\}_{n=1}^{\infty}$ of $rJ_m'(r) + kJ_m(r)$, and the series analogous to (6.28) will contain these roots. The resulting series has been called the *Dini* series and includes the Fourier–Bessel series as a particular case. Watson (1922, Section 18.3) discusses this series in some detail. For further examples and physical problems, the reader can refer to Churchill (1941), Relton (1946), Courant and Hilbert (1953, Section V-5), Morse and Feshbach (1953, Section 11.2), and Tolstov (1962, Chapter 9).

Tables of Bessel functions and their derivatives, products, and *roots* are necessary for any actual calculation. These tables have proliferated with the advent of electronic computation. See, for instance, the Bessel function tables of the British Association for the Advancement of Science (1950, 1952), the Royal Society Mathematical Tables (1960) (this includes zeros and associated values in Part III), and the National Physical Laboratory Mathematical Tables (1962). Tables of Bessel functions of large orders have been edited by the USSR Academy of Sciences (Fadeeva and Gavurin, 1950) and by the Harvard Computation Laboratory (1947–1951).

6.2.9. The Limit of Infinite Radius: Hankel Transforms

The expansion of functions $f(r)$ in terms of Bessel series need not be constrained to the interval $r \in (0, 1)$. A change of variables will allow for any interval $(0, R)$, as was done for simple Fourier series in Section 4.7. Let $q := rR$, and introduce the discrete variable $p_n := j_{mn}/R$ for fixed m, so that p_n takes on a discrete set of values proportional to the roots of the Bessel function, which can be numbered by the natural numbers n. If we further introduce $f_1(q) := (q/R)^{1/2} f(q/R)$, $f_1{}^H(p_n) := \pi^{-1/2} R f_n$, and $h_{mn} := (\pi j_{mn})^{-1/2} g_{mn}$, Eqs. (6.28) become

$$f_1(q) = \sum_{n \in \mathscr{Z}^+} h_{mn}(\pi/R) f_1{}^H(p_n)(p_n q)^{1/2} J_m(p_n q), \tag{6.29a}$$

$$f_1{}^H(p_n) = h_{mn} \int_0^R dq f_1(q)(p_n q)^{1/2} J_m(p_n q), \tag{6.29b}$$

$$\int_0^R dq f_1(q)^* g_1(q) = \sum_{n \in \mathscr{Z}^+} (\pi/R) f_1{}^H(p_n)^* g_1{}^H(p_n). \tag{6.29c}$$

The limit $R \to \infty$ of Eqs. (6.29) can be found. We have to watch the discrete variable $p_n := j_{mn}/R$. As $R \to \infty$, higher and higher roots of the Bessel function will correspond to finite values of p_n. For large values of the argument, the Bessel function $J_m(z)$ behaves (see Appendix B) like $(2/\pi z)^{1/2} \cos[z - \pi(m + \frac{1}{2})/2]$, i.e., the roots approach asymptotically the equally spaced sequence $\pi(n + m/2 + \frac{3}{4})$. The values of p_n hence also approach equal spacing $\Delta p := \pi/R$, which vanishes as $R \to \infty$. Finally, the values of h_{mn} approach unity. This is seen from (6.23b) and the asymptotic behavior of the Bessel function derivative evaluated at the roots. The factor $(2/\pi z)^{1/2}$ yields $g_{mn} \sim (\pi j_{mn})^{1/2}$ as $n \to \infty$ and thus $h_{mn} \to 1$. Introducing these considerations into (6.29), we observe that sums $\sum_p \Delta p \cdots$ of functions of p appear. As $R \to \infty$ these will become Riemann integrals $\int_0^\infty dp \cdots$, giving, finally,

$$f(q) = \int_0^\infty dp f^H(p)(pq)^{1/2} J_m(pq), \tag{6.30a}$$

$$f^H(p) = \int_0^\infty dq f(q)(pq)^{1/2} J_m(pq), \tag{6.30b}$$

$$\int_0^\infty dq f(q)^* g(q) = \int_0^\infty dp f^H(p)^* g^H(p), \tag{6.30c}$$

where we have dropped the subscripts. Equation (6.30b) defines the *Hankel integral transform* of $f(q)$ and (6.30a) its inverse, while (6.30c) is the corresponding Parseval identity. Although the derivation (6.28)–(6.30) has not been rigorous for basically the same reasons as in Section 4.7, the results (6.30) and their range of validity will be established independently in Section 8.4.

Exercise 6.12. Consider a similar limit for the Dini series.

The Bessel–Fourier series in the form (6.28) is but one of a family of similar series in Bessel and Neumann functions. These will be discussed in Section 6.3.

6.3. Sectorial and Annular Membranes

We continue our consideration of the Laplacian operator when the functions in its domain vanish on boundaries which follow polar coordinates in the plane. These are used for the description of sectorial and annular membranes. The results are nontrivial extensions of the results on the

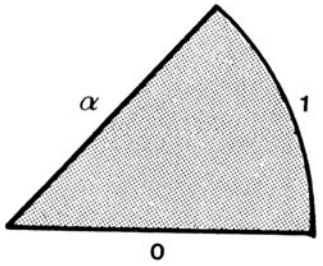


Fig. 6.8. Circular sector membrane.

circular membrane normal modes in Section 6.3 and are meant to illustrate the use of the normal mode method in finding explicit results for a variety of systems.

6.3.1. Inner Product on a Sector

Let the region $R_\triangleleft$ be a *sector* of the unit circle extending between the lines $\phi = 0$ and $\phi = \alpha$ (Fig. 6.8). The inner product on this region, in polar coordinates, will be

$$(\mathbf{f}, \mathbf{g})_\triangleleft = \int_0^1 r\, dr \int_0^\alpha d\phi f(r, \phi)^* g(r, \phi). \tag{6.31}$$

The space of functions we want to consider is $\mathscr{L}_0^2(R_\triangleleft)$: square-integrable functions under (6.31) which vanish on the boundary of $R_\triangleleft$, i.e., $f(r, 0) = 0 = f(r, \alpha)$ and $f(1, \phi) = 0$.

The expression for the Laplacian in polar coordinates is again (6.16), and the eigenfunction problem with the same coordinate separation is also (6.18). The solutions of the right-hand side of this equation, however, because of our new boundary conditions in ϕ, will be akin to the functions for a fixed-end string of length α, namely,

$$\Phi_m^\triangleleft(\phi) = (2/\alpha)^{1/2} \sin \mu\phi, \qquad \mu := m\pi/\alpha, \qquad m \in \mathscr{Z}^+, \tag{6.32}$$

and the separation constant in (6.18) will be $c = \mu^2$.

6.3.2. Solution to the Problem

The Bessel differential equation, which is the left-hand side of Eq. (6.18), is identical to (6.20), except that $m \in \mathscr{Z}$ is replaced by $\mu = m\pi/\alpha$, $m \in \mathscr{Z}^+$. This replacement applies also to the solutions, Eq. (6.23), which for $R_\triangleleft$ now read

$$\varphi_{mn}^\triangleleft(r, \phi) := (2/\alpha)^{1/2} g_{\mu n} J_\mu(j_{\mu n} r) \sin \mu\phi, \qquad m, n \in \mathscr{Z}^+, \tag{6.33}$$

where all quantities have the same meaning as before, $j_{\mu n}$ being the nth zero of the Bessel function of order μ. The main *difference* between (6.33) and (6.23) is that the "angular" label μ takes on equally spaced but in general noninteger values. The set of Laplacian eigenfunctions (6.33) will be orthogonal with respect to the inner product (6.31) and complete for $\mathscr{L}_0^2(R_<)$. A generalized Fourier series can be written for (6.33) identical to (6.24) except for the ranges of summation over m and integration over ϕ.

6.3.3. Normal Modes and Frequencies for a Sector Membrane

An elastic membrane governed by the wave equation over the region $R_<$ and fixed at its boundary will exhibit normal modes

$$\overset{<}{\varphi}_{mn}(r, \phi, t) = (2/\alpha)^{1/2} g_{\mu n} J_\mu(j_{\mu n} r) \sin \mu\phi \cos \omega_{\mu n} t, \tag{6.34}$$

and their time antiderivatives, the oscillation frequencies $\omega_{\mu n}$ being c times the nth zero of the Bessel function of order μ. In Fig. 6.9 are these allowed angular frequencies for the normal modes of a sectorial membrane of angle $\alpha = \pi/3$: the allowed μ's are positive integer multiples of 3. As the figure suggests, the opening of the angle α produces a "sliding down" of the allowed frequencies along their *trajectories*. In particular when α reaches π we have a half-circular membrane. The allowed values of μ are the positive

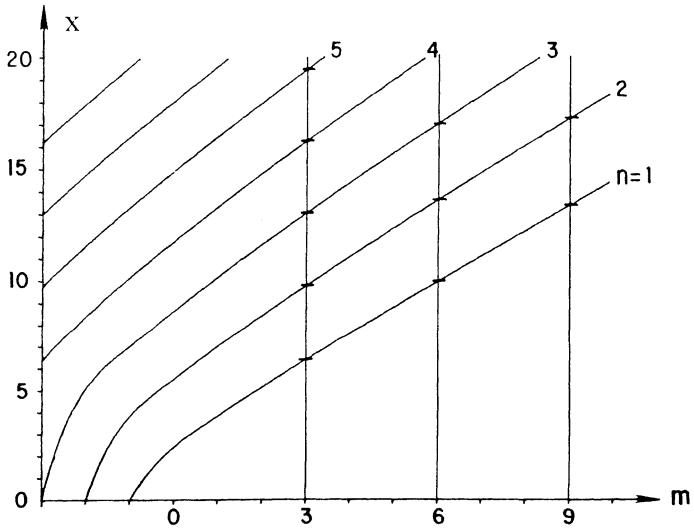


Fig. 6.9. Allowed angular frequencies of the normal modes of a sectorial membrane of angle $\alpha = \pi/3$. These are given by the zeros of $J_m(x)$ for m a nonzero multiple of 3.

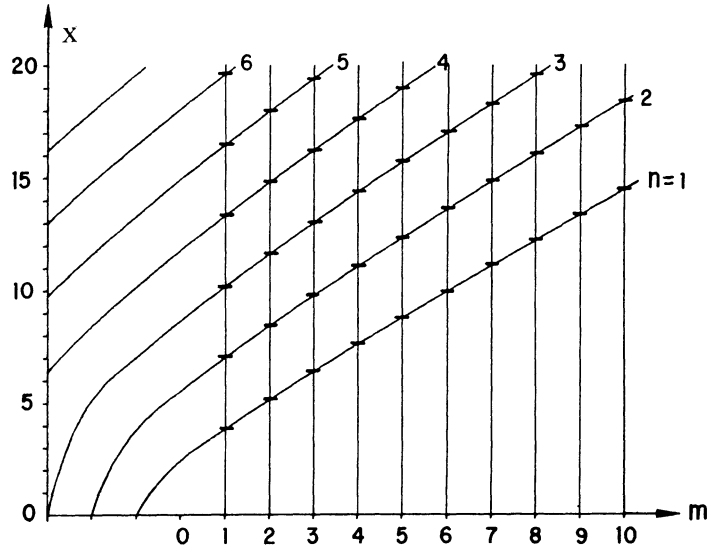


Fig. 6.10. Allowed angular frequencies of the normal modes of an $\alpha = \pi$ sectorial (semicircular) membrane.

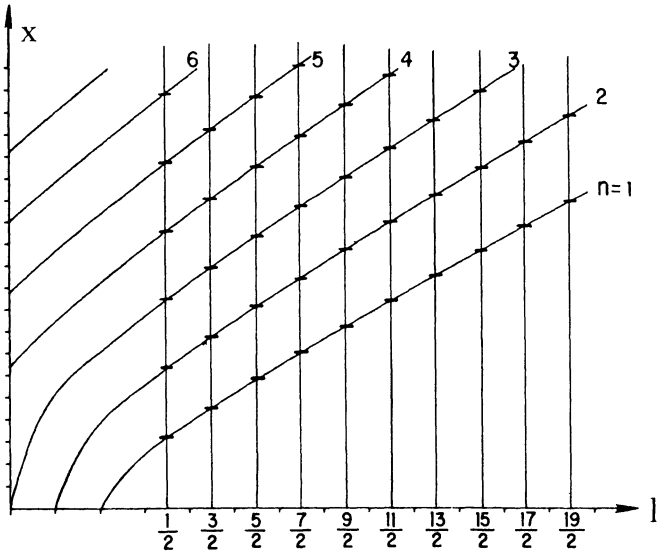


Fig. 6.11. Allowed angular frequencies of the normal modes in a spherical cavity.

integers (Fig. 6.10). Except for the $m = 0$ modes, therefore, the sounds one can produce on a circular drum are identical to those one can get from a half-drum. The mechanics of actual drumming, however, tend to generate mostly $m = 0$ normal modes. These are the only circular membrane modes where the center is in motion.

Exercise 6.13. Extend the sector angle α to 2π. You have then a circular membrane with a fixed strut extending to the center. The allowed angular frequencies will include $\omega_{1/2,n} = cn\pi$, capable of producing harmonic sounds. (See the particular function $J_{1/2}$ in Appendix B.) Describe the corresponding normal modes.

Exercise 6.14. Provided you are familiar with spherical harmonics, solve the wave equation for a resonating spherical cavity. Show that the allowed angular frequencies are only half-integers, as given by Fig. 6.11. These are the allowed ω's for Exercise 6.13, minus integers.

6.3.4. Bessel Series for Real Order

As in Section 6.2, in considering the generalized Fourier expansion of functions in $\mathscr{L}_0^2(R_\circlearrowleft)$ in series of $\phi_{mn}^{\circlearrowleft}(r, \phi)$, we can consider those which have the form $f(r)\Phi_m^{\circlearrowleft}(\phi)$ so that ϕ integration and cancellation can be made. This gives rise to the pair of Bessel series equations (6.28) for general *real* order m.

Exercise 6.15. Prove this in detail.

Exercise 6.16. Show that for $m = \frac{1}{2}$ the Bessel series (6.28) becomes the Fourier sine series.

6.3.5. Annular Boundary Conditions and Solutions

Consider now a region $R_\odot$ which is an *annulus* of interior and exterior radii ρ_1 and ρ_2 (Fig. 6.12). The relevant inner product is then

$$(\mathbf{f}, \mathbf{g})_\odot = \int_{\rho_1}^{\rho_2} r\, dr \int_{-\pi}^{\pi} d\varphi f(r, \varphi)^* g(r, \varphi), \tag{6.35}$$

defining a space $\mathscr{L}_0^2(R_\odot)$ in analogy with the former cases. The search for the eigenfunctions of ∇^2 in this space follows that of Section 6.2; the angular functions are here periodic and identical to (6.19), while the radial functions have the form (6.21). The boundary conditions on the latter are different, however:

$$R_m(\rho_1) = a_m J_m(\lambda^{1/2}\rho_1) + b_m N_m(\lambda^{1/2}\rho_1) = 0, \tag{6.36a}$$

$$R_m(\rho_2) = a_m J_m(\lambda^{1/2}\rho_2) + b_m N_m(\lambda^{1/2}\rho_2) = 0. \tag{6.36b}$$

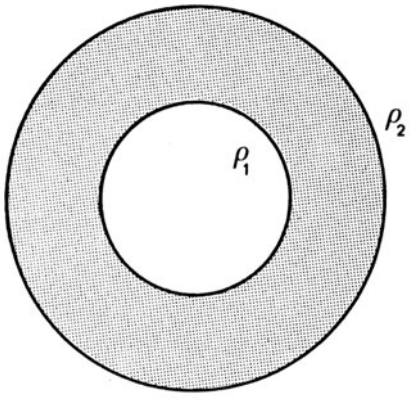


Fig. 6.12. Annular membrane.

This set of homogeneous equations will have a solution for the ratio b_m/a_m only if their determinant vanishes, i.e., for those values of $k := \lambda^{1/2}$ for which

$$D_m^{\rho_1\rho_2}(k) := J_m(\rho_1 k)N_m(\rho_2 k) - J_m(\rho_2 k)N_m(\rho_1 k) = 0. \tag{6.37}$$

6.3.6. Frequencies and Normal Modes for an Annular Membrane

The problem, then, is to find the zeros of the function $D_m^{\rho_1\rho_2}(k)$, which can be shown to be *simple*. This is not too difficult with standard numerical computer methods. See Fig. 6.13. Once these are found as $k_{m1}, k_{m2}, \ldots, k_{mn}, \ldots$, they can be introduced in (6.36) and the ratios $\rho_{mn} := b_m/a_m$ thereby determined for the nth zero of (6.37). The radial functions will then be

$$B_{mn}(r) := c_{mn}[J_m(k_{mn}r) + \rho_{mn}N_m(k_{mn}r)], \qquad m \in \mathscr{Z}, n \in \mathscr{Z}^+. \tag{6.38}$$

The normalization coefficient c_{mn} is chosen so that

$$\int_{\rho_1}^{\rho_2} r\, dr B_{mn}(r) B_{mn}(r) = \delta_{n'n}. \tag{6.39}$$

Bessel and Neumann functions are real, so no complex conjugation is necessary.

Exercise 6.17. Verify the orthogonality (6.39) of the $B_{mn}(r)$ with respect to the index n. This can be done as in Exercise 6.10.

Once the radial functions (6.38) have been found, the rest of the program follows as before: The eigenfunctions of ∇^2 on the annulus $R_\odot$ are $\varphi_{mn}^{\odot}(r, \phi) := B_{mn}(r)\Phi_m{}^{\odot}(\phi)$ and constitute a complete and orthonormal set of functions on $\mathscr{L}_0{}^2(R_\odot)$ [compare with (6.23) and (6.33)], giving rise to a generalized Fourier series on $R_\odot$. Normal modes for the annular membrane

can be built as the $\varphi^{\odot}_{mn}(r, \phi)$ times oscillating functions of time, of angular frequency $\omega_{mn} = ck_{mn}$ determined by the roots of (6.37). These can be plotted as in Fig. 6.6. In fact, Fig. 6.13, seen sidewise, is just such a diagram.

Exercise 6.18. Verify and explain the twofold degeneracy of ω_{mn} and ω_{-mn}.

Exercise 6.19. Investigate the case when the interior radius of the annulus, ρ_1, becomes zero. Show that, as $N_m(\rho) \to \pm\infty$ for $\rho \to 0$, $\rho_{mn} \to 0$ in (6.38). The annular normal modes thus become the circular ones, except for the $m = 0$ ones. Why are these absent?

Exercise 6.20. Consider an annular–sectorial membrane bounded between $r = \rho_1$ and ρ_2, $\phi = 0$ and α.

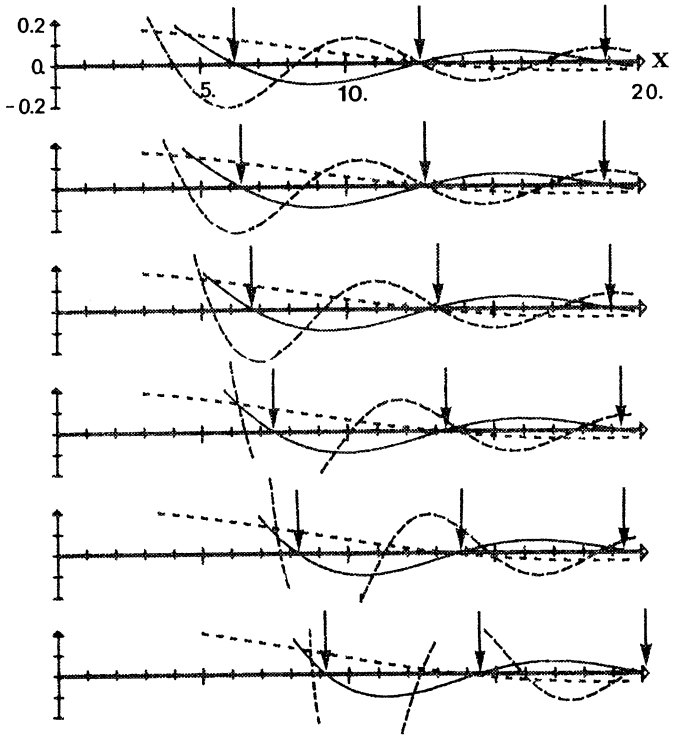


Fig. 6.13. The function $D_m^{\rho_1\rho_2}(k)$ in Eq. (6.37) for $m = 0, 1, \ldots, 5$. We draw three curves: long dashes for $\rho_1 = 0.25$, $\rho_2 = 1$; continuous for $\rho_1 = 0.5$, $\rho_2 = 1$, indicating the zeros by arrows; and short dashes for $\rho_1 = 0.75$, $\rho_2 = 1$. The zeros of the last function can be seen to lie at higher values of the argument and to tend toward equal spacing.

6.3.7. Bessel Series with the Annular Functions

The radial functions $B_{mn}(r)$ we have found for the annulus also provide an orthonormal (and *complete*) basis for the space of square-integrable functions on the interval (ρ_1, ρ_2). In fact, by arguments parallel to those which lead from the generalized Fourier expansions on $R_\bigcirc$ and $R_\diamond$ to the Bessel series in Eq. (6.28), we are led to the general Bessel series of order m,

$$f(r) = \sum_{n \in \mathscr{Z}^+} f_n^{B_m} B_{mn}(r), \tag{6.40a}$$

$$f_n^{B_m} = \int_{\rho_1}^{\rho_2} r\, dr f(r) B_{mn}(r), \tag{6.40b}$$

$$(\mathbf{f}, \mathbf{g})_B = \int_{\rho_1}^{\rho_2} r\, dr f(r)^* g(r) = \sum_{n \in \mathscr{Z}^+} f_n^{B_m *} g_n^{B_m}, \tag{6.40c}$$

which, as suggested by Exercise 6.20, is valid for real m.

The use of cylindrical functions for the series expansion of functions is not restricted to those types seen here, which arose out of the normal mode expansion in regions of the plane bounded by polar-coordinate boundaries. Among these "other" series expansions we should mention the *Neumann series*, which are of the form $\sum_{n=0}^{\infty} a_n J_{\nu+n}(r)$; the *Kapteyn series*, of the form $\sum_{n=0}^{\infty} b_n J_{\nu+n}[(\nu + n)r]$; and the *Schlömlich series*, of the form $\sum_{n=0}^{\infty} c_n J_\nu(nr)$. The region of convergence of the two first series is determined by the analytic properties of the functions to be expanded. In this sense, they are similar to the ordinary Taylor expansions. We shall not elaborate on these but refer the interested reader to Watson's treatise (1922, Chapters XVI, XVII, and XIX) for further details and applications. Neumann series also appear in the series on transcendental functions by Erdelyi *et al.* (1953–1955, Vol. 2, Chapter 7).

Tables of the roots of Eq. (6.37) are needed for any practical calculation. Two articles dealing with problems of this kind which offer reasonably extensive tables are those by Dwight (1948) and Bridge and Angrist (1962).

6.4. Other Series of Orthonormal Functions

In this chapter we have seen the Fourier and Bessel series—and many of their variants—arise in the description of the normal modes of an elastic medium enclosed by rectangular and polar-coordinate boundaries. There are at least two directions in which this approach can be generalized: first, by consideration of more general boundary conditions and surfaces in higher dimensions and, second, as "normal mode" solutions of other types of equations. In both cases, though, finding orthonormal and complete sets of functions is a *Sturm–Liouville* problem, which can be posed as follows.

6.4.1. The Sturm–Liouville Problem

Define an inner product over the interval (a, b) given by

$$(\mathbf{f}, \mathbf{g})_\omega = \int_a^b \omega(x)\, dx f(x)^* g(x), \qquad \omega(x) > 0,\ x \in (a, b), \tag{6.41}$$

with a positive *weight function* $\omega(x)$. Such an inner product defines the (*Hilbert*) space $\mathscr{L}_\omega^2(a, b)$ of functions $\mathbf{f}$ on (a, b) such that $(\mathbf{f}, \mathbf{f})_\omega < \infty$. Consider now a second-order differential operator with $p(x), q(x), r(x)$ real.

$$\mathbb{H} = p(x)\frac{d^2}{dx^2} + q(x)\frac{d}{dx} + r(x). \tag{6.42}$$

We want to examine the conditions under which $\mathbb{H}$ is *hermitian*, i.e., $(\mathbb{H}\mathbf{f}, \mathbf{g})_\omega = (\mathbf{f}, \mathbb{H}\mathbf{g})_\omega$. Performing the necessary integrations by parts, denoting d/dx by ∇ for the sake of brevity, and suppressing arguments, we find

$$\begin{aligned}(\mathbb{H}\mathbf{f}, \mathbf{g})_\omega &= \int_a^b \omega\, dx[(p\nabla^2 + q\nabla + r)f^*]g \\ &= \{\omega p(g\nabla f^* - f^*\nabla g) + [\omega q - \nabla(\omega p)]f^* g\}\Big|_a^b + \int_a^b \omega\, dx f^* \\ &\quad \times \{p\nabla^2 + \omega^{-1}[2\nabla(\omega p) - \omega q]\nabla + \omega^{-1}[\nabla^2(\omega p) - \nabla(\omega q)] + r\}g.\end{aligned} \tag{6.43}$$

So that (6.43) will equal $(\mathbf{f}, \mathbb{H}\mathbf{g})_\omega$ for arbitrary $\mathbf{f}$ and $\mathbf{g}$ it is sufficient that (a) $\nabla(\omega p) = \omega q$, which turns the operator in curly brackets into $\mathbb{H}$; the boundary term disappears if either (b) $\nabla h/h|_{x=a} = \nabla h/h|_{x=b}$ for $h = f$ and g or (b′) $\nabla h/h|_{x=a} = k_a$ and $\nabla h/h|_{x=b} = k_b$, k_a and k_b constants. These conditions direct us to consider operators (6.42) of the form

$$\mathbb{H} = [\omega(x)]^{-1}\frac{d}{dx}\omega(x)p(x)\frac{d}{dx} + r(x), \tag{6.44}$$

which, we are assured, are *hermitian* with respect to the inner product (6.41) in spaces of functions which satisfy boundary conditions which are either periodic or fix the logarithmic derivative at the interval ends.

We now pose ourselves the task of finding the solutions $\varphi_\lambda(x)$ to the eigenvalue equation

$$\mathbb{H}\varphi_\lambda(x) = \lambda\varphi_\lambda(x) \tag{6.45}$$

which are in $\mathscr{L}_\omega^2(a, b)$ and which satisfy the vanishing of the boundary term by (b) or (b′). We assume here for mathematical tractability that the set of values over which λ can range—the spectrum of $\mathbb{H}$—is an infinite, discrete set.

The solutions to (6.45), once they are explicitly found, will provide us with an *orthogonal* set of functions which can be normalized so that

$(\varphi_\lambda, \varphi_\mu)_\omega = \delta_{\lambda\mu}$. The proof of this fact is completely analogous to the proof in (1.106) for finite-dimensional vector spaces and was briefly commented upon following Eq. (6.4) in discussing eigenfunctions of the Laplacian which vanish on finite, closed boundaries.

Exercise 6.21. Verify the validity of the above construction for the operator d^2/dx^2, Eq. (6.44) with $\omega(x) = 1 = p(x)$, $r(x) = 0$, for the interval $(-\pi, \pi]$ with periodic boundary conditions (b) leading to the functions $(2\pi)^{-1/2} \exp(imx)$, $m \in \mathscr{Z}$, $\lambda = -m^2$. Note the slightly disturbing feature that the nonzero eigenvalues of d^2/dx^2 are doubly degenerate.

Exercise 6.22. Verify the validity for d^2/dx^2 under conditions (b′) in a general interval (a, b). The solutions to (6.45) have the general form $f_\mu(x) = c_\mu \sin(\mu x) + d_\mu \cos \mu x$, $\lambda = -\mu^2$. Assuming that $\nabla f_\mu/f_\mu|_{x=a} = k_a$ and $\nabla f_\mu/f_\mu|_{x=b} = k_b$, find the allowed values of μ and the corresponding ratio of c_μ/d_μ. Normalize. [See Titchmarsh (1946, Section 4.1).]

Exercise 6.23. Study the Bessel series of annular functions (6.38) as stemming from the eigenvalue equation (6.20), which has the form (6.44)–(6.45) with $\omega(x) = x$, $p(x) = 1$, $r(x) = -m^2/x^2$, $m > 0$. The solutions (6.21) are further curtailed by the boundary conditions on (ρ_1, ρ_2): $k_{\rho_1} = \infty = k_{\rho_2}$. Other boundary conditions will give versions of the Dini series. [See Titchmarsh (1946, Section 4.7 *et seq.*).]

Exercise 6.24. Consider Bessel's differential equation (B.12) written as an eigenfunction equation with eigenvalues m^2 of the form (6.44)–(6.45) with $\omega(x) = 1/x$, $p(x) = x^2 = r(x)$. What boundary conditions give the orthogonality relations for the expanding functions employed in the Neumann series?

6.4.2. On Eigenvalues, Orthogonality, and Completeness

It should be observed that only orthogonality of the eigenfunction set is guaranteed by the hermiticity of the operator $\mathbb{H}$. *Completeness* is a more difficult property to prove or verify. When the operator is *self-adjoint* (see the discussion in Section 4.6) and the spectrum as assumed above, the eigenfunction set *is* complete. An arbitrary function $f(x) \in \mathscr{L}_\omega^2(a, b)$ can then be written (approximated *in the norm*) as a normalized eigenfunction series

$$f(x) = \sum_{n=0}^{\infty} f_n \varphi_n(x), \qquad x \in (a, b), \tag{6.46a}$$

where the generalized Fourier coefficients f_n are

$$f_n = (\boldsymbol{\varphi}_n, \mathbf{f})_\omega = \int_a^b \omega(x)\, dx \varphi_n(x)^* f(x). \tag{6.46b}$$

The generalized Parseval identity reads

$$(\mathbf{f}, \mathbf{g})_\omega = \int_a^b \omega(x)\, dx f(x)^* g(x) = \sum_{n=0}^{\infty} f_n^* g_n. \tag{6.46c}$$

Quantum mechanics, in its Schrödinger formulation, is mathematically a Sturm–Liouville theory, the operator in question being typically the system's Hamiltonian $-\frac{1}{2}\nabla^2 + V(\mathbf{x})$, where $V(\mathbf{x})$ is the potential function. The region R where $\mathbf{x}$ is allowed to range is usually the whole three-dimensional space, so, in a sense, the wave-function expansion lies outside the class considered in this part. Yet if the potential is such that is classically constrains a particle with finite energy to a bounded region in space, or if we are using coordinate systems such as cylindrical or spherical where one or more of the coordinates range, due to geometry, over a bounded interval, the result is a wave-function *series*. Of particular importance are the *bound-state Coulomb* and *harmonic oscillator* systems. The eigenfunction expansions associated with the latter will be detailed in Section 7.5; those of the former can be seen in most quantum mechanics texts, such as Messiah (1964, Chapter 11).

6.4.3. Orthogonal Polynomial Series

Due to their ubiquity, a class of eigenfunction expansions which we can hardly escape mentioning is that of the classical *orthogonal polynomials*. There are three families of these, according to whether the interval (a, b) in (6.41) is finite, half-infinite [i.e., (a, ∞)], or infinite. The first family is that of *Jacobi* polynomials, $P_n^{(\alpha,\beta)}(x)$, orthogonal under (6.41) with $(a, b) = (-1, 1)$ and $\omega(x) = (1 - x)^\alpha(1 + x)^\beta$, $\alpha, \beta > -1$. When $\alpha = \beta =: \gamma - \frac{1}{2}$, i.e., $\omega(x) = (1 - x^2)^{\gamma - 1/2}$, these become the *Gegenbauer* polynomials $C_n^{(\gamma)}(x)$ which appear in connection with hyperspherical harmonics [for solutions to the angular part of the N-dimensional Laplacian, see Eqs. (8.77)]. For $\gamma = \frac{1}{2}$, $\omega(x) = 1$, we have the *Legendre* polynomials $P_n(x)$, which appear in three-dimensional spherical coordinate separation. The second case, half-infinite intervals $(0, \infty)$, leads to *Laguerre* polynomials $L_n^{(\alpha)}(x)$ when $\omega(x) = x^\alpha \exp(-x)$. The Coulomb and radial harmonic oscillator quantum systems are solved in terms of these functions. Finally, infinite intervals require *Hermite* polynomials for $\omega(x) = \exp(-x^2)$. These are present in the harmonic oscillator wave functions in Cartesian coordinates.

The three families of *classical* orthogonal polynomials are further related, with some rather technical restrictions, to the existence of a *Rodrigues* differential recursion formula as shown by Tricomi (1955) [this can be seen, in simplified version, in the text by Dennery and Krzywicki (1967, Section III-10)]. A result of this recursion formula is that the interval (a, b) determines uniquely the weight function $\omega(x)$ and the differential equation satisfied by the polynomials. For the above intervals, the Jacobi, Laguerre, and Hermite families satisfy (6.44)–(6.45) with $p(x) = 1 - x^2$, x, and 1, respectively.

Books on the series expansion in terms of orthogonal polynomials include the classic by Szegő (1939), Rainville (1960), and Boas and Buck (1964). The general subject of eigenfunction expansions including many

concrete examples can be seen in the two-volume work by Titchmarsh (1946, 1958). A more readable account can be found in Yoshida (1960).

6.4.4. Two- and Three-Variable Series Expansions

The wave equation, once the time dependence has been "factored off" and replaced by a $-\omega^2$ term, is a Helmholtz equation such as (6.4). In two-dimensional space, the Helmholtz equation is known to have separable solutions in (*only*) four coordinate systems: Cartesian, polar, parabolic, and elliptic. If the boundary conditions are given following these coordinate lines, the solutions will be given in terms of circular and Bessel functions in the first two cases and *parabolic cylinder* and *Mathieu* functions in the last two. Corresponding orthonormal and complete sets of normal modes can be obtained for elastic media enclosed in such boundaries, except that in the last two cases these remain as two-variable u-v function expansions of the form $U_{mn}(u)V_{mn}(v)$, where the separation constants, related to m and n, are *coupled* and do *not* simplify to single-variable series. Only Cartesian and polar coordinates have this property. A variety of problems involving the two-dimensional wave equation with various boundary conditions can be found in Morse and Feshbach (1953, Sections 5-1 and 11-2). For parabolic cylinder and Mathieu functions we have to turn to more specialized literature (see below). The latter are given concise treatment in the textbook by Hochstadt (1966).

The wave equation in three dimensions leads to further special functions, since the corresponding Helmholtz equation separates now in 11 coordinate systems. The four orthogonal coordinate systems which separate the two-dimensional Helmholtz equation yield, under translations along a normal, Cartesian, circular, parabolic, and elliptic cylinder coordinates. Under rotation around an axis in the plane they generate spherical, parabolic, and prolate and oblate spheroidal coordinates. In addition, there are the conical, ellipsoidal, and paraboloidal systems. The surfaces defined by these coordinates which can serve as boundaries are three-dimensional conic surfaces. New functions appear: associated Legendre polynomials and spheroidal, Lamé, Jacobian elliptic, and ellipsoidal functions. The three-variable normal mode expansions do not simplify to two- or single-variable series except for those obtained by translation. The spherical coordinates are somewhat special in that their normal modes have the structure $R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$. For $m = 0$ they yield the Legendre polynomial series in $\cos\theta$ and the Bessel–Fourier series in r.

The higher transcendental functions appearing in the solution of the Helmholtz equation in two and three dimensions are given a full discussion in volumes such as those by Hobson (1931), McLahlan (1947), Meixner and Schärfke (1954), and especially Arscott (1964). Of particular importance, the

spherical harmonics, orthogonal functions on the surface of a sphere, have many interesting group-theoretical properties. These have been presented in books by Edmonds (1957) and Rose (1957). Last, it should be mentioned that the theory of Lie algebras and groups offers a powerful method for the determination of certain operator eigenfunctions and their completeness. The works of Maurin (1968) and Olevskiĭ (1975) develop this field.

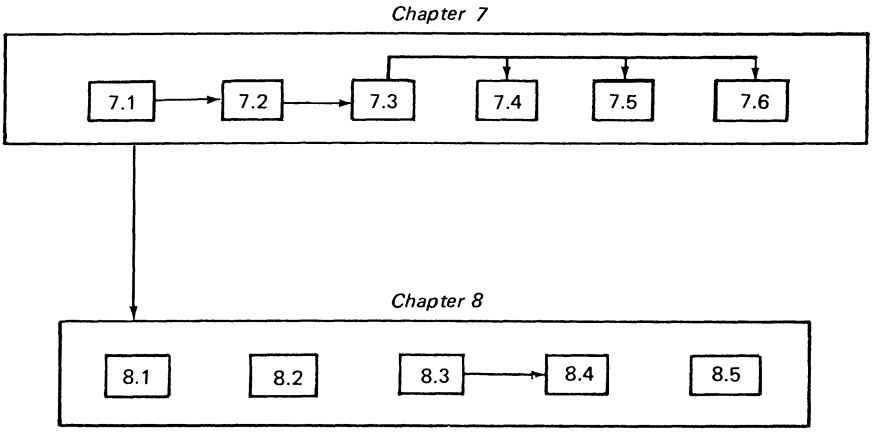
Part III

Fourier and Related Integral Transforms

Integral transforms traditionally refer to the generalized expansion—as an *integral* rather than a series sum—of a function in a continuum of oscillating exponential or related functions. Of these, the prime example is the Fourier transform discussed in Chapter 7; other commonly used integral transforms, those associated with the names of Laplace, Mellin, and Hankel, are studied in Chapter 8. Applications are interspersed with the study of their relevant properties.

The presentation of the Fourier transform starts with the classic Fourier integral theorem and a survey of the relevant function spaces. The main properties under transformations and differential operators are then explored. With the introduction of the Dirac δ and the related task of finding the Green's function for an evolution equation, the basics are given for more specialized applications in the last three sections. These include causality and its description, oscillator wave-function bases including coherent states, and uncertainty relations. The last two, in addition to their inherent mathematical interest, are ubiquitous in quantum mechanics.

In Chapter 8 integral transforms related to Fourier transforms are applied to the description of unbounded diffusive and elastic media in one and more dimensions. The closing section is intended to provide a panorama of other integral transforms which appear in various situations.



7

Fourier Transforms

The continuous partial-wave decomposition of a function over the full real line constitutes the Fourier analysis of the function. The precise formulation of this decomposition, a broad outline of its range of applicability, and its vector space aspects constitute Section 7.1. Its main properties are given in Section 7.2. Section 7.3 proceeds toward applications by the introduction of the Dirac δ and its role in finding the Green's function, which determines the time development of diffusive and elastic systems with source or driving-force terms. Except for a few connections, the following three sections are independent of each other. Section 7.4 deals with functions which have support (i.e., are not necessarily zero) on half-infinite or finite intervals. The former are interesting in that they can be used to describe causal processes. The Fourier transforms of these functions satisfy certain *dispersion relations* due to their behavior in the complex plane. Subtractions for band-absorption filters are described. Section 7.5 deals with the quantum oscillator wave functions. The *harmonic* oscillator wave functions constitute a denumerable complete and orthonormal basis for the space of square-integrable functions. The *repulsive* oscillator functions, on the other hand, though less well known, serve both as a generalized basis for that space and as a fine working ground for various Fourier analysis techniques. Finally, Section 7.6 describes a type of complementarity between a function and its Fourier transform which gives rise to the Heisenberg uncertainty relation between the dispersion in measurement of two quantum-mechanical observables.

7.1. The Fourier Integral Theorem

In this section we shall prove the reciprocity between a function $f(q)$, $q \in \mathscr{R}$ (the real line), and its Fourier transform $\tilde{f}(p)$, $p \in \mathscr{R}$, which was sug-

gested in two earlier sections. Its precise formulation constitutes the Fourier integral theorem. Several examples, useful later on, will be given.

7.1.1. Introduction

In Section 3.4 we followed the finite Fourier transform for spaces whose dimension was allowed to increase without bound [Eqs. (3.50) and (3.51)], while in Section 4.7 we expanded functions $f(q)$ periodic in a growing interval [Eqs. (4.138) and (4.139)]. In both cases we found the limiting expressions

$$f(q) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp \tilde{f}(p) \exp(ipq) =: (\mathbb{F}^{-1}\tilde{\mathbf{f}})(q), \tag{7.1a}$$

$$\tilde{f}(p) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f(q) \exp(-ipq) =: (\mathbb{F}\mathbf{f})(p). \tag{7.1b}$$

Provided the integrals exist—or can be made sense of—$\tilde{f}(p)$ is called the Fourier transform function corresponding to $f(q)$ and represents the partial-wave coefficients for its generalized expansion, as an integral, in the exponential functions $\exp(ipq)$. The Parseval identity

$$(\mathbf{f}, \mathbf{g}) := \int_{-\infty}^{\infty} dq f(q)^* g(q) = \int_{-\infty}^{\infty} dp \tilde{f}(p)^* \tilde{g}(p) = (\mathbb{F}\mathbf{f}, \mathbb{F}\mathbf{g}) \tag{7.2}$$

can be seen as an integral version of the Pythagorean theorem for spaces of a continuous infinity of dimensions.

7.1.2. Statement of the Theorem

The conditions for (7.1) and (7.2) to hold must include that the integral over an infinite interval exist and must specify what the meaning of (7.1a) is when $f(q)$ is discontinuous at some points. The *Fourier integral theorem* states that if $f(q)$ (a) is piecewise continuous (continuous except at most at a number of isolated points), (b) has bounded total variation (so that when approximated by any step function the sum of the absolute values of the step height differences is finite), and (c) is absolutely integrable [i.e., $\int_{-\infty}^{\infty} dq |f(q)| < \infty$], *then* for any $q' \in \mathscr{R}$,

$$\lim_{L\to\infty} (2\pi)^{-1/2} \int_{-L}^{L} dp \left[(2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f(q) \exp(-ipq) \right] \exp(ipq') = \lim_{\varepsilon\to 0} \tfrac{1}{2}[f(q' + \varepsilon) + f(q' - \varepsilon)]. \tag{7.3}$$

When the three conditions are satisfied, (7.3) tells us that (7.1a) indeed reproduces the $f(q)$ by the Fourier transform (7.1b) at all points of continuity of the function. If $f(q)$ is discontinuous at some point q_d, the integral in (7.1a)

yields the value of $f(q)$ at the midpoint of the discontinuity. This was also a characteristic of the Dirichlet theorem for Fourier series in Section 4.2. Again we shall work with the understanding that any two functions $f(q)$ and $g(q)$ which differ from each other at most on a denumerable set of points (a set of *measure zero* for *Lebesgue* integration) are equivalent.

7.1.3. Proof: The Case of the Rectangle Function

The strategy we shall follow in proving the Fourier integral theorem is first to establish the result—as if it were an example—for a *rectangle* function and then to use some of the limits obtained in order to prove that for any piecewise continuous and bounded function the result holds as well. Consider the *rectangle* function of width ε and height η:

$$R^{(\varepsilon,\eta)}(q) := \begin{cases} \eta, & -\varepsilon/2 < q \leqslant \varepsilon/2, \\ 0, & \text{otherwise.} \end{cases} \tag{7.4}$$

[This is identical to the rectangle function introduced in Section 4.2 except that the domain of (7.4) is $\mathscr{R}$, whereas in (4.24) it was the interval $(-\pi, \pi]$ which when extended to $\mathscr{R}$ carried an infinity of copies of itself spaced by 2π.] The Fourier transform of (7.4) can be easily calculated by (7.1b) as

$$\begin{aligned} \tilde{R}^{(\varepsilon,\eta)}(p) &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq R^{(\varepsilon,\eta)}(q) \exp(-ipq) \\ &= (2\pi)^{-1/2} \eta \int_{-\varepsilon/2}^{\varepsilon/2} dq \exp(-ipq) \\ &= (2\pi)^{-1/2} \varepsilon\eta \sin(p\varepsilon/2)/(p\varepsilon/2). \end{aligned} \tag{7.5}$$

See Fig. 7.1. Now, in proving (7.3) for this function we must evaluate

$$\begin{aligned} \bar{R}^{(\varepsilon,\eta)}(q) &:= \lim_{L\to\infty} (2\pi)^{-1/2} \int_{-L}^{L} dp \tilde{R}^{(\varepsilon,\eta)}(p) \exp(ipq) \\ &= \lim_{L\to\infty} \pi^{-1}\eta \int_{-L}^{L} dp p^{-1} \sin(p\varepsilon/2) \cos pq \\ &= \lim_{L\to\infty} \pi^{-1}\eta \int_{0}^{L} dp p^{-1} \{\sin[p(q + \varepsilon/2)] - \sin[p(q - \varepsilon/2)]\}. \end{aligned} \tag{7.6}$$

In the first step we have used the fact that the imaginary part is odd in p and hence vanishes, while the second is only a trigonometric identity and a halving of the integration range as the integrand is even. We are thus faced with limits of integrals of the kind

$$\begin{aligned} I(s) &:= \lim_{L\to\infty} \int_{0}^{L} dp p^{-1} \sin ps \\ &= \operatorname{sign} s \lim_{v\to\infty} \int_{0}^{b} dy y^{-1} \sin vy, \end{aligned} \tag{7.7}$$

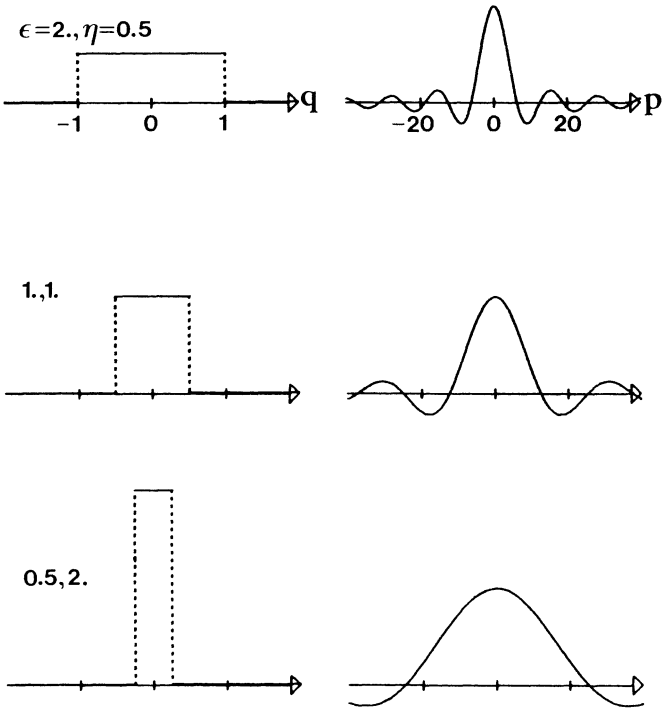


Fig. 7.1. The rectangle function $R^{(\varepsilon,\eta)}(q)$ (right) and its Fourier transform $\tilde{R}^{(\varepsilon,\eta)}(p)$ (left) for various values of ε and η such that $\varepsilon\eta = 1$.

where we have changed variables to $y \coloneqq bp/L$ and $v \coloneqq |s|L/b$, $b > 0$, thereby putting the onus of the limit on the argument of the trigonometric function. We have introduced the sign function, which takes the values 1, 0, or -1 according to whether $s > 0$, $s = 0$, or $s < 0$, so as to keep the upper integration limit positive. The last form is also valid when $s = 0$. We shall now show that the value of the integral in the last term of (7.7) is $\pi/2$. For this purpose we employ the result on the Dirichlet kernel, Eqs. (4.19)–(4.20), using the evenness of the integrand and a change of scale $x = \pi y/b$ in order to write it as

$$\lim_{v\to\infty} \int_0^b dy[\sin(\pi y/2b)]^{-1} \sin vy = b, \qquad v = \pi(k + \tfrac{1}{2})/b, \qquad k \in \mathscr{Z}^+ \tag{7.8}$$

($\mathscr{Z}^+$ is the set of positive integers). Now we subtract this from (7.7) as

$$[I(s)\,\mathrm{sign}(s) - \pi/2] = \lim_{v\to\infty} \int_0^b dy g(y) \sin vy, \tag{7.9a}$$

$$g(y) \coloneqq 1/y - \pi[2b \sin(\pi y/2b)]^{-1}. \tag{7.9b}$$

The proof that (7.9a) is zero proceeds very much as in the proof of the Dirichlet theorem in Section 4.2; namely, we note that $g(y)$ is bounded in the interval $[0, b]$ with a bound independent of v, as is its derivative $g'(y)$. We can integrate (7.9a) by parts and see that

$$\lim_{v\to\infty} v^{-1}\left[-g(y)\cos vy\Big|_0^b + \int_0^b dyg'(y)\cos vy\right] = 0. \tag{7.9c}$$

We conclude that

$$\lim_{v\to\infty} \int_0^b dyy^{-1}\sin vy = \pi/2, \tag{7.10a}$$

and hence

$$\lim_{L\to\infty} \int_{-L}^{L} dpp^{-1}\sin ps = \pi \operatorname{sign} s. \tag{7.10b}$$

Thus, the rectangle function is reconstructed in (7.6) as

$$\bar{R}^{(\varepsilon,\eta)}(q) = \eta[\operatorname{sign}(q + \varepsilon/2) - \operatorname{sign}(q - \varepsilon/2)]/2. \tag{7.11}$$

We note that (7.11) coincides with the original function (7.4) for all values of the argument except at $q = \pm\varepsilon/2$, where the original function is discontinuous while the integral (7.6) converges, as promised by (7.3), to the midpoint of the discontinuity: $\bar{R}^{(\varepsilon,\eta)}(\pm\varepsilon/2) = \eta/2$. The two functions are therefore equivalent.

Exercise 7.1. Show that the Fourier transform of a rectangle function $R^{(b-a,\eta)}(q - (a + b)/2)$ of height η whose nonzero values are in the interval $[a, b]$ is

$$\tilde{R}(p) = (2\pi)^{-1/2}\eta ip^{-1}[\exp(-ibp) - \exp(-iap)]. \tag{7.12}$$

Verify along the same lines as above that the Fourier integral theorem holds for this pair.

7.1.4. The Case of Piecewise Continuous Functions

The validity of the Fourier integral theorem for the rectangle function and Exercise 7.1 shows that this theorem also holds for step functions composed of a finite number of steps. Now, any continuous function with bounded total variation can be approximated uniformly by a sequence of step functions. Intuitively at least, we can expect that the Fourier integral theorem holds for these functions if, additionally, they are absolutely integrable so that the first integration in (7.3) is defined. We shall now set out to prove this using the results obtained above.

If $f(x)$ is absolutely integrable, as long as L is finite we can exchange the order of integration in (7.3) so that

$$(2\pi)^{-1}\int_{-\infty}^{\infty} dqf(q)\int_{-L}^{L} dp\,\exp[ip(q'-q)]$$
$$= \pi^{-1}\int_{-\infty}^{\infty} dqf(q+q')q^{-1}\sin Lq. \quad (7.13)$$

The limit $L\to\infty$ will thus require an integral of the kind (7.10a) with a function $f(y+b)$ placed in company with the oscillating sine. Now, Eq. (7.10a) is actually independent of b, which was only required to be finite and positive. As we can write $\int_0^b = \int_0^{b'} + \int_{b'}^b$ for $0 < b' < b$, the integrals $\int_0^b$ and $\int_0^{b'}$ being $\pi/2$, it follows that $\int_{b'}^b$ *vanishes*. Note that the argument (7.9) also applies for integrals $\int_a^0$, $a < 0$, as we need only set $b = -a$ in (7.8). Assume now that $f(y+c)$ is continuous and of bounded variation in $(a, 0)$ and $(0, b)$; then we state that

$$\lim_{v\to\infty}\int_a^b dyf(y+c)y^{-1}\sin vy = \begin{cases} \frac{1}{2}\pi[f(c^+)+f(c^-)] & \text{if } a<0<b,\\ \frac{1}{2}\pi f(c^+) & \text{if } a=0<b\\ \frac{1}{2}\pi f(c^-) & \text{if } a<0=b\\ 0 & \text{when } 0\notin[a,b], \end{cases} \quad (7.14)$$

where $f(c^+) \coloneqq \lim_{\varepsilon\to 0} f(c+\varepsilon)$, $\varepsilon > 0$. Indeed, for the second case we can break up the integral as $\int_0^b = \int_0^\delta + \int_\delta^b$ for $0 < \delta < b$ and δ as small as we please. Using the mean value theorem, we see that the first integral will yield $\frac{1}{2}\pi f(c^+)$, while the second one vanishes. These arguments can be applied to prove the other cases, constituting essentially the Riemann–Lebesgue theorem.

The infinite integral in (7.13) can be now broken up as $\int_{-\infty}^{\infty} = \int_{-\infty}^{a} + \int_a^b + \int_b^{\infty}$. Since $f(q+q')$ is assumed absolutely integrable on $\mathscr{R}$, for every preassigned $\varepsilon_a > 0$ and $\varepsilon_b > 0$ we can find integration limits a and b such that $\int_{-\infty}^a$ and $\int_b^\infty$, with the integrand in (7.13), are less than these numbers, leaving only the contribution from $\int_a^b$, to which Eq. (7.14) applies. In this way, the Fourier integral theorem (7.3) is proven.

Exercise 7.2. Consider the single-tooth "sawtooth" function

$$s_M(q) \coloneqq \begin{cases} q, & q\in(-M/2, M/2),\\ 0, & \text{otherwise,}\end{cases} \quad (7.15a)$$

and its Fourier transform

$$\tilde{s}_M(q) = (2\pi)^{-1/2}iMp^{-1}[\cos(pM/2) - (pM/2)^{-1}\sin(pM/2)]. \quad (7.15b)$$

Verify the workings of the proof of the Fourier integral theorem, in particular the use of the mean value theorem and the splitting of the integral over $\mathscr{R}$.

Following the usage in earlier sections we define the quadratic norm of **f** as

$$\|\mathbf{f}\| := (\mathbf{f}, \mathbf{f})^{1/2} = \left[\int_{-\infty}^{\infty} dq|f(q)|^2\right]^{1/2}. \tag{7.16}$$

Exercise 7.3. Prove the Parseval identity (7.2) in the form

$$\lim_{L\to\infty}\int_{-L}^{L} dp\tilde{f}(p)^*\tilde{g}(p) = \int_{-\infty}^{\infty} dqf(q)^*g(q). \tag{7.17}$$

You can replace $\tilde{f}(p)$ and $\tilde{g}(p)$ by their expressions (7.1b), exchange integrals for finite L, and then use (7.3). Note that, in particular, $\|\mathbf{f}\| = \|\tilde{\mathbf{f}}\|$.

Exercise 7.4. Prove the Schwartz inequality

$$|(\mathbf{f}, \mathbf{g})|^2 \leqslant (\mathbf{f}, \mathbf{f})(\mathbf{g}, \mathbf{g}), \tag{7.18a}$$

which here assumes the form

$$\left|\int_{-\infty}^{\infty} dqf(q)^*g(q)\right|^2 \leqslant \left[\int_{-\infty}^{\infty} dq|f(q)|^2\right]\left[\int_{-\infty}^{\infty} dq|g(q)|^2\right], \tag{7.18b}$$

and its Fourier-transformed version by the Parseval identity. This is nothing more than the proof in (1.13)–(1.15). The Schwartz inequality (7.18b) has been shown to be but a special case of the more general relation

$$\begin{aligned}\left|\int_{-\infty}^{\infty} dqf(q)^*g(q)\right| &\leqslant \int_{-\infty}^{\infty} dq|f(q)^*g(q)| \\ &\leqslant \left[\int_{-\infty}^{\infty} dq|f(q)|^p\right]^{1/p}\left[\int_{-\infty}^{\infty} dq|g(q)|^{p'}\right]^{1/p'}\end{aligned} \tag{7.18c}$$

for p and p' such that $p^{-1} + p'^{-1} = 1$. The last two members are known as *Hölder's inequality*. For $p = 2 = p'$ we recover (7.18b). When $p = 1$, $p' = \infty$, the corresponding expression for $g(q)$ becomes the supremum of the function.

Exercise 7.5. Write out the integral expressions which represent the triangle inequalities (1.19) and (1.21). These are a special $p = 2$ case of the *Minkowski inequality*

$$\left[\int_{-\infty}^{\infty} dq|f(q) + g(q)|^p\right]^{1/p} \leqslant \left[\int_{-\infty}^{\infty} dq|f(q)|^p\right]^{1/p} + \left[\int_{-\infty}^{\infty} dq|g(p)|^p\right]^{1/p}, \tag{7.19}$$

which is valid for $p \geqslant 1$.

7.1.5. Example: The Gaussian Bell Function

The unit *Gaussian bell function* of *width* ω,

$$G_\omega(q) := (2\pi\omega)^{-1/2}\exp(-q^2/2\omega), \tag{7.20}$$

will be used quite often. It is a function which is infinitely differentiable. It is positive, its maximum being $G_\omega(0) = (2\pi\omega)^{-1/2}$, and it decreases to

0.60653... of this value at $q = \pm\omega^{1/2}$. Due to the normalization chosen in (7.20), $G_\omega(q)$ can be shown by Euler's integral to enclose *unit area*,

$$\int_{-\infty}^{\infty} dq G_\omega(q) = 1, \tag{7.21}$$

independently of its width.

The Fourier transform of the Gaussian (7.20) can be calculated as

$$\begin{aligned}
\tilde{G}_\omega(p) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq G_\omega(q)\exp(-ipq) \\
&= (2\pi)^{-1}\omega^{-1/2}\int_{-\infty}^{\infty} dq \exp(-q^2/2\omega - ipq) \\
&= (2\pi)^{-1}\omega^{-1/2}\exp(-p^2\omega/2)\int_{-\infty}^{\infty} dq \exp[-(q + i\omega p)^2/2\omega] \\
&= (2\pi)^{-1/2}\exp(-p^2\omega/2)\int_{-\infty}^{\infty} dq' G_\omega(q') \\
&= \omega^{-1/2}G_{1/\omega}(p).
\end{aligned} \tag{7.22}$$

The fourth equality requires a common complex integration result: The integrand is analytic and free from singularities in any band parallel to the real axis and decreases rapidly at $|\mathrm{Re}\, q| \to \infty$; hence $\int_{-\infty+i\omega p}^{+\infty+i\omega p} = \int_{-\infty}^{\infty}$. Thus, *the Fourier transform of a Gaussian of width ω is another Gaussian of width $1/\omega$.* See Fig. 7.2.

Exercise 7.6. Verify the Parseval identity for the Gaussian bell function. Show that

$$\|\mathbf{G}_\omega\| = (4\pi\omega)^{-1/4} = \|\tilde{G}_\omega\|. \tag{7.23a}$$

You can use the value of the Euler integral (7.21) for 2ω. Differentiating the last equation with respect to ω, show that

$$\|\mathbb{Q}\mathbf{G}_\omega\| = (\omega/\pi)^{1/4}/2, \tag{7.23b}$$

where $(\mathbb{Q}\mathbf{G}_\omega)(q) = qG_\omega(q)$. This is related to the *second moment* of the Gaussian function and will be used in Section 7.6.

7.1.6. On the Function Spaces $\mathscr{C}_\downarrow^\infty$, $\mathscr{L}^2(\mathscr{R})$, $\mathscr{L}^1(\mathscr{R})$, and $\mathscr{S}'$

The theory of Fourier transforms includes a much greater amount of information and caveats than meets the eye in Eqs. (7.1) and (7.2) or the more rigorous (7.3) and (7.17). First, let us emphasize that we can have *two* geometric interpretations of the pair of functions $f(q)$ and its Fourier transform $\tilde{f}(p)$: (a) the view developed in Parts I and II, which regards $f(q)$ and $\tilde{f}(p)$ as *the coordinates, in two bases, of the same* **f**, an element of some

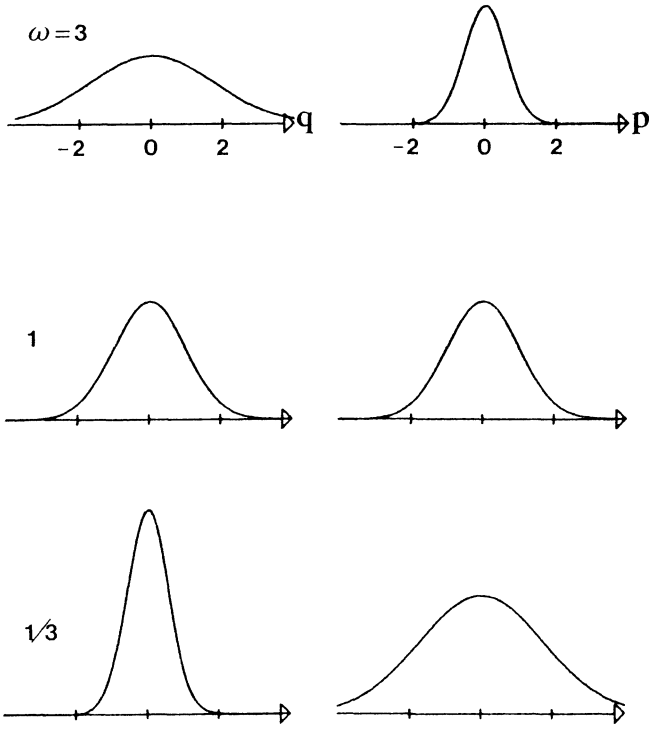


Fig. 7.2. The Gaussian function $G_\omega(q)$ (left) and its Fourier transform (right) for various values of the width. Note that the maximum of the latter is independent of ω.

appropriate vector space $\mathscr{V}$ of functions with domain $\mathscr{R}$ (see Section 4.5), and (b) the Fourier transformation as an *active* transformation of this vector space into itself as $\mathbf{f} \mapsto \tilde{\mathbf{f}} = \mathbb{F}\mathbf{f}$. The two points of view, passive and active transformations of $\mathscr{V}$, are conceptually different ways of interpreting Eqs. (7.1). Both are useful. The first picture is widely used in quantum mechanics where $\psi(q)$ and its Fourier transform $\tilde{\psi}(p)$ represent the configuration- and momentum-space wave functions, respectively, of the same *state* vector $\boldsymbol{\psi}$ which describes a quantum system. The second picture, to which we subscribe in most of this chapter, is to regard the Fourier transform as an *operator* $\mathbb{F}$ mapping various function spaces $\mathscr{V}$ onto themselves or onto other spaces $\mathbb{F}\mathscr{V}$, not coincident with $\mathscr{V}$. We shall take the argument of the original function $\mathbf{f}$ to be q and that of $\tilde{\mathbf{f}} = \mathbb{F}\mathbf{f}$ to be p.

We shall now present some function spaces which are of interest in their relation with Fourier analysis. We define $\mathscr{C}_\downarrow^\infty$ as the space of infinitely differentiable functions of *fast decrease* (i.e., such that for all m and n, $q^m d^n f(q)/dq^n \to 0$ as $|q| \to \infty$). Examples of functions in this space are the

Gaussian bell function (7.20), all its derivatives, and any polynomial times these functions. It is rather easy to prove (Section 7.2) that the Fourier transformation $\mathbb{F}$ maps $\mathscr{C}_{\downarrow}^{\infty}$ onto itself. Next, we recall the definition of $\mathscr{L}^2(\mathscr{R})$, the space of square-integrable functions over $\mathscr{R}$ in the sense of Lebesgue, i.e., $\mathbf{f} \in \mathscr{L}^2(\mathscr{R})$ when $\|\mathbf{f}\| < \infty$. As mentioned in Section 4.5, this is a definition of integration which is wider and more powerful than the ordinary Riemann integral; it coincides with the latter for integrands which satisfy the conditions of the Dirichlet or the Fourier integral theorem. The Parseval identity suggests that, as the square norm of $\mathbf{f}$ and $\tilde{\mathbf{f}} = \mathbb{F}\mathbf{f}$ are equal, $\mathscr{L}^2(\mathscr{R})$ is also mapped onto *itself* under $\mathbb{F}$. This can be shown rigorously to be true. The Parseval identity (7.2) assures us that the Fourier operator $\mathbb{F}$ is *isometric* (i.e., angle and length preserving) in $\mathscr{C}_{\downarrow}^{\infty}$; moreover, as $\mathscr{L}^2(\mathscr{R})$ is a *Hilbert* space (Section 4.5), the domains of $\mathbb{F}$ and$\mathbb{F}^{\dagger} = \mathbb{F}^{-1}$ [the adjoint of an operator being defined as in (1.57)] are equal and characterize $\mathbb{F}$ as a *unitary* operator in $\mathscr{L}^2(\mathscr{R})$.

It is easy to see that $\mathscr{C}_{\downarrow}^{\infty} \subset \mathscr{L}^2(\mathscr{R})$, but further it can be proven that the first space is *dense* in the second. This is quite important and means that any $\mathbf{f} \in \mathscr{L}^2(\mathscr{R})$ can be approximated *in the norm* as close as desired by a sequence of functions which are elements of $\mathscr{C}_{\downarrow}^{\infty}$. The implication of denseness of one space in another is that certain operators defined in $\mathscr{C}_{\downarrow}^{\infty}$ can have their domains extended to $\mathscr{L}^2(\mathscr{R})$, much the in same way that one can extend continuous functions from the rationals to $\mathscr{R}$. Thus, although most of our results will be proven for functions in $\mathscr{C}_{\downarrow}^{\infty}$, their validity will extend to $\mathscr{L}^2(\mathscr{R})$.

Two more function spaces are important in the context of Fourier transforms. One is the space $\mathscr{L}^1(\mathscr{R})$ of absolutely integrable functions in the sense of Lebesgue. This is the space for which we proved the Fourier integral theorem *minus* the continuity conditions: Lebesgue integration allows us to disregard these. The image of $\mathscr{L}^1(\mathscr{R})$ under $\mathbb{F}$ does *not* coincide with $\mathscr{L}^1(\mathscr{R})$. Finally, there is the space of generalized functions which we denoted in Section 4.5 by $\mathscr{S}'$. The action of $\mathbb{F}$ on this space will appear in Section 7.3 when the Dirac δ on $\mathscr{R}$ is introduced.

Bringing up these notions—mere definitions and statements—from functional analysis may seem discouraging to the reader who is meeting Fourier transforms for the first time. He is urged to continue with the next few sections so as to get a better grasp of the Fourier pair of equations (7.1) by exploring its properties and applications. The development will be done with as little hairsplitting as necessary, with the assurance that (most of) the formal manipulations can be rigorously justified.

The existing bibliography is very wide. Functional analysis volumes such as those by Gel'fand *et al.* (1964–1968), Yoshida (1965), and Kato (1966) tackle the general structure of function spaces. Fourier analysis is in the foreground of several books, e.g., those by Titchmarsh (1937), Bochner and Chandrasekharan (1949), Sneddon (1951), Lighthill (1958), Bochner (1959),

Arsac (1966), and Butzer and Nessel (1971). The book by Dym and McKean (1972) proceeds with an agile pace through many areas of interest to physicists. The applied literature is equally solid: Carslaw and Jaeger (1947) and three books by Papoulis (1962, 1965, and 1977), to cite only a few. Further, most books on mathematical physics include at least one chapter on the subject of Fourier transforms. Classics which have been mentioned earlier are Whittaker and Watson (1903), Morse and Feshbach (1953), Courant and Hilbert (1953), and L. Schwartz (1966). A table of Fourier transforms of functions of practical use has been compiled by Oberhettinger (1973b).

7.2. Various Operators and Operations under Fourier Transformation

Given a function $f(q)$ and its Fourier transform $\tilde{f}(p) = (\mathbb{F}\mathbf{f})(p)$, we shall apply certain operators to the former—translation, differentiation, etc.—and explore the corresponding transformed operators as applied to the latter. Next, operations such as function multiplication and convolution will be studied. In this way, (a) we can find Fourier transforms of new functions in terms of known ones, and (b) we can study the ways in which the Fourier transform operator meshes with others. This will indicate the range of problems for which the Fourier transform becomes the natural solution tool.

7.2.1. Linear Combination

The first operation in the function vector space which comes to mind is that of linear combination of functions. Assume $f(q)$ and $g(q)$ have their corresponding Fourier transforms $\tilde{f}(p)$ and $\tilde{g}(p)$. Their linear combination $h(q) := af(q) + bg(q)$, $a, b \in \mathbb{C}$, quite obviously has $\tilde{h}(p) = a\tilde{f}(p) + b\tilde{g}(p)$ for its Fourier transform, as can be verified in a single line. The Fourier transformation is thus a *linear* operator:

$$\mathbb{F}(a\mathbf{f} + b\mathbf{g}) = a\mathbb{F}\mathbf{f} + b\mathbb{F}\mathbf{g}, \qquad \text{i.e.,} \quad \widetilde{(a\mathbf{f} + b\mathbf{g})}(p) = a\tilde{f}(p) + b\tilde{g}(p). \tag{7.24}$$

7.2.2. Powers of the Fourier Transformation

We can apply the Fourier transform *twice* as $[\mathbb{F}(\mathbb{F}\mathbf{f})](q)$. Assuming that $\mathbb{F}\mathbf{f}$ is in the domain of $\mathbb{F}$ [for spaces $\mathscr{C}_\downarrow^\infty$, $\mathscr{L}^2(\mathscr{R})$, or others mentioned in Section 7.1], it is not difficult to see, changing the sign of q' in (7.3), that we obtain

$$(\mathbb{F}^2\mathbf{f})(q) = f(-q) =: (\mathbb{I}_0\mathbf{f})(q), \qquad \text{i.e.,} \quad \tilde{\tilde{f}}(q) = f(-q), \tag{7.25}$$

where we have defined $\mathbb{I}_0 = \mathbb{I}_0^{-1}$ as the operator which *inverts* the real line through the origin. Note that $\mathbb{I}_0^2 = \mathbb{1}$ is the identity operator, and hence the Fourier operator is a *unitary fourth root* of the identity:

$$\mathbb{F}^4 = \mathbb{1}. \tag{7.26}$$

7.2.3. The Translation and Multiplication-by-Exponential Operators

The *translation* operator, defined by its action on an arbitrary function

$$(\mathbb{T}_y\mathbf{f})(q) \coloneqq f(q + y), \tag{7.27}$$

has the following property under Fourier transformation:

$$\begin{aligned}(\widetilde{\mathbb{T}_y\mathbf{f}})(p) &= \big(\mathbb{F}(\mathbb{T}_y\mathbf{f})\big)(p) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq(\mathbb{T}_y\mathbf{f})(q)\exp(-ipq)\\ &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dqf(q + y)\exp(-ipq)\\ &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq'f(q')\exp[-ip(q' - y)]\\ &= \exp(iyp)(\mathbb{F}\mathbf{f})(p) = \exp(iyp)\tilde{f}(p).\end{aligned} \tag{7.28}$$

[Compare with Eqs. (4.36).] If we define $\mathbb{E}_x$ as the operator which multiplies a function $f(q)$ by $\exp(ixq)$, i.e.,

$$(\mathbb{E}_x\mathbf{f})(q) \coloneqq \exp(ixq)f(q) \tag{7.29}$$

(where we remind the reader that q and p are dummy variables), we can write Eq. (7.28) as an operator equation,

$$\mathbb{F}\mathbb{T}_y = \mathbb{E}_y\mathbb{F}, \qquad \mathbb{F}\mathbb{T}_y\mathbb{F}^{-1} = \mathbb{E}_y, \tag{7.30}$$

valid when applied to any function in the common domain of the operators. It tells us, as does (7.28), that the Fourier transform of a translated function is $\exp(iyp)$ times the Fourier transform of the original function. Now

$$\mathbb{I}_0\mathbb{T}_y\mathbb{I}_0^{-1} = \mathbb{T}_{-y}, \qquad \mathbb{I}_0\mathbb{E}_x\mathbb{I}_0^{-1} = \mathbb{E}_{-x}, \tag{7.31}$$

which is proven applied to an arbitrary function. It follows thus that (7.30) can be written as

$$\mathbb{F}\mathbb{E}_y = \mathbb{T}_{-y}\mathbb{F}, \qquad \mathbb{F}\mathbb{E}_y\mathbb{F}^{-1} = \mathbb{T}_{-y}, \tag{7.32}$$

which states that the Fourier transform of an $f(q)$ times $\exp(iyq)$ equals the Fourier transform of $f(q)$ translated by $-y$. See Table 7.1.

Exercise 7.7. The translation operator $\mathbb{T}_y$ maps $\mathscr{L}^2(\mathscr{R})$ onto itself and fulfills $(\mathbb{T}_y\mathbf{f}, \mathbb{T}_y\mathbf{g}) = (\mathbf{f}, \mathbf{g})$. It is hence a *unitary* operator. Show that unitarity of $\mathbb{T}_y$ implies that of $\mathbb{E}_x$ by (7.30)–(7.32). Of course this can also be verified directly. Each set of operators (7.27) or (7.29) forms a one-parameter continuous *group* since $\mathbb{T}_y\mathbb{T}_{y'} = \mathbb{T}_{y+y'}$, $\mathbb{E}_x\mathbb{E}_{x'} = \mathbb{E}_{x+x'}$, and $\mathbb{T}_0 = \mathbb{1} = \mathbb{E}_0$.

Exercise 7.8. Show that

$$\mathbb{T}_y\mathbb{E}_x = \exp(ixy)\mathbb{E}_x\mathbb{T}_y. \tag{7.33}$$

This is the *Weyl commutation relation*. Its physical interpretation is one of the cornerstones of quantum mechanics [see Weyl (1928), and for the corresponding harmonic analysis, see Wolf (1975)].

7.2.4. The Dilatation Operator

We turn now to the *dilatation* operator, which we define as

$$(\mathbb{D}_a \mathbf{f})(q) := a^{-1/2} f(a^{-1}q), \qquad 0 < a \in \mathscr{R}. \tag{7.34}$$

[Compare with Eq. (4.44a), where a was constrained to be an integer; the change of scale by $a^{-1/2}$ has been kept here so that dilatation will be a unitary operation. See Exercise 7.9.] The Fourier transform of (7.34) is, by a change of variables involving a,

$$\begin{aligned}\widetilde{\mathbb{D}_a \mathbf{f}}(p) = \big(\mathbb{F}(\mathbb{D}_a \mathbf{f})\big)(p) &= (2\pi)^{-1/2} a^{-1/2} \int_{-\infty}^{\infty} dq f(a^{-1}q) \exp(-ipq) \\ &= (2\pi)^{-1/2} a^{1/2} \int_{-\infty}^{\infty} dq' f(q') \exp(-iapq') \\ &= \big(\mathbb{D}_{1/a}(\mathbb{F}\mathbf{f})\big)(p) = a^{1/2} \tilde{f}(ap).\end{aligned} \tag{7.35}$$

Hence the Fourier transform of a function dilated by a factor a is dilated by a factor of $1/a$. See the corresponding entry in Table 7.1, where the factor $a^{-1/2}$ in (7.34) is omitted. Thus as an operator equation,

$$\mathbb{F}\mathbb{D}_a = \mathbb{D}_{1/a}\mathbb{F}, \qquad \mathbb{F}\mathbb{D}_a\mathbb{F}^{-1} = \mathbb{D}_{1/a}. \tag{7.36}$$

In particular, $\mathbb{D}_1 = \mathbb{1}$.

Exercise 7.9. Show that the dilatation operators are *unitary*, i.e.,

$$(\mathbb{D}_a \mathbf{f}, \mathbb{D}_a \mathbf{g}) = (\mathbf{f}, \mathbf{g}), \tag{7.37}$$

mapping $\mathscr{L}^2(\mathscr{R})$ onto itself. They also form a one-parameter group since $\mathbb{D}_a\mathbb{D}_{a'} = \mathbb{D}_{aa'}$. Study the workings of (7.36) on the unit Gaussian (7.20).

Exercise 7.10. Consider the most general linear transformation of $\mathscr{R}$ as brought about by

$$(\mathbb{T}_y\mathbb{D}_a \mathbf{f})(q) = a^{-1/2} f(a^{-1}q + y) = (\mathbb{D}_a\mathbb{T}_{ay}\mathbf{f})(q). \tag{7.38}$$

Show that the set of all these operators forms a two-parameter group.

Exercise 7.11. Equation (7.38) implies the operator equation

$$\mathbb{T}_y\mathbb{D}_a = \mathbb{D}_a\mathbb{T}_{ay}. \tag{7.39a}$$

By multiplying both sides by $\mathbb{F}$ and $\mathbb{F}^{-1}$, show that

$$\mathbb{E}_x\mathbb{D}_a = \mathbb{D}_a\mathbb{E}_{a^{-1}x}. \tag{7.39b}$$

Exercise 7.12. Show that the Fourier transform of an even function [$f(-q) = f(q)$] is even, and that of an odd function [$f(-q) = -f(q)$] is odd.

Exercise 7.13. Show that if $f^*(q)$ is the function complex conjugate of $f(q)$ and if $\tilde{f}(p)$ is the latter's Fourier transform, the Fourier transform of the former will be

$$\widetilde{f^*}(p) = [\tilde{f}(-p)]^*. \tag{7.40}$$

In particular, if $f(q)$ is a real function of q, the real part of $\tilde{f}(p)$ will be even in p, while the imaginary part will be odd. Results of this kind are collected in Table 7.2.

7.2.5. Product and Convolution

We now turn to the subject of product and convolution of functions under Fourier transformation. The ordinary *product* of two functions is

$$(f \cdot g)(q) \coloneqq f(q)g(q), \qquad q \in \mathscr{R}, \tag{7.41}$$

while we define the *convolution* of $f(q)$ and $g(q)$ as

$$(f * g)(q) \coloneqq \int_{-\infty}^{\infty} dq' f(q')g(q - q') = \int_{-\infty}^{\infty} dq' f(q - q')g(q'), \qquad q \in \mathscr{R}. \tag{7.42}$$

The results we shall prove are that (a) the Fourier transform of the product of two functions equals $(2\pi)^{-1/2}$ times the convolution of their Fourier transforms and that (b) the Fourier transform of the convolution of two functions equals $(2\pi)^{1/2}$ times the product of their Fourier transforms. The operations (7.41) and (7.42) are thus mapped into each other under Fourier transformation.

The properties of integrability and continuity of the convolution will be collected after the proof of the preceding statements. For the moment we only have to assume that we can exchange the integration order in two following two equations. Statement (a) follows from

$$\begin{aligned}
\widetilde{f \cdot g}(p) &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f(q)g(q) \exp(-ipq) \\
&= (2\pi)^{-1} \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dp' \tilde{f}(p')g(q) \exp(ip'q) \exp(-ipq) \\
&= (2\pi)^{-1} \int_{-\infty}^{\infty} dp' \tilde{f}(p') \int_{-\infty}^{\infty} dq g(q) \exp[-i(p - p')q] \\
&= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp' \tilde{f}(p')\tilde{g}(p - p') = (2\pi)^{-1/2}(\tilde{f} * \tilde{g})(p),
\end{aligned} \tag{7.43a}$$

i.e.,

$$\mathbb{F}(\mathbf{f} \cdot \mathbf{g}) = (2\pi)^{-1/2}(\mathbb{F}\mathbf{f}) * (\mathbb{F}\mathbf{g}), \tag{7.43b}$$

while statement (b) is proven similarly by exchanging f and $\tilde{f}$, etc., and inverting the sign of the exponentials, leading to

$$\widetilde{f * g}(p) = (2\pi)^{1/2}\tilde{f}(p)\tilde{g}(p) \tag{7.44a}$$

$$\mathbb{F}(\mathbf{f} * \mathbf{g}) = (2\pi)^{1/2}(\mathbb{F}\mathbf{f})\cdot(\mathbb{F}\mathbf{g}). \tag{7.44b}$$

[These formulas are the analogues of Eqs. (3.6) and (3.8) for finite Fourier transforms and of Eqs. (4.59) and (4.61) for Fourier series. See Table 7.1.] In Part II we saw that convolution "smooths" functions. This is the case here too. Some results on convolution are the following: (a) If $\mathbf{f}, \mathbf{g} \in \mathscr{L}^2(\mathscr{R})$, their convolution (7.42) exists at every $q \in \mathscr{R}$, is bounded since

$$|(f * g)(q)| \leqslant \|\mathbf{f}\| \, \|\mathbf{g}\|, \tag{7.45}$$

is *uniformly continuous*, and tends toward zero for $|q| \to \infty$. [The convolution need not be in $\mathscr{L}^2(\mathscr{R})$; compare with (3.9)–(3.10) and with (4.70a).] (b) If $\mathbf{f} \in \mathscr{L}^1(\mathscr{R})$ and $\mathbf{g}$ is bounded, $g(q) \leqslant \gamma$, then their convolution (7.42) exists at every q, is bounded since

$$|(f * g)(q)| \leqslant \gamma \int_{-\infty}^{\infty} dq' |f(q')|, \tag{7.46}$$

and is uniformly continuous. (c) If $\mathbf{f} \in \mathscr{L}^1(\mathscr{R})$ and $g(q)$ is uniformly continuous either in $\mathscr{L}^1(\mathscr{R})$ or in $\mathscr{L}^2(\mathscr{R})$, then so will be, correspondingly, their convolution. (d) If $\mathbf{f} \in \mathscr{C}^\infty$ and $\mathbf{g}$ is such that $(f * g)(q)$ is finite for all finite q, then $\mathbf{f} * \mathbf{g} \in \mathscr{C}^\infty$. Other properties are given in Exercise 7.15.

Exercise 7.14. Prove the relation between convolution and inner product.

$$(f * g)(q) = (\mathbf{f}^*, \mathbb{T}_q \mathbb{I}_0 \mathbf{g}) = (\tilde{\mathbf{f}}^*, \mathbb{E}_{-q}\tilde{\mathbf{g}}), \tag{7.47}$$

where $\mathbf{f}^*$ represents the function $[f(q)]^*$. This is the analogue of Eq. (4.71) and reduces the proof of (7.45) to the Schwartz inequality. The proof of the uniform continuity of the convolution requires a form of the triangle inequality using (7.47) for $\mathbb{T}_q$ and $\mathbb{T}_{q+\varepsilon}$ for small, arbitrary $\varepsilon > 0$. Proofs for the other statements can be found in the literature. See Dym and McKean (1972).

Exercise 7.15. Prove the following properties of the convolution: (a) commutativity, $\mathbf{f} * \mathbf{g} = \mathbf{g} * \mathbf{f}$; (b) associativity, $\mathbf{f} * (\mathbf{g} * \mathbf{h}) = (\mathbf{f} * \mathbf{g}) * \mathbf{h}$; and (c) distributivity, $\mathbf{f} * (a\mathbf{g} + b\mathbf{h}) = a\mathbf{f} * \mathbf{g} + b\mathbf{f} * \mathbf{h}$.

Exercise 7.16. Show that the convolution between an arbitrary function $f(q)$ and the rectangle function (7.4) of unit area ($\eta = 1/\varepsilon$) is the *ε-smoothed* function

$$(f * R^{(\varepsilon, 1/\varepsilon)})(q) = \varepsilon^{-1} \int_{q-\varepsilon/2}^{q+\varepsilon/2} dq' f(q'). \tag{7.48}$$

Exercise 7.17. A function can be "cut" between $-\varepsilon/2$ and $\varepsilon/2$ by multiplication with the rectangle function of unit height. Show that the Fourier transform of the cut function, using (7.5), will be

$$\widetilde{f \cdot R^{(k,1)}}(p) = 2\pi^{-1} \int_{-\infty}^{\infty} dp' \tilde{f}(p - p') p'^{-1} \sin(p'k/2). \tag{7.49}$$

Comparison with (7.14) for the limit $k \to \infty$ should be suggestive.

Exercise 7.18. Show that the convolution of two Gaussian functions (7.20) is a Gaussian, viz.,

$$(G_\omega * G_{\omega'})(q) = G_{\omega+\omega'}(q). \tag{7.50}$$

Compare with Eq. (5.11).

7.2.6. Differentiation

We shall now analyze the relationship between differentiation and Fourier transformation. Assume that a function $f(q)$ and its derivative $f'(q) := df(q)/dq$ satisfy the conditions of the Fourier integral theorem. The transform of the latter will be

$$\begin{aligned} \widetilde{f'}(p) &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f'(q) \exp(-ipq) \\ &= (2\pi)^{-1/2} \left[f(q) \exp(-ipq) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dq f(q) \frac{d}{dq} \exp(-ipq) \right] \\ &= ip\tilde{f}(p). \end{aligned} \tag{7.51}$$

Here we have integrated by parts, used the fact that the Fourier integral theorem requires $f(q) \to 0$ for $|q| \to \infty$ in order to eliminate the constant term, and recognized $\tilde{f}(p)$ in the final expression. By repeated application of (7.51) we can state that if the functions involved satisfy the conditions of the Fourier integral theorem, then

$$\widetilde{f^{(n)}}(p) = (ip)^n \tilde{f}(p), \tag{7.52}$$

i.e., the Fourier transform of the nth derivative of a function is $(ip)^n$ times the Fourier transform of the original function.

This relation is quite symmetric. If we search for the Fourier transform of $(-iq)^m f(q)$, this will be

$$\begin{aligned} &(2\pi)^{-1/2} \int_{-\infty}^{\infty} dq (-iq)^m f(q) \exp(-ipq) \\ &\qquad = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq f(q) \frac{d^m}{dp^m} \exp(-ipq). \end{aligned} \tag{7.53}$$

That is,

$$\widetilde{(-iq)^m f(p)} = \frac{d^m}{dp^m}\tilde{f}(p); \tag{7.54}$$

the *inverse* Fourier transform of the mth derivative of a function is $(-iq)^m$ times the inverse transform of the function.

7.2.7. The Operators $\mathbb{Q}$ and $\mathbb{P}$

Equation (7.54) is a rather clumsy way of writing a result as the variables q and p must be explicitly referred to as the arguments of f and $\tilde{f}$. To improve the notation we shall introduce the operator $\mathbb{Q}$ whose role is to multiply the function it is acting upon by its argument, i.e.,

$$(\mathbb{Q}\mathbf{f})(z) \coloneqq zf(z), \tag{7.55}$$

where z may be q, p, or any other dummy variable. Similarly, letting

$$(\mathbb{P}\mathbf{f})(z) \coloneqq -i\frac{d}{dz}f(z) \tag{7.56}$$

represent $-i$ times the operator of differentiation, we can put Eqs. (7.52) and (7.54) in operator form as

$$\mathbb{F}\mathbb{P} = \mathbb{Q}\mathbb{F}, \qquad \mathbb{F}\mathbb{Q} = -\mathbb{P}\mathbb{F}, \tag{7.57a}$$

respectively; that is,

$$\mathbb{F}\mathbb{P}\mathbb{F}^{-1} = \mathbb{Q}, \qquad \mathbb{F}\mathbb{Q}\mathbb{F}^{-1} = -\mathbb{P}. \tag{7.57b}$$

Similarity transformation by $\mathbb{F}$ thus turns $\mathbb{P}$ into $\mathbb{Q}$ and conversely with a minus sign.

It requires only one line to prove that $\mathbb{Q}$ and $\mathbb{P}$ are *hermitian* operators: For functions $f(q)$, $g(q)$ such that $qf(q)g(q)$ is integrable,

$$(\mathbf{f}, \mathbb{Q}\mathbf{g}) = \int_{-\infty}^{\infty} dq f(q)^* q g(q) = (\mathbb{Q}\mathbf{f}, \mathbf{g}), \tag{7.58a}$$

while if they are differentiable functions whose derivatives are in $\mathscr{L}^2(\mathscr{R})$, integration by parts yields

$$(\mathbf{f}, \mathbb{P}\mathbf{g}) = -i\int_{-\infty}^{\infty} dq f(q)^* \frac{d}{dq} g(q) = -if(q)^* g(q)\Big|_{-\infty}^{\infty}$$
$$+ i\int_{-\infty}^{\infty} dq \left[\frac{d}{dq}f(q)\right]^* g(q) = (\mathbb{P}\mathbf{f}, \mathbf{g}). \tag{7.58b}$$

For both operators one can find *extensions* in the domain which turn these into *self-adjoint* operators. Some of the relevant properties of these operators

—possibility of exponentiation into unitary operators and existence of a complete basis of generalized eigenvectors—were sketched in Section 4.5.

A further important property of the operators of differentiation and multiplication by the argument is their *commutator*:

$$[(\mathbb{Q}\mathbb{P} - \mathbb{P}\mathbb{Q})\mathbf{f}](z) = \left(-i\mathbb{Q}\frac{d}{dz} - \mathbb{P}z\right)f(z)$$

$$= \left(-iz\frac{d}{dz} + i\frac{d}{dz}z\right)f(z) = if(z); \qquad (7.59a)$$

that is,

$$[\mathbb{Q}, \mathbb{P}] \coloneqq \mathbb{Q}\mathbb{P} - \mathbb{P}\mathbb{Q} = i\mathbb{1}. \qquad (7.59b)$$

A pair of self-adjoint operators with the properties (7.57) and (7.59) are said to be *canonically conjugate*. Later on we shall study the various consequences of these simple relations. The appropriate physical interpretation of these equations is one of the cornerstones of quantum mechanics, where $\mathbb{Q}$ and $\hbar\mathbb{P}$ are the position and momentum operators, $\hbar$ being Planck's constant h divided by 2π. Equation (7.59b) is the *Heisenberg commutation relation.*

Exercise 7.19. Show that from (7.57) it follows that

$$\mathbb{F}S(\mathbb{Q}, \mathbb{P})\mathbb{F}^{-1} = S(-\mathbb{P}, \mathbb{Q}), \qquad (7.60)$$

where $S(\mathbb{Q}, \mathbb{P})$ is any polynomial or series function of $\mathbb{Q}$ and $\mathbb{P}$ which specifies the order of the entries in its expansion.

7.2.8. Example: Free-Fall Schrödinger Equation

In some instances, the property (7.60) allows one to reduce the degree of a differential operator and simplify the process of finding a solution. Consider the second-order differential equation whose explicit form is

$$\mathbb{H}'\psi(q) \coloneqq (\tfrac{1}{2}\mathbb{P}^2 + \mathbb{Q})\psi(q) = \left(-\tfrac{1}{2}\frac{d^2}{dq^2} + q\right)\psi(q) = 0. \qquad (7.61)$$

Application of $\mathbb{F}$ on the left and (7.60) lead to

$$(\tfrac{1}{2}\mathbb{Q}^2 - \mathbb{P})\tilde{\psi}(p) = \left(\tfrac{1}{2}p^2 + i\frac{d}{dp}\right)\tilde{\psi}(p) = 0. \qquad (7.62)$$

The last two members of (7.62) are the transformed, simplified equation which, being of first order, can be immediately solved as

$$\tilde{\psi}(p) = c\exp(ip^3/6), \qquad c \in \mathscr{C}. \qquad (7.63)$$

Now the inverse Fourier transform of (7.63) yields a solution to (7.61) as

$$\psi(q) = c(2\pi)^{-1/2}\int_{-\infty}^{\infty} dp\exp(ip^3/6 - ipq) =: c(2\pi)^{1/2}2^{1/3}\,\mathrm{Ai}\,(2^{1/3}q). \qquad (7.64)$$

The integral in (7.64) is not trivial. It is known in the literature as Airy's integral and gives rise to the Airy function Ai(z) (see Appendix B). It is related to the Bessel function of order $\frac{1}{3}$. Note that the Fourier transform method served to find the solution in spite of the fact that $\tilde{\psi}(p)$ is neither in $\mathscr{L}^2(\mathscr{R})$ nor in $\mathscr{L}^1(\mathscr{R})$. In Fig. B.3 we show a plot of the Airy function. It decreases exponentially for $q > 0$ and oscillates increasingly faster for $q < 0$. The *second* solution of Airy's differential equation (7.61), the Bi(z) function, *increases* faster than $\exp z$ for $z > 0$ but does not appear in (7.62). Actually, quite ordinary-looking differential equations possess generalized function solutions which, we may surmise, lead to linearly independent solutions. Equation (7.61) is related to the free-fall (or *linear* potential) quantum Schrödinger Hamiltonian, which will be further investigated in Sections 8.5 and 10.1.

Exercise 7.20. Regarding the commutator symbol defined in (7.59b), show that for any three linear operators $\mathbb{A}$, $\mathbb{B}$, $\mathbb{C}$ with a common domain the commutator is *distributive* with respect to linear combination,

$$[\mathbb{A}, b\mathbb{B} + c\mathbb{C}] = b[\mathbb{A}, \mathbb{B}] + c[\mathbb{A}, \mathbb{C}], \tag{7.65}$$

and that a *Leibnitz rule* of sorts holds:

$$[\mathbb{A}, \mathbb{B}\mathbb{C}] = [\mathbb{A}, \mathbb{B}]\mathbb{C} + \mathbb{B}[\mathbb{A}, \mathbb{C}]. \tag{7.66}$$

Exercise 7.21. Show that the commutator of $\mathbb{Q}^m$ and $\mathbb{P}^n$ is

$$[\mathbb{Q}^m, \mathbb{P}^n] = -\sum_{k=1}^{\min(m,n)} \binom{m}{k}\binom{n}{k} k!(-i)^k \mathbb{Q}^{m-k}\mathbb{P}^{n-k}, \tag{7.67}$$

where $\binom{m}{k} = m!/(m-k)!\,k!$ is the binomial coefficient. This can be done by induction, first on m and then on n, using the basic Heisenberg commutation relation (7.59b) and the Leibnitz rule (7.66).

7.2.9. Integration

The validity of Eq. (7.52) can be extended to negative indices, i.e., to integration $f^{(-1)}(x) \coloneqq \int_c^x dx' f(x')$, as long as the new function is also integrable. For this it is necessary that $\tilde{f}(0) = 0$, which means that the definite integral $\int_{-\infty}^{\infty} dx f(x)$ vanishes. In this case, if $f(q)$ satisfies the conditions of the Fourier integral theorem, $f^{(-1)}(q)$ will do so as well.

7.2.10. Differentiability and Asymptotic Behavior under Fourier Transformation

Repeated differentiation of a function $f(q)$ with Fourier transform $\tilde{f}(p)$ may, as Eq. (7.52) suggests, eventually produce a function whose Fourier transform $\widetilde{f^{(n)}}(p)$ fails to be integrable because of the growing factor $(ip)^n$. In that case, although (7.52) may still be formally written, it ceases to be the

Fourier transform of an ordinary function. Because of (7.1a), the latter would have to be the improper integral of a growing function.

Deferring the introduction of such divergent integrals until Section 7.3, we can look closer at those functions $f(q)$ which are n times differentiable and whose asymptotic behavior is that of a negative power m of the argument. One such result can be easily proven. Assume $f(q)$ and $q^m d^n f(q)/dq^n$ belong to $\mathscr{L}^2(\mathscr{R})$. If this holds, it also follows that $q^r d^s f(q)/dq^s \in \mathscr{L}^2(\mathscr{R})$ for $0 \leqslant r \leqslant m$ and $0 \leqslant s \leqslant n$. As all these functions have finite norm, we can use the Parseval identity and triangle inequality in writing

$$\begin{aligned} \|\mathbb{Q}^n\mathbb{P}^m\tilde{\mathbf{f}}\| &= \|\mathbb{F}^{-1}\mathbb{Q}^n\mathbb{P}^m\tilde{\mathbf{f}}\| = \|\mathbb{P}^n\mathbb{Q}^m\mathbf{f}\| = \|(\mathbb{Q}^m\mathbb{P}^n - [\mathbb{Q}^m, \mathbb{P}^n])\mathbf{f}\| \\ &\leqslant \|\mathbb{Q}^m\mathbb{P}^n\mathbf{f}\| + \|[\mathbb{Q}^m, \mathbb{P}^n]\mathbf{f}\| < \infty, \end{aligned} \tag{7.68}$$

where we have used the commutator (7.67) of $\mathbb{Q}^m$ and $\mathbb{P}^n$, noting that it involves only powers of $\mathbb{Q}$ and $\mathbb{P}$ which are less than m and n. Hence *if* $f(q)$ *and* $q^m d^n f(q)/dq^n \in \mathscr{L}^2(\mathscr{R})$, *it follows that* $p^r d^s \tilde{f}(p)/dp^s \in \mathscr{L}^2(\mathscr{R})$ *for* $0 \leqslant r \leqslant n$ *and* $0 \leqslant s \leqslant m$. The converse of this result is a consequence of exchanging f and $\tilde{f}$ in (7.68).

If in the preceding result we let m and n be arbitrarily large and note that $\mathscr{L}^2(\mathscr{R})$ functions must vanish asymptotically, we can validate the statement that the Fourier transformation maps $\mathscr{C}_\downarrow^\infty$ onto itself.

7.2.11. Hyperdifferential Form for the Translation Operator

We shall now proceed to show some operator identities involving the Fourier transformation, translations, multiplications, dilatation, and differentiation. We shall work in a naïve way on a space of $\mathscr{C}_\downarrow^\infty$ functions which have convergent Taylor expansions and whose Fourier transforms have the same properties. The results are valid—in the appropriately generalized sense—for other function spaces as well.

We show first that [as for Fourier series in (4.124)],

$$\mathbb{T}_y = \exp(iy\mathbb{P}) \coloneqq \sum_{n=0}^{\infty} \frac{(iy)^n}{n!} \mathbb{P}^n. \tag{7.69}$$

This can be proven by writing out the Taylor expansion of $f(q + y)$ around q and isolating the operator acting on $f(q)$. We can follow an alternative proof as, clearly,

$$\exp(ix\mathbb{Q})f(q) \coloneqq \sum_{n=0}^{\infty} \frac{(ix)^n}{n!} \mathbb{Q}^n f(q) = \exp(ixq)f(q) =: \mathbb{E}_x f(q). \tag{7.70}$$

Now, by applying $\mathbb{F}$ to the left of this equation and using (7.30) and (7.32) for $\mathbb{E}_x$ and $\mathbb{T}_x$ or (7.57) and (7.60) for $\mathbb{Q}$ and $\mathbb{P}$, Eq. (7.69) follows from (7.70) for $y = -x$.

7.2.12. Hyperdifferential Form for the Dilatation Operator

One new hyperdifferential relation is that of the dilatation operator (7.34). We state that

$$\mathbb{D}_a = \exp[-i \ln a \cdot \tfrac{1}{2}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q})], \qquad a > 0. \tag{7.71}$$

To prove this assertion, we apply it first to the function q^k, recalling that $q\, dq^k/dq = kq^k$. Expanding the exponential series and using (7.59) for the exponent, we can write

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{(-i \ln a)^n}{n!} (\mathbb{Q}\mathbb{P} - i/2)^n q^k &= \exp(-\tfrac{1}{2} \ln a) \sum_{n=0}^{\infty} \frac{(-\ln a)^n}{n!} \left(q \frac{d}{dq}\right)^n q^k \\ &= a^{-1/2} \sum_{n=0}^{\infty} \frac{(-\ln a)^n}{n!} k^n q^k \\ &= a^{-1/2} \exp(-k \ln a) q^k = a^{-1/2}(a^{-1}q)^k.\end{aligned} \tag{7.72}$$

The result (7.71) is thus proven for monomials q^k. Expanding any analytic function in q as its Taylor series implies the validity of (7.71) for the space of functions where the series involved converge.

Exercise 7.22. Verify (7.36) using (7.71) and (7.60).

Exercise 7.23. Detail the validity of (7.71) for $a < 0$. It is clearest to work in the complex a-plane and see that no multivaluedness appears in the final result.

7.2.13. Convolution Operators

Assume $S(\mathbb{P})$ is an operator function of $\mathbb{P}$ defined in terms of a formally convergent series. We saw that $S = \exp$ had the rather simple effect of translation on functions $f(q)$. What about other such functions? We can write, using (7.60) and (7.44b)

$$\begin{aligned}S(\mathbb{P})\mathbf{f} = \mathbb{F}^{-1}[\mathbb{F}S(\mathbb{P})\mathbb{F}^{-1}]\mathbb{F}\mathbf{f} = \mathbb{F}^{-1}S(\mathbb{Q})\mathbb{F}\mathbf{f} = \mathbb{F}^{-1}(\mathbf{S} \cdot \mathbb{F}\mathbf{f}) \\ = (2\pi)^{-1/2}(\mathbb{F}^{-1}\mathbf{S}) * \mathbf{f}.\end{aligned} \tag{7.73}$$

The action of $S(\mathbb{P})$ on a function $\mathbf{f}$ is easiest to write down after Fourier transformation, as $S(\mathbb{Q})$ only multiplies the function $\tilde{f}(p)$ by the function $S(p)$. The inverse Fourier transform of this product of functions is thus $(2\pi)^{1/2}$ times the inverse Fourier transform of the function $\mathbf{S}$ in convolution over q with $\mathbf{f}$.

7.2.14. Gaussian Operator

As an example to be used later in connection with the time evolution of the solutions of the diffusion equation, consider the *Gaussian operator*, which we define as

$$\mathbb{G}_\omega := \exp(-\tfrac{1}{2}\omega\mathbb{P}^2) = (2\pi/\omega)^{1/2}G_{1/\omega}(\mathbb{P}). \tag{7.74}$$

Equation (7.73) together with the property that the Gaussian function be proportional to its own Fourier transform [Eq. (7.22)] leads to

$$\begin{aligned}(\mathbb{G}_\omega\mathbf{f})(q) &= (2\pi/\omega)^{1/2}[G_{1/\omega}(\mathbb{P})\mathbf{f}](q) = (\mathbf{G}_\omega * \mathbf{f})(q)\\ &= (2\pi\omega)^{-1/2}\int_{-\infty}^{\infty} dq'\exp[-(q-q')^2/2\omega]f(q'). \end{aligned}\tag{7.75}$$

7.2.15. Solution of Inhomogeneous Differential Equations and Green's Functions

A second example of the use of (7.73) which reaches a broad range of applications refers to the solution of inhomogeneous differential equations with constant coefficients,

$$[U(\mathbb{P})\mathbf{f}](q) := \sum_n c_n \frac{d^n}{dq^n}f(q) = \varphi(q), \tag{7.76}$$

where $\varphi(q)$ may be a constant—in case (7.76) is, for instance, a step in the solution of a partial differential equation—or a *source* function representing input of heat into a system. The operator on the left-hand side can involve terms with negative values of n representing indefinite integration. Equation (7.76) thus has the structure

$$U(\mathbb{P})f(q) = \varphi(q), \qquad U(z) = \sum_n c_n(iz)^n, \tag{7.77}$$

where the $\varphi(q)$ is known and fixed and $f(q)$ is to be found. Formally, we can divide by $U(\mathbb{P})$, call $S(\mathbb{P}) := [U(\mathbb{P})]^{-1}$, and use (7.73) for $\boldsymbol{\varphi}$ replacing $\mathbf{f}$. We shall do this explicitly: the Fourier transform of (7.76) is

$$[\mathbb{F}U(\mathbb{P})\mathbf{f}](p) = [U(\mathbb{Q})\tilde{\mathbf{f}}](p) = \sum_n c_n(ip)^n\tilde{f}(p) = \tilde{\varphi}(p). \tag{7.78}$$

Hence

$$\tilde{f}(p) = \tilde{\varphi}(p)\Big/\sum_n c_n(ip)^n \tag{7.79}$$

is the Fourier transform of the solution. To recover the latter, we apply the inverse transform, thus expressing $f(q)$ as a *convolution* of the inhomogeneous part $\varphi(q)$ of the equation with a kernel:

$$f(q) = (\mathbf{V} * \boldsymbol{\varphi})(q), \tag{7.80a}$$

$$V(q) = (2\pi)^{-1}\int_{-\infty}^{\infty} dp\Big[\sum_n c_n(ip)^n\Big]^{-1}\exp(ipq) = (2\pi)^{-1/2}(\mathbb{F}^{-1}\mathbf{U}^{-1})(q). \tag{7.80b}$$

This is Eq. (7.73) with φ for f and U^{-1} for S. The actual calculation of $V(q)$ may require more techniques than we have at this point: the function U, usually a polynomial, can have roots on the real axis, forcing us to run the integration over a set of poles. The formal solution (7.80) is presented for the moment as a general strategy to be followed. Some tactics will be given in Section 7.4.

7.2.16. Domain Distinctions for Hyperdifferential and Integral Operators

Various features in the above equations may seem perplexing. Hyperdifferential operators $S(\mathbb{P})$, as such, can be properly applied only to infinitely differentiable functions (and even then questions about convergence may arise). Yet the last member of (7.73) and certainly the examples (7.75) and (7.77) tell us that in its *integral form*, if the operator *kernel* $(\mathbb{F}^{-1}\mathbf{S})(q)$ is a "decent" function, the domain of the operator $S(\mathbb{P})$ can include discontinuous functions and in fact need not even be constrained to integrable or $\mathscr{L}^2(\mathscr{R})$ functions. [See, in retrospect, Eqs. (4.99) and (4.100).] It is sufficient that the convolution integral exist. The question is, then, what is the domain of definition of the operators? If the "ordinary" forms (7.27), (7.34), or (7.75) are used to define the translation, dilatation, and Gaussian operators, their domain includes all functions in $\mathscr{L}^2(\mathscr{R})$ (and of course, much larger classes such as the *generalized* function of Section 7.3), while if the hyperdifferential forms (7.69), (7.71), and (7.74) are used, the domain is restricted at least to $\mathscr{C}_{\downarrow}^{\infty}$ functions (although other $\mathscr{C}^{\infty}$-spaces may be proposed). The two sets of definitions lead, rigorously, to *different* operators. By abuse of notation we have employed the same symbol for both. This has been for economy rather than through carelessness, however, since one can show—it

Table 7.1 A Function and Its Fourier Transform under Various Operators and Operations

Operation	$f(q)$	$\tilde{f}(p)$
Linear combination	$af(q) + bg(q)$	$a\tilde{f}(p) + b\tilde{g}(p)$
Translation	$f(q + y)$ $\exp(-ixq)f(q)$	$\exp(iyp)\tilde{f}(p)$ $\tilde{f}(p + x)$
Dilatation	$f(aq)$	$a^{-1}\tilde{f}(p/a)$
Complex conjugation	$f(q)^*$	$\tilde{f}(-p)^*$
Multiplication	$f(q)g(q)$	$(2\pi)^{-1/2}(\tilde{f} * \tilde{g})(p)$
Convolution	$(f * g)(q)$	$(2\pi)^{1/2}\tilde{f}(p)\tilde{g}(p)$
Differentiation	$d^n f(q)/dq^n$ $(-iq)^n f(q)$	$(ip)^n\tilde{f}(p)$ $d^n\tilde{f}(p)/dp^n$

Table 7.2 Relation between Some Properties of a Function and Those of Its Fourier Transform

Property	$f(q)$	$\tilde{f}(p)$
Parity	Even Odd	Even Odd
Complex conjugation	Real Imaginary	$\tilde{f}(-p)^* = \tilde{f}(p)$ $\tilde{f}(-p)^* = -\tilde{f}(p)$
Differentiability and decrease	$q^r d^s f(q)/dq^s \in \mathscr{L}^2(\mathscr{R})$, $0 \leqslant r \leqslant m, 0 \leqslant s \leqslant n$	$p^s d^r \tilde{f}(p)/dp^r \in \mathscr{L}^2(\mathscr{R})$, $0 \leqslant s \leqslant n, 0 \leqslant r \leqslant m$
Positivity	Positive: $f(q) > 0, q \in \mathscr{R}$	Positive definite: $\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \tilde{f}(p - p')\phi(p)^*\phi(p') > 0$
Support (Section 7.4)	$f(q) = 0, q < a$	$\lvert\tilde{f}(p)\rvert \leqslant C \exp(-a\lvert\operatorname{Im} p\rvert)$; $\tilde{f}(p)$ entire analytic in $\operatorname{Im} p < 0$ half-plane
	$f(q) = 0, q > b$	$\lvert\tilde{f}(p)\rvert \leqslant C' \exp(b \operatorname{Im} p)$; $\tilde{f}(p)$ entire analytic in $\operatorname{Im} p > 0$ half-plane
	$f(q) = 0, q \notin [a, b]$	$\tilde{f}(p)$ entire analytic on the whole complex p-plane

has been mentioned before in Section 4.5—that $\mathscr{C}_{\downarrow}^{\infty}$ is *dense* in the space $\mathscr{S}'$ of generalized functions. One can always contrive sequences of $\mathscr{C}_{\downarrow}^{\infty}$ functions $\{f_n(q)\}_{n=1}^{\infty}$ such that $\lim_{n\to\infty}(\mathbf{g}, \mathbf{f}_n) = (\mathbf{g}, \mathbf{f})$, where $\mathbf{f} \in \mathscr{S}'$ and $\mathbf{g}$ is any "test" function in an appropriate space $\mathscr{S}$. *Extending* the domain of the hyperdifferential forms amounts to adding the limit points of all these sequences and thus arriving at the domain of the integral operator forms. The two forms are thus *weakly* equivalent. Certain manipulations and proofs will be easier on one or another form. The Fourier transform, as a prime example, has been given by an integral form [Eq. (7.1b)]. We shall see below that it also has a differential realization.

Exercise 7.24. The Gaussian operators (7.74) have the manifest property of multiplying as

$$\mathbb{G}_{\omega}\mathbb{G}_{\omega'} = \mathbb{G}_{\omega+\omega'}, \qquad \mathbb{G}_0 = \mathbb{1}. \tag{7.81}$$

Using the associativity of operators and of the convolution product (Exercise 7.15), you can show rather trivially that the Gaussian convolution relation (7.50) holds.

Exercise 7.25. The multiplication of Gaussian hyperdifferential operators (7.81) is formally valid for all $\omega, \omega' \in \mathscr{R}$, telling us that these form a one-parameter continuous *group* of operators. Yet, in their integral form (7.75), only $\mathbb{G}_{\omega}$ for $\omega > 0$ can be applied to $\mathscr{L}^1(\mathscr{R})$ functions. Excluding the case $\omega = 0$, show that *on* $\mathscr{L}^1(\mathscr{R})$ the set of integral operators (7.75) forms a *semigroup*.

Exercise 7.26. Show that if a function $f(q)$ is *positive* [i.e., $f(q) > 0$ for all $q \in \mathscr{R}$] then its Fourier transform $\tilde{f}(p)$ is *positive definite*, i.e.,

$$\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \tilde{f}(p - p')\varphi(p)^*\varphi(p') > 0 \tag{7.82}$$

for all $\varphi(p) \in \mathscr{L}^2(\mathscr{R})$. This can be proven by writing $\tilde{\mathbf{f}}$ as the Fourier transform of $\mathbf{f}$ and exchanging integrals. This result and its converse constitute *Bochner's theorem*. Compare with Exercises 1.19 and 4.6 for Fourier finite transforms and series.

7.3. The Dirac δ and the Green's Function for a System

The Dirac δ, as a generalized function, has already appeared in Section 4.5 in relation to spaces of periodic functions of period 2π. Here, a parallel Dirac δ will be introduced as a generalized function on the full real line. Most concepts developed here will thus have their analogues for spaces of periodic functions, but some will be new. We show that the Green's function of a system governed by a differential equation is the solution of the inhomogeneous version of that equation where the inhomogeneous part is a Dirac δ.

7.3.1. Three Function Sequences and a Limit

Among the functions we have worked with, we shall select three whose common properties merit that we place them under the same symbol. These are the rectangle function (7.4), its Fourier transform (7.5), and the Gaussian bell function (7.20). We denote them by

$$\delta^k(q) \coloneqq \tilde{R}^{[k,(2\pi)^{-1/2}]}(q) = (\pi q)^{-1} \sin(kq/2), \qquad R^{(1/k,k)}(q), \qquad G_{1/k}(q). \tag{7.83}$$

They are all real and even and enclose unit area. See Figs. 7.1 and 7.2. When we examine the *convolution* of (7.83) with an arbitrary continuous function $f(q)$ we obtain, for every k, a function

$$f^k(q) \coloneqq \int_{-\infty}^{\infty} dq' f(q - q')\delta^k(q'). \tag{7.84}$$

Now, upon letting k grow without bound, we assert that we reproduce the original function: $\lim_{k\to\infty} f^k(q) = f(q)$. Indeed, for the Fourier transform of the rectangle function in (7.83), the limit of (7.84) is the content of the Fourier integral theorem given in Section 7.1. Equation (7.14), in particular, for $y = -q'$ and $c = q$ is the desired expression for q a point of continuity of the function, together with the ensuing discussion on the extension of the result on $\int_a^b$ to $\int_{-\infty}^{\infty}$. For the rectangle and Gaussian function in (7.83) we can use the mean value theorem. For the former this is just (7.48) since $k = 1/\varepsilon \to \infty$, while for the latter, since $\lim_{k\to\infty} G_{1/k}(q) = 0$ for $q \neq 0$, integration limits $q \pm \varepsilon'$ similar to the former can be found such that the integral $\int_{q-\varepsilon'}^{q+\varepsilon'}$ approximates $\int_{-\infty}^{\infty}$ as closely as desired. As $k \to \infty$, $\varepsilon' \to 0$, and (7.21) ensures that in (7.84) $f(q)$ is regained.

[We have followed the presentation of the limit of (7.83) in complete analogy with that of Fourier series in (4.75) up to the choice of sequences, $\tilde{R}$ being the analogue of the Dirichlet kernel and the Gaussian being the counterpart of the Jacobi theta function. Convolution rather than translated inner product only was chosen here for convenience.]

7.3.2. The Dirac δ Symbol

We shall introduce the symbol of the Dirac δ on $\mathscr{R}$,

$$\lim_{k\to\infty} \delta^k(q) =: \delta(q), \tag{7.85}$$

adding that the interpretation is, as in (4.79), that the limit is to be taken outside the integral under which the $\delta^k(q)$ are placed in company with a continuous *test* function $f(q)$. The Dirac δ and several other symbols with similar definition are said to be *generalized functions*, since they obey many

of the formal manipulations usually associated with ordinary functions, as will be seen below. As a symbol, the main property of the Dirac δ is

$$\int_{-\infty}^{\infty} dq' f(q')\delta(q - q') = (f * \delta)(q) = f(q) \tag{7.86}$$

for any continuous $f(q)$. It is thus the *reproducing kernel* for (Lebesgue) integration and acts as a "unit function" for the operation of convolution (see Exercise 7.15). Note that (7.85)–(7.86) is consistent for function sequences (7.83) whether or not $f(q)$ is absolutely integrable. Also, it is not necessary that $\lim_{k\to\infty} \delta^k(q) = 0$ for $q \neq 0$ (as it is sometimes stated when introducing the Dirac δ): The δ^k sequences can also become infinitely oscillatory, as was the case with the $\tilde{R}$ sequence.

7.3.3. Derivatives of the Dirac δ

Among the three sequences of functions in (7.83), the $\tilde{R}$ and the Gaussian sequences are composed of infinitely differentiable functions (the latter are, in addition, $\mathscr{C}_{\downarrow}^{\infty}$ functions). We can consider their nth derivatives and introduce the nth derivative of the Dirac δ,

$$\lim_{k\to\infty} d^n\delta^k(q)/dq^n =: \delta^{(n)}(q), \tag{7.87}$$

with the same interpretation for this symbol as for (7.85). It has the property that, for any $\mathscr{C}^n$ function $f(q)$ [whose nth derivative $f^{(n)}(q)$ is continuous],

$$\int_{-\infty}^{\infty} dq' f(q')\delta^{(n)}(q - q') = (f * \delta^{(n)})(q) = f^{(n)}(q), \tag{7.88a}$$

as can be easily verified before the limit (7.87) is taken. One minor point in the proof of (7.88a) which should be noted is that

$$\delta^{(n)}(q - q') = \partial^n\delta(q - q')/\partial q^n = (-1)^n\partial^n\delta(q - q')/\partial q'^n. \tag{7.88b}$$

The first form may be extracted from the integral, while the second can be used to integrate by parts, ending the verification with (7.88a) for $f^{(n)}(q')$.

7.3.4. The Heaviside Θ-Function

The Dirac $\delta^{(n)}$ symbolism can be extended consistently to negative values of n, that is, to the antiderivatives,

$$\delta^{(-1)}(q) = \int_{-\infty}^{q} dq'\delta(q') = \begin{Bmatrix} 1, & q > 0 \\ \frac{1}{2}, & q = 0 \\ 0, & q < 0 \end{Bmatrix} =: \Theta(q), \tag{7.89}$$

where we have defined $\Theta(q)$, the *Heaviside step function*. Note that $\Theta(0)$ is undefined from the integral (7.89) alone, although if we were to use any of the sequences defining the δ, the value $\Theta(0) = \frac{1}{2}$ would appear. The converse of (7.89),

$$\delta(q) = \frac{d}{dq}\Theta(q) =: \Theta'(q), \tag{7.90}$$

can also be used to *define* the Dirac δ, as its placement in convolution with a differentiable function (which vanishes at $\pm\infty$) yields, by integration by parts,

$$(\Theta' * f)(q) = \int_{-\infty}^{\infty} dq'\Theta'(q')f(q-q') = -\int_{-\infty}^{\infty} dq'\Theta(q')\, df(q-q')/dq'$$

$$= -\int_{0}^{\infty} dq'\, df(q-q')/dq' = f(q) = (\delta * f)(q). \tag{7.91}$$

Exercise 7.27. Justify (7.89)–(7.91) by any of the sequences of functions (7.83). The $\tilde{R}$ sequence will lead to the use of the $\mathrm{Si}(q)$ (sine integral) function, while the Gaussian sequence requires the $\mathrm{erf}(q)$ (error) function. For a list of their asymptotic properties, see the Abramowitz–Stegun tables (1964, Chapters 5 and 7).

7.3.5. Divergent Integral Representation of the Dirac δ

The Fourier transform of the Dirac δ or its derivatives may be defined either as the limit of the Fourier transforms of the sequences (7.83) or directly by the use of (7.88) with the Fourier kernel for f, yielding

$$\widetilde{\delta^{(n)}}(p) = (2\pi)^{-1/2}(ip)^n. \tag{7.92}$$

Equation (7.52), treating the δ as an ordinary function, leads to the same result.

Exercise 7.28. Consider the Fourier transforms of the sequences (7.83) and show that the $k \to \infty$ limit of these is indeed (7.92). Examine the norms: show that the limit of these is infinity, so that the $\delta^{(n)}$ do *not* belong to $\mathscr{L}^2(\mathscr{R})$.

As every function in the sequences (7.83) satisfies the conditions of the Fourier integral theorem, it follows that [if we keep in mind the definition (7.87) and take appropriate account of the exchange of limits, $k \to \infty$ and integration $\int_{-L}^{L} \to \int_{-\infty}^{\infty}$] we can write the *inverse* Fourier transform of (7.92), regaining $\delta^{(n)}$ as

$$\delta^{(n)}(q) = (2\pi)^{-1}\int_{-\infty}^{\infty} dp(ip)^n \exp(-ipq). \tag{7.93}$$

[Compare Eq. (7.93) with the divergent Fourier series representation of the periodic Dirac δ in Eqs. (4.82) and (4.94).]

At the risk of becoming repetitious, we must emphasize that the integral (7.93) does not exist in the ordinary sense but is a symbolic equality between the limits of two sequences of integrals, one containing the functions $d^n\delta^k(q)/dq^n$ and the other its integrated Fourier transform, both in company with an arbitrary $\mathscr{C}^n$ test function. The reason for introducing these expressions is that they allow us to verify directly in convenient shorthand, and disregarding the difficulties in justifying exchange of integrals, many of the calculations which otherwise require more circuitous, if rigorous, derivations. As an example of its use we shall rederive the convolution equation (7.43):

$$\begin{aligned}
\widetilde{f\cdot g}(p) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq f(q)g(q)\exp(-ipq) \\
&= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq\left[(2\pi)^{-1/2}\int_{-\infty}^{\infty} dp'\tilde{f}(p')\exp(ip'q)\right] \\
&\quad\times\left[(2\pi)^{-1/2}\int_{-\infty}^{\infty} dp''\tilde{g}(p'')\exp(ip''q)\right]\exp(-ipq) \\
&= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dp'\int_{-\infty}^{\infty} dp''\tilde{f}(p')\tilde{g}(p'') \\
&\quad\times\left\{(2\pi)^{-1}\int_{-\infty}^{\infty} dq\exp[i(p'+p''-p)q]\right\} \\
&= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dp'\int_{-\infty}^{\infty} dp''\tilde{f}(p')\tilde{g}(p'')\delta(p-p'-p'') \\
&= (2\pi)^{-1/2}(\tilde{f}*\tilde{g})(p).
\end{aligned}$$

In the last expression we have a divergent integral of the type (7.93) for $n = 0$. By replacing this by $\delta(p - p' - p'')$, one of the two integrals is canceled, setting either $p' = p - p''$ or $p'' = p - p'$. [In this form, the proof of the convolution result can be compared with its finite-dimensional counterpart in Section 3.1, Eqs. (3.1)–(3.3), the *coupling* coefficient (3.5) being the Dirac δ.]

Exercise 7.29. Using (7.93), verify the result (7.52), showing that the inverse Fourier transform of $(ip)^n\tilde{f}(p)$ is $f^{(n)}(q)$. Note that the former is a product between $(ip)^n$ and $\tilde{f}(p)$, so the latter should be the convolution of the inverse Fourier transforms. Show that Eq. (7.93) actually embodies—in symbolic form—the Fourier integral theorem.

Exercise 7.30. Show that the Fourier coefficients (7.92) and divergent integral representation (7.93) also represent correctly—up to an arbitrary additive constant—the antiderivatives of the Dirac δ. The Heaviside step function—minus $\frac{1}{2}$—is obtained from (7.93), with $n = -1$, when Eq. (7.10b) is used. The reason the

constant does not appear is that in validating (7.52) for negative derivatives we disregarded the constant term in the integration by parts, arguing that this should be zero. This now forces us to obtain functions such that

$$\lim_{L\to\infty} f(q)\exp(-ipq)\Big|_{-L}^{L} = 0.$$

The result is thus that the sign, rather than the Heaviside, function appears in the Fourier synthesis.

Exercise 7.31. Prove that the convolution of two Dirac δ's is a δ:

$$\int_{-\infty}^{\infty} dq\, \delta(q - q')\,\delta(q - q'') = \delta(q' - q'').$$

This is immediate if seen naïvely. It can also be proven by sequence limits on Gaussian or rectangle functions using Eq. (7.50) or (7.48).

Exercise 7.32. Consider functions $f(q)$ which are *periodic* in q with period 2π—or any period, for that matter. Show that the Fourier transform $\tilde{f}(p)$ is a sum of Dirac δ's sitting on p = integer with coefficients which are the Fourier *series* expansion coefficients. In this way one regains Fourier series from the transforms.

7.3.6. $\delta(q^2 - a^2)$

The Dirac δ will appear time and again in the description of diffusive, elastic, and quantum systems. One of its applications will involve $\delta(q^2 - a^2)$, so let us analyze what happens when the argument of the δ is a function of q. We shall not refer here to sequences of functions but to the intuitive picture of $\delta(q)$ as an infinitely high, narrow "function" with unit area sitting at the origin. In this picture, $\delta(q^2 - a^2)$ must have two peaks, one at $q = a$ and another at $q = -a$, as for both points the argument of the δ is zero. We shall analyze the effect of $\delta(q^2 - a^2)$ on a test function, changing variables to $v = q^2 - a^2$. We have to be careful about the ranges, though: define $q := -(v_1 + a^2)^{1/2}$ for $q < 0$ and $q := +(v_2 + a^2)^{1/2}$ for $q \geqslant 0$. We thus write

$$\begin{aligned}
\int_{-\infty}^{\infty} dq\, \delta(q^2 - a^2)f(q) &= \left(\int_{-\infty}^{0} + \int_{0}^{\infty}\right) dq\, \delta(q^2 - a^2)f(q) \\
&= -\int_{\infty}^{-a^2} \tfrac{1}{2}(v_1 + a^2)^{-1/2}\, dv_1\, \delta(v_1) f\big(-(v_1 + a^2)^{1/2}\big) \\
&\quad + \int_{-a^2}^{\infty} \tfrac{1}{2}(v_2 + a^2)^{-1/2}\, dv_2\, \delta(v_2) f\big((v_2 + a^2)^{1/2}\big) \\
&= (2|a|)^{-1} f(|a|) + (2|a|)^{-1} f(-|a|) \\
&= \int_{-\infty}^{\infty} dq (2|a|)^{-1}[\delta(q - |a|) + \delta(q + |a|)] f(q).
\end{aligned} \tag{7.94a}$$

Hence, we can state that

$$\delta(q^2 - a^2) = (2|a|)^{-1}[\delta(q - |a|) + \delta(q + |a|)]. \tag{7.94b}$$

7.3.7. $\delta(F(q))$

This result can be generalized to the expression $\delta(F(q))$, where $F(q)$ is any differentiable function with simple zeros. (See Fig. 7.3.) Assume the roots of $F(q)$ are $a_1, a_2, \ldots, a_N$, and let $I_1, I_2, \ldots, I_N$ be intervals such that (a) $a_i \in I_i$ and (b) $F(q)$ is monotonic on I_i so that $q = F^{-1}(v)$ on I_i is uniquely defined. The natural change of variable is to let $v_i := F(q)$ for $q \in I_i$ and $dq = dv_i/F'(F^{-1}(v_i))$. We can thus write

$$\int_{-\infty}^{\infty} dq\delta(F(q))f(q) = \sum_i \int_{I_i} dq\delta(F(q))f(q)$$

$$= \sum_i \int_{F(I_i)} dv_i\delta(v_i)f(F^{-1}(v_i))/F'(F^{-1}(v_i)). \tag{7.95a}$$

Now, whenever $F(q)$ is a decreasing function of q, $F'(q) < 0$ and $F(I_i)$ is an integration interval where the ordinary bound order is reversed. By placing an absolute value on the denominator of the last integral, the normal bound order is restored. Use of $\delta(v_i)$ now yields

$$\sum_i f(F^{-1}(0))/|F'(F^{-1}(0))| = \sum_i f(a_i)/|F'(a_i)|. \tag{7.95b}$$

Hence,

$$\delta(F(q)) = \sum_i |F'(a_i)|^{-1}\delta(q - a_i). \tag{7.96}$$

Equation (7.94b) is derived from (7.96) for $F(q) = q^2 - a^2$, $a_{1,2} = \mp|a|$, and $F'(q) = 2q$. In particular, the behavior of the Dirac δ under change of scale of the argument is thus

$$\delta(cq) = |c|^{-1}\delta(q). \tag{7.97}$$

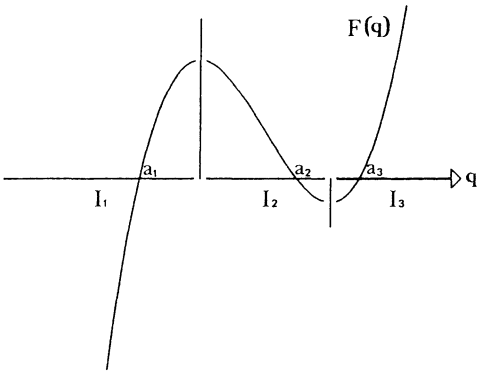


Fig. 7.3. A function broken into its monotonic segments.

7.3.8. The Dirac δ and the Solution of Inhomogeneous Differential Equations

The Dirac δ appears as a natural tool in the solution of *inhomogeneous* differential equations, i.e., those of the form

$$S\left(q, \frac{d}{dq}\right) f(q) = \varphi(q), \tag{7.98}$$

where $S(q, d/dq)$ is a differential operator involving sums of functions of q times derivatives in q, $\varphi(q)$ is a fixed *source* function, and we must solve for $f(q)$. [An equation of this type was seen to describe a damped, forced harmonic oscillator in Section 2.1, where we postponed the general inhomogeneous solution. A particular case of (7.98) was also briefly given in (7.61)–(7.64) and in (7.77) for the case when S is a function only of d/dq.] In Sections 5.1 and 5.2 when we analyzed the solutions to the heat and wave equations in continuous, finite media, we saw that arbitrary initial conditions could be seen as an integrated superposition of Dirac δ's. Here, too, the source function in (7.98) can be interpreted as such a superposition:

$$\varphi(q) = \int_{-\infty}^{\infty} dq' \varphi(q') \delta(q - q'). \tag{7.99}$$

If we can find a solution to the *reduced* inhomogeneous equation

$$S\left(q, \frac{d}{dq}\right) G(q, q') = \delta(q - q'), \tag{7.100}$$

then the solution of (7.98) will follow as

$$f(q) = \int_{-\infty}^{\infty} dq' \varphi(q') G(q, q'). \tag{7.101}$$

This can be verified simply by substituting (7.101) into (7.98), assuming the differentiation in q can be exchanged with integration and applying (7.100). An identity follows. The meaning of $G(q, q')$ in the solution of the reduced equation (7.100) is that of the *Green's function* of the process described by (7.98): the behavior of the system under a *unit* (a Dirac δ) source or impulse function. This is the same Green's function which has appeared time and again in connection with the solution of *homogeneous* differential equations and which carried the disturbance due to initial conditions. The connection between initial conditions and source functions will be made afterwards. Here, we shall find a general solution to the reduced equation (7.100) for the case when the differential operator S is independent of q, i.e., when it appears as $U(\mathbb{P})$, $\mathbb{P} := -id/dq$, a function of the derivatives alone. This special case is quite important: it describes the damped, driven harmonic oscillator proposed in Section 2.1. The damped harmonic oscillator equation in turn is

instrumental in the solution of the heat and wave equations in one or more dimensions, which will be the subjects of Chapter 8.

7.3.9. The Green's Function of an Operator

Consider

$$[U(\mathbb{P})\mathbf{G}_{q'}](q) = \delta(q - q'). \tag{7.102}$$

The Fourier transform of this equation is, due to (7.30), (7.57), and (7.92) for $n = 0$,

$$[U(\mathbb{Q})\tilde{\mathbf{G}}_{q'}](p) = U(p)\tilde{G}_{q'}(p) = (2\pi)^{-1/2}\exp(-ipq'). \tag{7.103}$$

This equation may be solved algebraically:

$$\tilde{G}_q(p) = [(2\pi)^{1/2}U(p)]^{-1}\exp(-ipq') = (\mathbb{E}_{-q'}\tilde{\mathbf{V}})(p), \tag{7.104a}$$

$$\tilde{V}(p) \coloneqq (2\pi)^{-1/2}/U(p). \tag{7.104b}$$

The inverse Fourier transformation thus gives the solution of (7.102) as

$$\begin{aligned} G_{q'}(q) &= (\mathbb{F}^{-1}\mathbb{E}_{-q'}\tilde{\mathbf{V}})(q) \\ &= (\mathbb{T}_{-q'}\mathbb{F}^{-1}\tilde{\mathbf{V}})(q) \\ &= (2\pi)^{-1/2}[\mathbb{F}^{-1}(1/\mathbf{U})](q - q'). \end{aligned} \tag{7.105}$$

This function will be actually calculated below for the damped harmonic oscillator case. The result (7.105), however, gives us the general result that the Green's function for any inhomogeneous differential equation with constant coefficients is a function of $q - q'$, q' being the source position and q the location where the effect is felt. Such systems are thus *translationally invariant*. In Section 7.4 *causality* will come into the picture for partial differential equations in space and time variables. Equation (7.105) tells us that the Green's function of an operator is a function such that the operator turns it into a Dirac δ.

The solution (7.102)–(7.105) for $\tilde{V}(p) =: \tilde{f}(p)$ and $\tilde{f}(p)^{-1} \coloneqq 1/\tilde{f}(p)$ allows us to write a neat formula binding an operator and its Green's function as

$$\tilde{f}\left(-i\frac{d}{dq}\right)^{-1} f(q) = (2\pi)^{1/2}\delta(q). \tag{7.106}$$

Exercise 7.33. Use Eq. (7.106) in order to prove that, for the Gaussian function (7.20),

$$\exp\left(-\tfrac{1}{2}t\frac{d^2}{dq^2}\right)G_t(q) = \delta(q). \tag{7.107}$$

This formally represents the backward time evolution of a Gaussian temperature distribution to the point where it becomes a Dirac δ.

Exercise 7.34. Formally rederive Eq. (7.106) in the form

$$f(q) = (2\pi)^{1/2}\tilde{f}\left(-i\frac{d}{dq}\right)\delta(q), \tag{7.108}$$

noting that $\tilde{f}(-id/dq)$ can be written in terms of the translation operator (7.69) as

$$\begin{aligned}\tilde{f}\left(-i\frac{d}{dq}\right) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq' f(q')\exp\left(-q'\frac{d}{dq}\right)\\ &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq' f(q')\mathbb{T}_{-q'},\end{aligned} \tag{7.109}$$

whose action on any generalized function is well defined.

Exercise 7.35. Using the results of Exercise 7.34, show that the convolution of two functions can be given an operator form as

$$(f * g)(q) = (2\pi)^{1/2}\tilde{f}\left(-i\frac{d}{dq}\right)g(q) = (2\pi)^{1/2}\tilde{g}\left(-i\frac{d}{dq}\right)f(q). \tag{7.110}$$

7.3.10. Application to the Driven, Damped Harmonic Oscillator

A concrete example of a differential equation with constant coefficients is given by the forced, damped harmonic oscillator, whose solutions $f(q)$—using q for time—obey

$$\left(M\frac{d^2}{dq^2} + c\frac{d}{dq} + k\right)f(q) = F(q), \qquad c \geqslant 0, \tag{7.111}$$

[See Eq. (2.1). We maintain the coefficients of inertia, dissipation, and restitution as M, c, and k.] This is a differential equation of the kind (7.98)–(7.102) with

$$U(p) = -Mp^2 + icp + k = -M(p - p_+)(p - p_-) = [(2\pi)^{1/2}\tilde{G}(p)]^{-1}, \tag{7.112}$$

where the roots of the polynomial are

$$p_\pm \coloneqq ic/2M \pm [k/M - (c/2M)^2]^{1/2} =: i\Gamma \pm p_e, \tag{7.113a}$$

$$\Gamma \coloneqq c/2M \geqslant 0, \qquad p_e \coloneqq (p_0^2 - \Gamma^2)^{1/2}, \qquad p_0 \coloneqq (k/M)^{1/2}. \tag{7.113b}$$

The Green's function of the differential operator (7.111) is

$$G(q) = -(2\pi M)^{-1}\int_{-\infty}^{\infty} dp[(p - p_+)(p - p_-)]^{-1}\exp(ipq). \tag{7.114}$$

The integrand in the last equation, we note, has two poles in the upper complex p-half-plane. These are depicted in Fig. 7.4(a) as a function of the damping constant c.

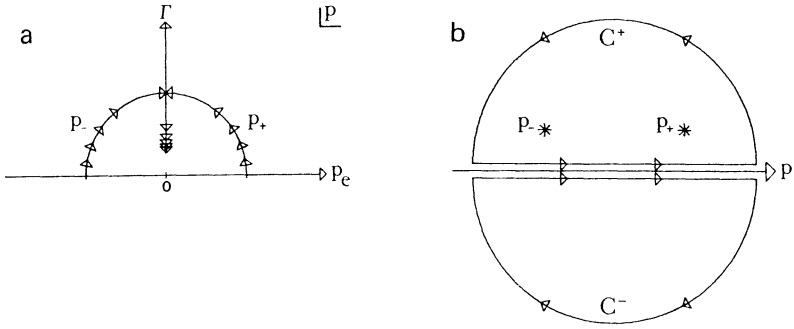


Fig. 7.4. (a) Migration of the complex oscillation frequency poles as a function of the damping constant c. The arrows indicate the points in the complex p-plane where $c = 2(kM)^{1/2}\kappa$ for $\kappa = 0.2, 0.4, \ldots, 1$ (damped oscillating and critical cases) and $\kappa = 1.2, 1.4, \ldots, 2$ (overdamped case). (b) Complex integration contours in the p-plane for $q > 0$ and $q < 0$ for a fixed pole pair.

The techniques of complex integral calculus are a handy tool for evaluation of the integral (7.114). The factor $\exp(ipq)$ for $q > 0$ makes the integrand vanish asymptotically for large $\operatorname{Im} p$ in the upper half-plane, while for $q < 0$ the vanishing occurs for large $|\operatorname{Im} p|$ in the lower half-plane. Cauchy's residue theorem can be used to construct integration paths C^+ and C^- as shown in Fig. 7.4(b). When $q > 0$, C^+ encloses the two poles, the integration along the real axis is the one in (7.114), and the contribution of the semicircle at infinity is zero due to Jordan's lemma. For $q < 0$, C^- encloses no singularities and hence the integral (7.114) is zero. For the former case, $q > 0$,

$$\begin{aligned} G(q) &= 2\pi i \sum \operatorname{Res}\{[(p - p_+)(p - p_-)]^{-1} \exp(ipq)\} \\ &= 2\pi i[(p_+ - p_-)^{-1} \exp(ip_+ q) + (p_- - p_+)^{-1} \exp(ip_- q)] \\ &= -4\pi(p_+ - p_-)^{-1} \exp(-\Gamma q) \sin p_e q. \end{aligned} \tag{7.115}$$

The Green's function (7.114) turns out to be, then,

$$G(q) = \begin{cases} (Mp_e)^{-1} \exp(-\Gamma q) \sin p_e q, & q \geqslant 0, \\ 0, & q < 0. \end{cases} \tag{7.116}$$

The value at $q = 0$ is zero for both cases.

The solution to the original forced damped oscillator equation (7.111) is thus

$$f(q) = \int_{-\infty}^{q} dq' F(q') G(q - q') \tag{7.117}$$

plus a general solution of the homogeneous equation.

The Green's function (7.116) can be compared with the solutions of the free damped harmonic oscillator [Eqs. (2.11a), (2.12), and (2.13) for the

oscillatory, critical, and overdamped cases for Γ less than, equal to, and larger than $(k/M)^{1/2}$ (see Fig. 2.4); in fact, they are the same function for $q = t$]. This leads us to interpret the initial condition $f(q')$ in the latter as the result of the action of a unit impulse force $F(q) = f(q')\delta(q - q')$ in (7.111), which is a homogeneous differential equation for $q > q'$. Similarly, an initial velocity $\dot{f}(q')$ results from the action of a force $\dot{f}(q')\,\partial\delta(q - q')/\partial q$ and gives rise to a solution which is the derivative of (7.116) with respect to q:

$$\frac{dG(q)}{dq} = \begin{cases} -\Gamma G(q) + M^{-1}\exp(-\Gamma q)\cos p_e q, & q > 0, \\ 1/2M, & q = 0, \\ 0, & q > 0. \end{cases} \tag{7.118}$$

For times earlier than that of the initial conditions, the system is considered to be undisturbed, as indicated by (7.116) and (7.118). This property of the solution indicates that the system is *causal*. Causality assures us that the effect of a force $\delta(q - q')$ will reach the system only for times q later than q'.

7.3.11. Causality and Poles in the Complex Plane

The statement of *causality* is again present in (7.117), telling us that the disturbance at a point q in time depends only on the *past* history of the driving force: $q' \in (-\infty, q)$. Any equation which governs the time development of a physical process is expected to exhibit this fundamental requirement. Given any differential equation with constant coefficients characterized by $U(\mathbb{P})$ as in (7.102), one can verify easily whether it leads to causal solutions or not. Generally, *if* $U(p)$, as a function of p, *has roots in the upper complex p-plane only, the system will be causal.* The proof of this fact follows closely the above development. We have said "generally," since equations can be contrived where the function $U(p)$ grows faster than the decrease of the exponential factor in (7.114), making the use of the Jordan lemma impossible. Other cases which fall outside the statement are those where $U(p)$ has an infinity of poles accumulating into an essential singularity or branch cuts which complicate the use of the Cauchy theorem.

7.3.12. "Cut" Functions of Time as Causal Solutions

Having examined the property of causality and its relation to Fourier transformation, we shall examine again the solutions of the forced, damped harmonic oscillator, assuming that all the observable quantities are zero up to an initial time a and beyond a final time b. The first requirement corresponds physically to either the situation where the measured quantities and driving force are actually zero up to that moment or where the measuring process starts at $q = a$. At that instant, the observed values are $f_a := f(a)$ and

$f'_a \coloneqq df(q)/dq|_{q=a}$. The second requirement [$f(q) = 0$ for $q > b$] similarly means either that the system is in equilibrium, that we have turned off the measuring apparatus, or that a power failure has ended our day's work. The boundary values $f_b \coloneqq f(b)$ and $f'_b \coloneqq df(q)/dq|_{q=b}$ are not expected to be present, however, in the prediction of $f(q)$ for $a < q < b$. We consider functions $f_{ab}(q)$ which are zero outside the finite interval $[a, b]$. Consequently, their derivatives include Dirac δ's at a and b because of the discontinuities at these points:

$$(f_{ab})'(q) = \delta(q-a)f_a - \delta(q-b)f_b + (f')_{ab}(q), \tag{7.119a}$$

$$(f_{ab})''(q) = \delta'(q-a)f_a - \delta'(q-b)f_b + \delta(q-a)f'_a - \delta(q-b)f'_b + (f'')_{ab}(q). \tag{7.119b}$$

We must take some care in distinguishing the derivatives of cut functions $(f_{ab})'$, etc., from the cut derivatives of functions $(f')_{ab}$. See Fig. 7.5. It is the former which appear in the damped oscillator differential equation (7.111). Fourier transformation of (7.119) yields

$$\widetilde{(f')}_{ab}(p) = (2\pi)^{-1/2}\exp(-ipq)f(q)|_{q=a}^{b} + ip\tilde{f}_{ab}(p), \tag{7.120a}$$

$$\widetilde{(f'')}_{ab}(p) = (2\pi)^{-1/2}ip\exp(-ipq)f(q)|_{q=a}^{b} + (2\pi)^{-1/2}\exp(-ipq)f'(q)|_{q=a}^{b} - p^2\tilde{f}_{ab}(p). \tag{7.120b}$$

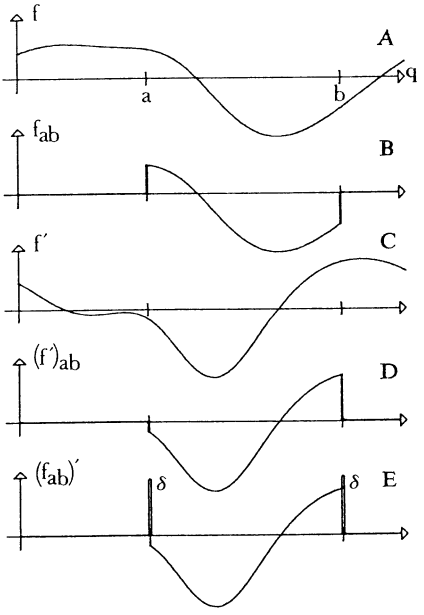


Fig. 7.5. Cuts, derivatives, and cut derivatives. (A) An "arbitrary" uncut function $f(q)$. (B) The cut function $f_{ab}(q)$. (C) The derivative of $f(q)$. (D) The cut derivative. (E) Derivative of the cut function.

The Fourier-transformed differential equation thus yields, after some rearrangement and solving for $\tilde{f}_{ab}(p)$,

$$\tilde{f}_{ab}(p) = \tilde{f}_F(p) + \tilde{f}_a(p) - \tilde{f}_b(p), \tag{7.121a}$$

where, using (7.112),

$$\tilde{f}_F(p) := -M^{-1}[(p - p_+)(p - p_-)]^{-1}\tilde{F}(p) = (2\pi)^{1/2}\tilde{G}(p)\tilde{F}(p) \tag{7.121b}$$

is the part of the solution determined by the driving force, and, for $d = a$ or b, the boundary conditions appear as

$$\begin{aligned}\tilde{f}_d(p) &= -(2\pi)^{-1/2}[(p - p_+)(p - p_-)]^{-1}\exp(-idp)[(ip + c/M)f_d + f_d'] \\ &= [(cf_d + Mf_d') + ipMf_d](\widetilde{\mathbb{T}_{-d}\mathbf{G}})(p),\end{aligned} \tag{7.121c}$$

where $\mathbb{T}_{-d}$ is the translation operator (7.27)–(7.30). The cut solution to the problem is finally the inverse Fourier transform of (7.121). Using results on translation, convolution, and differentiation, we can write

$$f_{ab}(q) = f_F(q) + f_a(q) - f_b(q), \tag{7.122a}$$

$$f_F(q) = (F * G)(q) = \int_a^{\min(q,b)} dq' F(q')G(q - q'), \tag{7.122b}$$

$$\begin{aligned}f_d(q) &= [(cf_d + Mf_d') + Mf_d d/dq]G(q - d) \\ &= f_d[cG(q - d) + MdG(q - d)/dq] + Mf_d'G(q - d).\end{aligned} \tag{7.122c}$$

7.3.13. Stationary and Transient Solutions

The solution $f_{ab}(q)$ is composed of three parts. The first, $f_F(q)$, is the response of the system to the driving force $F(q)$ and equals (7.117) for a force which may be nonzero only for $q \in [a, b]$. It is referred to as the *stationary* solution of the inhomogeneous differential equation. Next, we have two *transient* terms which depend on the boundary values of $f_{ab}(q)$ at a and b and which are solutions to the homogeneous differential equation. We now analyze the way the three summands in (7.122a) combine, referring to Fig. 7.6. The first part, $f_F(q)$ [Fig. 7.6(B)], is due to the source function [Fig. 7.6(A)]. It is zero for $q \leqslant a$, and because of the $\Theta(q - q')$ behavior of the Green's function, it will only contain information about the source for $a < q' < q$. This is causality. For $q > b$, $F(q)$ is zero and leaves $f_F(q)$ to oscillate freely with the damping of the medium. Next, we have the boundary term $f_a(q)$ in Fig. 7.6(C). It is zero up to $q = a$, where it jumps to f_a with slope f_a' and oscillates freely thereafter. The third part, $f_b(q)$ in Fig. 7.6(D), is zero up to $q = b$; jumps to f_b, the value of the first two terms at $q = b$, with slope f_b'; and oscillates freely. The sign of $f_b(q)$ in (7.122a) is *negative*, how-

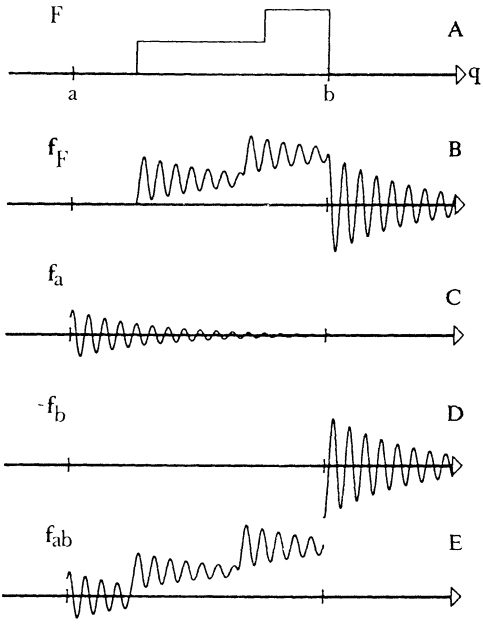


Fig. 7.6. Driving force and causal response. (A) The applied driving force during the time interval $[a, b]$. (B) The pure time-unlimited response of the system to the driving force. (C) "Arbitrary" initial conditions to the measurement process. (D) Boundary conditions at $q = b$ due to the the cut of the observation interval. (E) Total measured response of the system in the time interval $[a, b]$.

ever. This means that the latter function combines with the first two to yield a total value of *zero* for $f_{ab}(q)$, $q > b$. This is shown in Fig. 7.6(E).

The overall statement of causality is then that, for $a < q < b$, $f_{ab}(q)$ contains information about the initial conditions and the source function up to the time of measurement. The boundary conditions at $q = b$ do not enter the solution at all. As expected, a hypothetical future power failure cannot affect the outcome of the experiment.

The mathematical aspects of causality will be further analyzed in Section 7.4 from the point of view of Fourier transforms. Laplace transforms will be used in Section 8.1.

7.4. Causality and Dispersion Relations

In this section we shall investigate some properties of functions $f_{a\infty}(q)$, $f_{-\infty b}(q)$, and $f_{ab}(q)$ which have *support* on the intervals $[a, \infty)$, $(-\infty, b]$, and $[a, b]$, i.e., $f_{..}(q) = 0$ for q outside these intervals. The constraints on the Fourier transforms of such "cut" functions will lead us to some basic requirements—called dispersion relations—which enter the description of causal filters, refractive media, and scattering amplitudes between elementary particles.

7.4.1. Causal Functions

Consider the *causal* exponentially damped function with support on the half-line $[a, \infty)$:

$$\Theta_\varepsilon(q-a) = (\mathbb{T}_{-a}\boldsymbol{\Theta}_\varepsilon)(q) \coloneqq \begin{cases} \exp[-\varepsilon(q-a)], & q < a, \\ \frac{1}{2}, & q = a, \\ 0, & q < a, \ \mathrm{Re}\,\varepsilon > 0. \end{cases} \tag{7.123}$$

Note that for $\mathrm{Im}\,\varepsilon \neq 0$ the function oscillates as well. Its Fourier transform can be easily found as

$$\begin{aligned} (\mathbb{F}(\mathbb{T}_{-a}\boldsymbol{\Theta}_\varepsilon))(p) &= (2\pi)^{-1/2}\int_a^\infty dq \exp[-\varepsilon(q-a) - ipq] \\ &= -i(2\pi)^{-1/2}(p - i\varepsilon)^{-1}\exp(-iap). \end{aligned} \tag{7.124}$$

It is a function with a single, simple pole at $p = i\varepsilon$ in the upper complex p-half-plane, with residue $-i(2\pi)^{-1/2}\exp(a\varepsilon)$. The Heaviside step function $\Theta(q)$ in Eq. (7.89) is the limit of (7.123) as $\varepsilon \to 0^+$ from the upper complex ε-half-plane.

7.4.2. Two Results on Fourier Transforms of Causal Functions

Equations (7.123) and (7.124) will be used later on. Certain characteristics of the latter, however, are common to Fourier transforms of all functions with support on the half-line $[a, \infty)$. Consider one such function

$$f_{a\infty}(q) = \begin{cases} f(q), & q > a, \\ \frac{1}{2}f(a), & q = a, \\ 0, & q < a, \end{cases} \tag{7.125}$$

which we assume satisfies the conditions of the Fourier integral theorem. Its transform is thus

$$\tilde{f}_{a\infty}(p) = (2\pi)^{-1/2}\int_a^\infty dq f(q)\exp(-ipq). \tag{7.126}$$

We shall now explore the general properties of (7.126) which result from the restriction (7.125). These turn out to be rather recognizable features as a function of *complex* $p = \mathrm{Re}\,p + i\,\mathrm{Im}\,p$. We state that *the Fourier transform of a causal function* which has support on $[a, \infty)$ is (a) an *entire analytic function in the lower complex half-plane* $\mathrm{Im}\,p < 0$ (entire functions in some region, we recall, are those which do *not* exhibit singularities of any kind in that region), and (b) its growth in the lower half-plane is bounded by $C_f \exp(-a|\mathrm{Im}\,p|)$, where C_f is a constant. Moreover, the *inverse* Fourier transform of a function satisfying (a) and (b) is one with support on $[a, \infty)$.

We prove the second statement first by the estimate on (7.126),

$$|\tilde{f}_{a\infty}(p)| \leqslant (2\pi)^{-1/2} \int_a^\infty dq\, |f(q)| \cdot |\exp(-ipq)|$$

$$= (2\pi)^{-1/2} \int_a^\infty dq\, |f(q)| \exp(q \operatorname{Im} p). \tag{7.127}$$

As q is not bounded from above, the estimate is vacuous for $\operatorname{Im} p > 0$ since the last term is infinity. For $\operatorname{Im} p < 0$, as $a < q$, $\exp(a \operatorname{Im} p)$ majorizes the exponential factor and hence, as anticipated,

$$|\tilde{f}_{a\infty}(p)| \leqslant (2\pi)^{-1/2} \exp(a \operatorname{Im} p) \int_a^\infty dq\, |f(q)|$$

$$=: C_f \exp(-a|\operatorname{Im} p|). \tag{7.128}$$

The constant C_f is finite if $f(q)$ is assumed to be in $\mathscr{L}^1(\mathscr{R})$.

Exercise 7.36. Since by assumption $f(q)$ is of bounded total variation, find from (7.127) the alternative estimate for

$$|\tilde{f}_{a\infty}(p)| \leqslant (2\pi)^{-1/2} \max_{q\in[a,\infty)} |f(q)| \cdot |\operatorname{Im} p|^{-1} \exp(-q|\operatorname{Im} p|). \tag{7.129}$$

To show that $\tilde{f}_{a\infty}(p)$ is an analytic function in the lower half-plane $\operatorname{Im} p < 0$, the basic argument is that the total derivative of (7.126) with respect to complex p exists as the factor $\exp(-ipq)$ is entire and analytic in the complex plane p and

$$d\tilde{f}_{a\infty}(p)/dp = (2\pi)^{-1/2} \int_a^\infty dq(-iq) f(q) \exp(-iq \operatorname{Re} p) \exp(q \operatorname{Im} p). \tag{7.130}$$

For all complex p with $\operatorname{Im} p < 0$ the existence of the integral is guaranteed in spite of the extra factor $-iq$ because of the decreasing exponential term. The bounds (7.128)–(7.129) assure us that no infinities are present. This argument extends to all derivatives in the Taylor series for $\tilde{f}_{a\infty}(p)$.

7.4.3. The Converse Result

The proof of the converse, namely that if $\tilde{f}_{a\infty}(p)$ is an entire analytic function and majorized by (7.128)–(7.129) in the lower complex half-plane, its inverse Fourier transform is zero in $(-\infty, a)$, is performed straightforwardly:

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

$$= (2\pi)^{-1/2} \int_{-\infty}^\infty dp \tilde{f}_{a\infty}(p) \exp(iq \operatorname{Re} p) \exp(-q \operatorname{Im} p). \tag{7.131}$$

For $\operatorname{Im} p < 0$ the integrand is analytic, entire, and, moreover, due to (7.128)–(7.129), contains a factor $\exp[(q - a)|\operatorname{Im} p|]$. For $q < a$ this is decreasing. The Jordan lemma and the Cauchy integral theorem can now be used, as in Section 7.3, in order to show, by the integration contour in Fig. 7.4(b), that (7.131) is zero. For $q > a$ there is no general condition since $f(q)$ in (7.125) is arbitrary.

Exercise 7.37. Use Cauchy's theorem and Jordan's lemma in order to perform the inverse Fourier transform of (7.124) and recover the $\Theta_\varepsilon(q)$ function in (7.123) for $q > a$. In this case it happens to be possible to use complex contour integration for the upper complex p-half-plane as well. This was also possible for the damped oscillator Green's function in Section 7.3. The workings of this technique for $q = a$ will be discussed below.

Exercise 7.38. Show the Fourier transform of the exponentially damped anticausal function $\Theta_\varepsilon(b - q)$ with support on $(-\infty, b]$ to be

$$(\mathbb{FT}_b \mathbb{I}_0 \Theta_\varepsilon)(p) = i(2\pi)^{-1/2}(p + i\varepsilon)^{-1} \exp(-ibp), \tag{7.132}$$

which exhibits a pole in the lower half-plane. As in Exercise 7.37, verify that the inverse Fourier transform of (7.132) is the original function.

Exercise 7.39. Consider *anticausal* functions $f_{-\infty b}(q)$ with support on the half-axis $(-\infty, b]$. Following the proof of the corresponding statements for causal functions, show that the Fourier transforms of $f_{-\infty b}(q)$ are (a) entire analytic functions in the upper complex half-plane $\operatorname{Im} p > 0$ and that (b) their growth is bounded by

$$|\tilde{f}_{-\infty b}(p)| \leqslant C_f' \exp(b \operatorname{Im} p), \tag{7.133a}$$

$$C_f' = (2\pi)^{-1/2} \int_{-\infty}^{b} dq\,|f(q)| \quad \text{or} \quad (2\pi)^{-1/2} \max_{q \in (-\infty, b]} |f(q)| \cdot (\operatorname{Im} p)^{-1}. \tag{7.133b}$$

Conversely, show that if $\tilde{f}_{-\infty b}(p)$ satisfies (a) and (b), it is the Fourier transform of a function which vanishes on (b, ∞).

7.4.4. Fourier Transforms of Functions with Finite Support

Last, the Fourier transforms of functions $f_{ab}(q)$ with support on a *finite* interval $[a, b]$ can be analyzed. They will be shown to be *entire analytic functions on the whole complex plane* (excluding the point at infinity, of course, since otherwise the function would be a constant). These functions lie in the intersection of the classes of causal and anticausal functions with support on $(-\infty, b]$ and $[a, \infty)$. Their properties will thus be the union of the properties of the two classes, and hence $\tilde{f}_{ab}(p)$ will be analytic in the upper and lower complex half-planes. Moreover, as the Fourier transform integral is over a finite range in q and $f_{ab}(q)$ is integrable, the expansion of the Fourier kernel $\exp(ipq)$ in Taylor series will produce a series of integrals which constitutes the Taylor expansion of $\tilde{f}_{ab}(p)$ for real p. The circle of convergence

is the whole complex plane. The growth of this function will be bounded for $\operatorname{Im} p < 0$ and $\operatorname{Im} p > 0$ by (7.128)–(7.129) and (7.133), respectively. Finally, the inverse Fourier transform of functions which are entire and analytic on $\mathscr{C}$ with the above bound conditions will have support on the finite interval $[a, b]$. Results of this kind, relating support, analyticity, and growth, are referred to as *Paley–Wiener theorems.*

7.4.5. The "Cutting" Process

Having found the properties of Fourier transforms of functions which vanish on a half-axis, we can explore further the "cutting" process. Assume $f(q)$ is a function satisfying the conditions of the Fourier integral theorem. The three "cuts" one can perform on it are

$$f_{a\infty}(q) = \lim_{\varepsilon \to 0^+} \Theta_\varepsilon(q - a) f(q), \tag{7.134a}$$

$$f_{-\infty b}(q) = \lim_{\varepsilon \to 0^+} \Theta_\varepsilon(b - q) f(q), \tag{7.134b}$$

$$f_{ab}(q) := f_{a\infty}(q) - f_{b\infty}(q) = f_{-\infty b}(q) - f_{-\infty a}(q), \tag{7.134c}$$

$$f(q) = f_{-\infty c}(q) + f_{c\infty}(q), \qquad c = a \text{ or } b. \tag{7.134d}$$

The Fourier transforms of (7.134) can be found as the convolutions of the Fourier transforms of the Θ_ε functions, Eqs. (7.124) and (7.132), and $\tilde{f}(p)$:

$$\tilde{f}_{a\infty}(p) = \lim_{\varepsilon \to 0^+} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p' - i\varepsilon)^{-1} \exp[-ia(p - p')] \tilde{f}(p'), \tag{7.135a}$$

$$\tilde{f}_{-\infty b}(p) = -\lim_{\varepsilon \to 0^+} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p' + i\varepsilon)^{-1} \exp[-ib(p - p')] \tilde{f}(p'), \tag{7.135b}$$

$$\tilde{f}_{ab}(p) = (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p')^{-1} \times \{\exp[-ia(p - p')] - \exp[-ib(p - p')]\} \tilde{f}(p'), \tag{7.135c}$$

$$\tilde{f}(p) = \lim_{\varepsilon \to 0} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'[(p - p' - i\varepsilon)^{-1} - (p - p' - i\varepsilon)^{-1}] \times \exp[-ic(p - p')] \tilde{f}(p'). \tag{7.135d}$$

In the expression for $f_{ab}(q)$ and its Fourier transform, the limit $\varepsilon \to 0^+$ disappears from the expression, since a rectangle function with value 1 between a and b can be used. We keep the form, however, for purposes of uniformity.

7.4.6. Boundary Values of Analytic Functions in a Half-plane

Equations (7.135) involve the expression

$$\hat{f}_c(p) \coloneqq (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p')^{-1} \exp[-ic(p - p')]\tilde{f}(p'), \qquad \operatorname{Im} p \neq 0, \tag{7.136}$$

associated to the functions $\tilde{f}(p)$. In (7.136), the pole of the integrand lies on the integration path, so we can only give meaning to $\hat{f}_c(p)$ for values of p which lie off the real axis. It is not difficult to show that $\hat{f}_c(p)$ is an entire analytic function for $\operatorname{Im} p \neq 0$: the factors of the integrand containing p are entire and analytic in this region, and their derivatives with respect to p do not worsen the integrability with respect to p'. In terms of (7.136) we can write (7.135) as

$$\tilde{f}_{a\infty}(p) = \lim_{\varepsilon \to 0^+} \hat{f}_a(p - i\varepsilon) \qquad \text{for } \operatorname{Im} p \leqslant 0, \tag{7.137a}$$

$$\tilde{f}_{-\infty b}(p) = -\lim_{\varepsilon \to 0^+} \hat{f}_b(p + i\varepsilon) \qquad \text{for } \operatorname{Im} p \geqslant 0, \tag{7.137b}$$

$$\begin{aligned} \tilde{f}_{ab}(p) &= \lim_{\varepsilon \to 0^+} (\hat{f}_a - \hat{f}_b)(p - i\varepsilon) \\ &= \lim_{\varepsilon \to 0^+} (\hat{f}_a - \hat{f}_b)(p + i\varepsilon), \end{aligned} \tag{7.137c}$$

$$\tilde{f}(p) = \lim_{\varepsilon \to 0^+} [\hat{f}_c(p - i\varepsilon) - \hat{f}_c(p + i\varepsilon)] \qquad \text{for } \operatorname{Im} p = 0. \tag{7.137d}$$

There are several observations to be made about these equations. The first ones pertain to Eqs. (7.137a) and (7.137b) and in fact were implicit in the discussion of Fourier transforms of functions with half-axis support. They tell us that Fourier transforms of causal and anticausal functions are *boundary values* of entire analytic functions in the lower and upper half-planes, respectively. For these, we have interesting relations if the limit $\varepsilon \to 0^+$ is symbolically placed on the integrand, which then becomes $(p' \mp i0^+)^{-1}$ times an integrable function $F(p) = \exp(-ip'a)\tilde{f}(p - p')$. The pole now slides onto the real axis, and the integration contour must be deformed into the lower or upper half-planes (Fig. 7.7), conveniently as a semicircle $C_\delta^{\mp}$

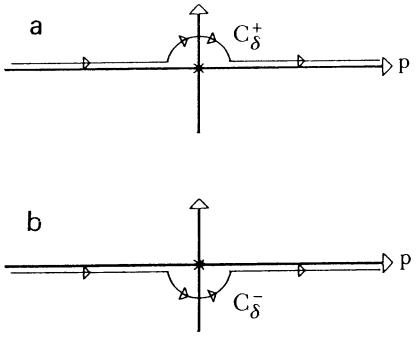


Fig. 7.7. Deformation of the integration contour as the integrand poles slide onto the real axis (a) from below and (b) from above.

of radius $\delta > 0$. The integral can be split in two parts, one along the real axis minus the interval $(-\delta, \delta)$ and the other along the semicircle around the pole. The former is called the *principal value* of the integral:

$$\mathscr{P}\int_{-\infty}^{\infty} dpp^{-1}F(p) \coloneqq \lim_{\delta\to 0}\left(\int_{-\infty}^{-\delta} + \int_{\delta}^{\infty}\right) dpp^{-1}F(p). \tag{7.138}$$

This definition is extended to any integrand with singularities on the integration interval by taking limits on both sides of each pole. The other part of the integral, over $C_\delta{}^{\mp}$, uses Cauchy's theorem to evaluate

$$\int_{C_\delta{}^{\mp}} dpp^{-1}F(p) = \pm i\pi F(0), \tag{7.139}$$

which is valid only if the function is *continuous* at $p = 0$.

7.4.7. $(p \pm i0^+)^{-n}$

The placing of the limit $\varepsilon \to 0^+$ on the integrand thus entails the following symbolic relation,

$$\lim_{\varepsilon\to 0^+}(p \mp i\varepsilon)^{-1} = \mathscr{P}p^{-1} \pm i\pi\delta(p), \tag{7.140a}$$

where all members are defined in terms of the corresponding quantities under integration in company with continuous functions. By formal differentiation one arrives at

$$\lim_{\varepsilon\to 0^+}(p \mp i\varepsilon)^{-n} = \mathscr{P}p^{-n} \pm i\pi(-1)^{n-1}(n!)^{-1}\delta^{(n-1)}(p). \tag{7.140b}$$

As applied to Eqs. (7.135a) and (7.135b), Eq. (7.140a) tells us that

$$\left.\begin{matrix}\tilde{f}_{c\infty}(p)\\ \tilde{f}_{-\infty c}(p)\end{matrix}\right\} = \pm(2\pi i)^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'p'^{-1}\exp(-ip'c)\tilde{f}(p-p') + \tfrac{1}{2}\tilde{f}(p). \tag{7.141}$$

It should be emphasized that the principal value of an integral avoids the poles of the integrand by excluding a vanishing segment *symmetric* around the pole.

Exercise 7.40. Verify that (7.140) yields, as in Exercise 7.38, the correct $f_{c\infty}(q)$ and $f_{-\infty c}(q)$, Eqs. (7.134a)–(7.134b). To this end, perform the inverse Fourier transform of (7.141) by integration over p. The second summand will yield $\frac{1}{2}f(q)$, while the first will be $f(q)$ times

$$\begin{aligned}&(2\pi i)^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'p'^{-1}\exp[ip'(q-c)]\\ &\quad = \pi^{-1}\lim_{\substack{\delta\to 0\\ L\to\infty}}\int_{\delta}^{L} dp'p'^{-1}\sin[p'(q-c)] = \tfrac{1}{2}\operatorname{sign}(q-c),\end{aligned} \tag{7.142}$$

thereby reconstituting (7.134a)–(7.134b) as $\frac{1}{2}(\pm\operatorname{sign} s + 1) = \Theta(\pm s)$. To prove (7.142), use the parity of the integrand, its behavior at the origin, and (7.10b).

The use of the last equation underlines the importance of considering integration intervals symmetric around the origin.

7.4.8. Cauchy Representation of Functions

Equation (7.137d) presents a result which is of great interest by itself. Assume we have a function $\tilde{f}(p)$ which is quite arbitrary: it may have discontinuities or be zero on segments. The analytic continuation of such a function into the complex plane is generally impossible since, by a well-known theorem, if an analytic function is zero on a segment, it must be zero everywhere. What Eq. (7.137d) tells us, then, is that one can find a function $\hat{f}_c(p)$ by (7.136), which is analytic everywhere off the real axis such that the *jump* of $\hat{f}_c(p)$ *across* this axis is the original function $\tilde{f}(p)$.

Exercise 7.41. Consider $\tilde{f}(p)$ to be a rectangle function of value 1 between a and b. Show that Eq. (7.136) for $c = 0$ yields $\hat{f}_0(p) = (2\pi i)^{-1} \ln[(b - p)/(a - p)]$. The logarithm function has branch points at zero and infinity, and the branch cut is usually placed along the negative real axis. This segment corresponds to $a \leqslant p \leqslant b$. Verify that the jump in the imaginary part of logarithm of $(b - p)/(a - p)$ across the branch cut $[a, b]$ is thus $2\pi i$. The support of $\tilde{f}(p)$ is the segment where $\hat{f}_0(p)$ is nonanalytic. For every $c \in \mathscr{R}$ you have such a representation.

The representation of functions by "jumps" of analytic functions in $\mathscr{C} - \mathscr{R}$ given by Eqs. (7.136)–(7.137d) for $c = 0$ is called their *analytic* or *Cauchy* representation. It is important because it also holds for generalized functions as the Dirac δ and its derivatives: If we place $\delta(p)$ in (7.136) for $c = 0$, we obtain $\hat{\delta}_0(p) = -(2\pi i p)^{-1}$. Now, this function is a bona fide analytic function except at $p = 0$, where it has a simple pole of residue $-(2\pi i)^{-1}$. The jump across this pole in the direction of the imaginary axis is infinite, and Eq. (7.137d) assures us that

$$\delta(p) = -(2\pi i)^{-1} \lim_{\varepsilon \to 0^+} [(p - i\varepsilon)^{-1} - (p + i\varepsilon)^{-1}] \tag{7.143}$$

holds. This is actually a result we have obtained before in (7.140) and which must have been noted by the attentive reader in Eq. (7.135d), where the right-hand side of (7.143) appears in the integrand and acts as a reproducing kernel under integration.

The treatment of generalized functions by complex variable theory and Fourier transforms can be made completely in terms of the Cauchy representation (7.136)–(7.137d). The interested reader is referred to the book by Bremermann (1965) for this approach.

7.4.9. Dispersion Relations

The relations we have developed for Fourier transforms of functions with support on various segments become a handy tool for the further

description of causality. Consider the function $f(q)$ in Eq. (7.134a) cut to $f_{a\infty}(q)$. As the Heaviside function $\Theta(q-a)$ acts as the *unit* function for this space of causal functions, Eqs. (7.135a) and (7.136)–(7.137a) become the *identity*

$$\tilde{f}_{a\infty}(p) = (2\pi i)^{-1}\int_{-\infty}^{\infty} dp'(p-p')^{-1}\exp[-ia(p-p')]\tilde{f}_{a\infty}(p'), \qquad \operatorname{Im} p < 0, \quad (7.144)$$

valid for *all* causal functions with support on $[a, \infty)$. For real p we can use (7.140) for the factor $(p-p'-i\varepsilon)^{-1}$, which replaces (7.144) with the principal value of the integral plus $\frac{1}{2}\tilde{f}_{a\infty}(p)$. Subtracting this last term, we find the relation

$$\tilde{f}_{a\infty}(p) = (\pi i)^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p-p')^{-1}\exp[-ia(p-p')]\tilde{f}_{a\infty}(p), \qquad p \text{ real}, \quad (7.145)$$

which is also valid for all causal functions satisfying the conditions of the Fourier integral theorem. The real and imaginary parts of this equation read

$$\operatorname{Re}\tilde{f}_{a\infty}(p) = \pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p-p')^{-1}\operatorname{Im}\{\exp[-ia(p-p')]\tilde{f}_{a\infty}(p')\}, \quad (7.146a)$$

$$\operatorname{Im}\tilde{f}_{a\infty}(p) = -\pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p-p')^{-1}\operatorname{Re}\{\exp[-ia(p-p')]\tilde{f}_{a\infty}(p')\}. \quad (7.146b)$$

Equations binding together the real and imaginary parts of a function are called *dispersion relations*. They are usually found in the literature in the form (7.146) for $a = 0$. We shall now proceed to bring out the physical meaning of the dispersion relations (7.146) in connection with the causal filtering of signals.

Exercise 7.42. Show the dispersion relations for an *anti*causal function $\tilde{f}_{-\infty b}(p)$ to be identical with (7.144)–(7.146) but for a *minus* sign in front of the integrals.

7.4.10. Description of Causal Filters

We consider a given causal function $s_{a\infty}(q)$ to represent a *signal* which up to time $q = a$ is zero and which from then on represents some measured time-dependent quantity. We can feed this signal as input to a "black box" processor and obtain an output signal $s'(q)$. This abstract mechanism applies to an electronic device receiving and encoding information, the attenuation and selective color filtering of light through a dispersive medium, and the

elastic scattering of an incident elementary particle beam (represented by its wave function) by an atomic or nuclear traget. The common properties one can require for a meaningful description of these processes are that they obey the following: (a) *linearity*: if $\mathbf{s}_1$ and $\mathbf{s}_2$ are input signals whose separate output is $\mathbf{s}_1'$ and $\mathbf{s}_2'$, the output of $c_1\mathbf{s}_1 + c_2\mathbf{s}_2$, where $c_1, c_2 \in \mathscr{C}$, should be $c_1\mathbf{s}_1' + c_2\mathbf{s}_2'$; (b) *time invariance*, that is, if the signal $s(q)$ is converted into $s'(q)$, any time-shifted version of the same input $s(q + q_0)$ for fixed q_0 should be converted into the corresponding time-shifted output $s'(q + q_0)$; and (c) *causality*, which means that the output shall not precede the input: if $s(q)$ starts at $q = a$, $s'(q)$ should not start before $q = a$.

From these requirements we can say that if we are able to know the output $\varphi_{0\infty}(q)$ corresponding to an idealized input $\delta(q)$, then for any input function

$$s_{a\infty}(q) = \int_a^\infty dq'\delta(q - q')s_{a\infty}(q') \tag{7.147}$$

[the $s_{a\infty}(q')$ being now generalized linear combination coefficients], the output will be

$$s'_{a\infty}(q) = \int_{-\infty}^q dq'\varphi_{0\infty}(q - q')s_{a\infty}(q') = (\varphi_{0\infty} * s_{a\infty})(q) =: (\Phi\mathbf{s}_{a\infty})(q). \tag{7.148}$$

The filtering process (Fig. 7.8) is thus described by a linear operator Φ whose action on the input signal is given by the convolution with the causal filter function $\varphi_{0\infty}(q)$. [This operator Φ can be given a differential form; see Eq. (7.110).] Causality of the filter's function implies that a value of the output $s'(q)$ at time q depends on the input $s(q')$ for q' *before* q ($q' < q$). The output signal does not appear before the input. There can be *delay* filters whose describing functions have support on $[b, \infty)$, $b > 0$, causing any output to be delayed by b with respect to the input. Another possibility are *finite-memory* filters described by functions with support on a finite interval $[b, c]$, $0 < b < c$. [In Sections 3.1 and 3.2 we described filters acting on signals which were sets of N data points, asking for linearity and for the property that waveforms be converted into waveforms of the same frequency. The latter amounts to property (b) above. We did not ask for causality in Section 3.1, since all components were counted modulo N, with the consequence, that, as can be seen in Fig. 3.2, the output signals could propagate in both directions, the filtering being seen as a "simultaneous" processing of the input points. There, waveform rather than unit-impulse filtering is in the fore.]

Equation (7.148) can be Fourier-transformed into

$$\widetilde{s'_{a\infty}}(p) = (2\pi)^{1/2}\tilde{\varphi}_{0\infty}(p)\tilde{s}_{a\infty}(p). \tag{7.149}$$

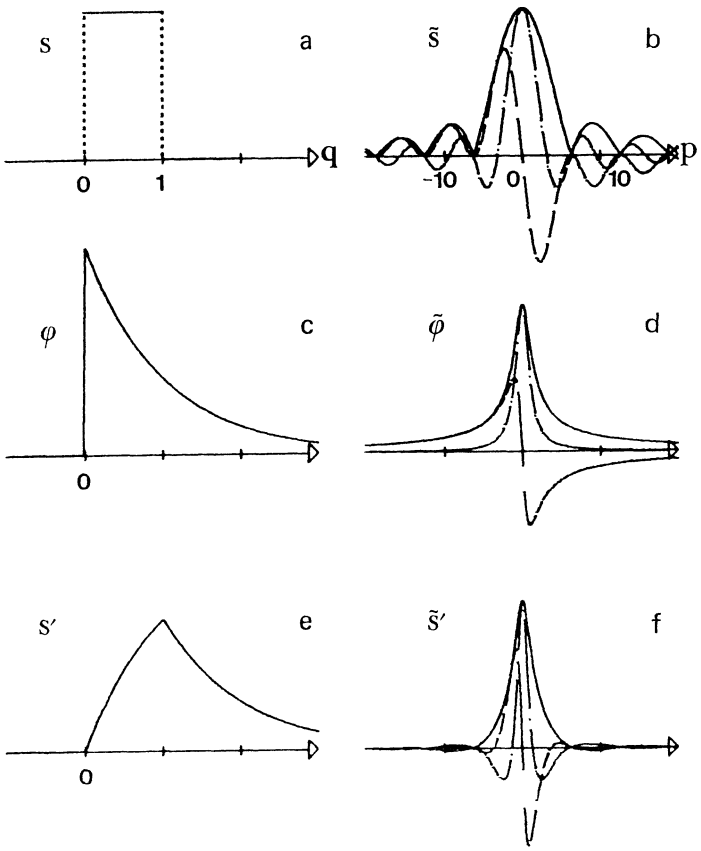


Fig. 7.8. Causal filtering. (a) "Rectangular" signal and (b) its Fourier transform, showing the real and imaginary parts (broken lines) and absolute value (continuous line). (c) Causal filter function $\varphi_{0\infty}$, a decreasing exponential, and (d) its Fourier transform. (e) Causal output signal, convolution of the input and filter function, and (f) its Fourier transform [product of (b) and (d)].

In this form we display the *filter transfer function* as the coefficient function of p, which modifies each of the input partial waves. [Compare with (3.12).]

Now, the filter's transfer function cannot be arbitrary, as it is the Fourier transform of a function with support on $[0, \infty)$. Physically the argument can be seen as follows. Assume that $\tilde{\varphi}(p)$ were 1 for all values of p except for $p \in [r, s]$, so that all p partial waves would be unaffected by the filter except those in the band $[r, s]$, which are absorbed. The filter would then subtract from the signal its partial-wave content in this range. If the latter is roughly constant, the subtracted part would be the Fourier transform of a

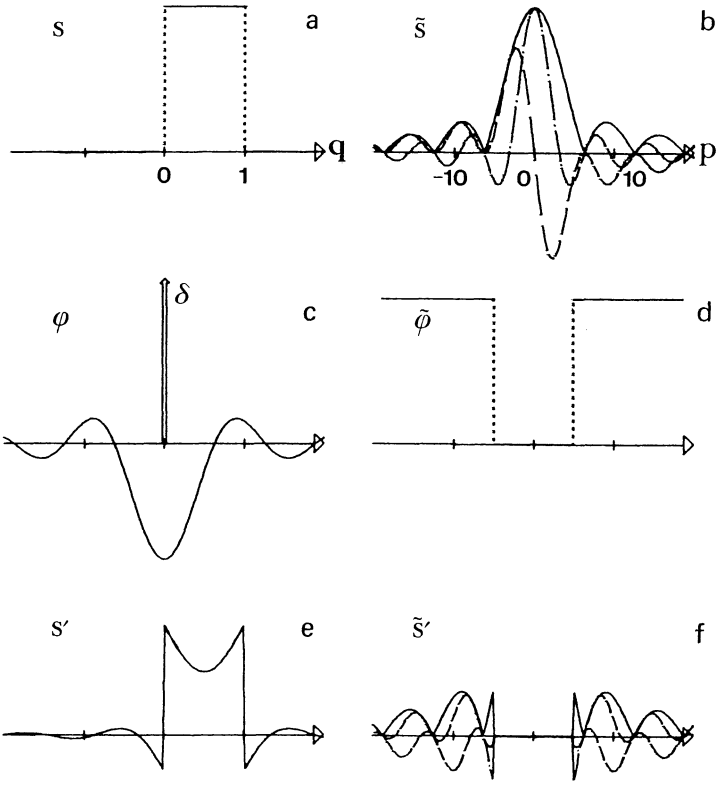


Fig. 7.9. Noncausal filtering. (a) The signal and (b) its Fourier transform—the same as in Figure 7.8. (c) Noncausal filter function built by specifying that its Fourier transform (d) eliminate all partial waves $p \in (-5, 5)$: it is a Dirac δ due to the "background" minus the Fourier transform of the subtracted rectangle. (e) Output signal and (f) its Fourier transform. The former has support on the entire q line and hence the filter is noncausal.

rectangle function, Fig. 7.1. The output signal would undergo the process drawn in Fig. 7.9, which has turned a causal input into a noncausal output. The requirement of a filter to be causal is then that if some partial-wave bands are absorbed, the *phase* of the remaining ones be modified in such a way that the output remains causal. Mathematically, if the signal partial-wave content $\tilde{s}_{a\infty}(p)$ in (7.149) is entire and analytic in the lower half-plane and the output $\tilde{s}'_{a\infty}(p)$ is required to be likewise, the transfer function $\tilde{\varphi}(p)$ must have the same property.

The condition for a causal filter is thus that its transfer function satisfy the dispersion relations (7.146) for $a = 0$. We shall now relate this to its absorptive and dispersive characteristics.

7.4.11. Absorptive and Dispersive Characteristics

We can write the transfer function in (7.149) as

$$\tilde{\varphi}(p) = (2\pi)^{-1/2}[\alpha(p) + i\beta(p)], \qquad \alpha(p), \beta(p) \text{ real for } p \text{ real.} \quad (7.150)$$

If we insist on having a filter which transforms real input signals into real output ones, as only real quantities are meaningful (exception taken of quantum-mechanical measurements, where phases of the wave function, although not directly measurable, have measurable effects), then $\varphi(q)$ must be real, whence (Table 7.2) $\tilde{\varphi}(p)^* = \tilde{\varphi}(-p^*)$. This implies that $\alpha(p)$ must be an *even* function of p, while $\beta(p)$ must be odd. Assume the input signal is a single wave:

$$s(q) = \cos \omega q, \quad (7.151a)$$

$$\tilde{s}(p) = (\pi/2)^{1/2}[\delta(p - \omega) + \delta(p + \omega)]. \quad (7.151b)$$

By taking into account the parity of $\alpha(p)$ and $\beta(p)$ in (7.150), the output signal will be

$$\begin{aligned}\tilde{s}'(p) &= (\pi/2)^{1/2}\{\alpha(p)[\delta(p - \omega) + \delta(p + \omega)] + i\beta(p)[\delta(p - \omega) + \delta(p + \omega)]\} \\ &= (\pi/2)^{1/2}\{\alpha(\omega)[\delta(p - \omega) + \delta(p + \omega)] + i\beta(\omega)[\delta(p - \omega) - \delta(p + \omega)]\}\end{aligned} \quad (7.152a)$$

$$s'(q) = \alpha(\omega) \cos \omega q + \beta(\omega) \sin \omega q. \quad (7.152b)$$

We can thus identify $\alpha(p)$ with the *absorptive* characteristics of the filter, $\alpha(p) = 1$ meaning perfect transparency, and $\beta(p)$, which shifts the phase of the input monochromatic waves, with its *dispersive* properties. These are, of course, not independent but, if the filter is to be causal, must satisfy the dispersion relations (7.146). These read

$$\alpha(p) = \pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}\beta(p), \quad (7.153a)$$

$$\beta(p) = -\pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}\alpha(p). \quad (7.153b)$$

In deriving the dispersion relations (7.146) we assumed the causal function to satisfy the conditions of the Fourier integral theorem. Now, for band-absorbing filters, $\alpha(p) < 1$ for some finite bands on the p-line, but $\alpha(p) = 1$, perfect transparency, may be the case for all other values—or it may be constant. In this case Eqs. (7.153) cease to be valid as the addition of a constant term to $\alpha(p)$ in (7.153b) does nothing to $\beta(p)$ since

$$\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1} = 0$$

while (7.153a) is changed by the constant's addition. Worse cases are those in which we want to represent *differencer* filters, i.e., where $s'(q) \sim d^n s(q)/dq^n$, as there we need $\varphi(q) \sim \delta^{(n)}(q)$ in (7.148) and hence $\tilde{\varphi}(p) \sim p^n$ in (7.150). The transfer function still qualifies as causal, but the dispersion relations (7.153) lose their meaning. For these functions we can still write, however, *dispersion relations with n subtractions.*

7.4.12. Subtractions

We shall assume that $(p - p_1 - i\varepsilon')^{-n}\tilde{f}_{0\infty}(p)$, $\varepsilon' > 0$, is absolutely integrable and, it will turn out, $\tilde{f}_{0\infty}(p)$ must be $n - 1$ times differentiable. This function is still causal since it is entire and analytic in the lower half-plane as the newly introduced n-fold pole lies on $+i\varepsilon'$. We write the usual dispersion relation (7.145) for the new function ($a = 0$ here), letting $\varepsilon' \to 0^+$ and taking note that the principal value in (7.145) does *not* refer to the new limit, for which (7.140b) must be used. We have

$$(p - p_1)^{-n}\tilde{f}_{0\infty}(p) = (\pi i)^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1} \times \{(p' - p_1)^{-n} + (-1)^n i\pi[(n-1)!]^{-1}\delta^{(n-1)}(p' - p_1)\} \times \tilde{f}_{0\infty}(p'). \tag{7.154}$$

We thus write the new n-times-subtracted dispersion relation

$$\tilde{f}_{0\infty}(p) = (\pi i)^{-1}(p - p_1)^n\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}(p' - p_1)^{-n}\tilde{f}_{0\infty}(p') + \sum_{m=0}^{n-1}(m!)^{-1}(p - p_1)^m d^m\tilde{f}_{0\infty}(p_1)/dp_1{}^m. \tag{7.155}$$

For $n = 0$ we recover (7.145). The addition of a constant to $\tilde{f}_{0\infty}(p)$ now requires one subtraction, for which the second term in (7.155) is $\tilde{f}_{0\infty}(p_1)$, which means in turn that the value of $\tilde{f}_{0\infty}(p)$ must be known at least at one point p_1. For n subtractions we must know n data values about the function $\tilde{f}_{0\infty}(p)$. The real and imaginary parts of (7.155) will finally relate the absorptive and dispersive parts of the filter transfer function.

Exercise 7.43. Repeat the subtraction procedure using different points $p_1, p_2, \ldots, p_s$ in factors raised to powers $n_1, n_2, \ldots, n_s$ such that $\sum_k n_k = n$. The n data values can thus be the values of $\tilde{f}_{0\infty}(p)$ and/or its derivatives at one/several points p_k.

Exercise 7.44. Repeat the subtraction procedure for functions $\tilde{f}_{a\infty}(p)$ and functions $\tilde{f}_{-\infty b}(p)$.

7.4.13. Further Comments and References

There are many directions in which the interested reader can continue in the subject sketched in this section. Bremmerman's book (1965) has been suggested before for its unified treatment of complex variable theory, generalized functions, and Fourier transforms. Growth conditions of Fourier transforms of functions analytic in strips lead to a number of results of the *Paley–Wiener* type. A digest of these can be found in Dym and McKean (1972, Section 3.3) or in the introduction of the original book by Paley and Wiener (1934). Communication theory, as can be expected, makes full use of dispersion relations in describing filter networks with complex impedance. On this subject, see the book by Friedland *et al.* (1961). Related to this subject is the description of the behavior of an electromagnetic signal in a dispersive medium, where the phenomena of phase vs. group velocities and forerunner waves appear. Brillouin (1960) has written a book on the subject with contributions due to Sommerfeld. It does not use the language of dispersion relations. A more recent and unified treatment can be found in a book by Müller (1969).

The application of dispersion relations in elementary particle physics has grown into a major field including *S*-matrix theory and Regge poles. The fundamental requirement of causality allows the specification of several necessary properties of the *S matrix*, an operator describing a scattering process. Subtraction constants are related to interaction strengths. A book by Hilgevoord (1960) contains the results up to 1960, before the current surge of interest in the field. Many texts on quantum mechanics contain chapters on this subject. Among the books specializing in this subject, see those by Newton (1964, 1966), Nussenzveig (1972), and Simon (1976).

7.5. Oscillator Wave Functions

There is one rather interesting *denumerable* orthonormal basis $\{\Psi_n\}_{n=0}^{\infty}$ for $\mathscr{L}^2(\mathscr{R})$ whose properties under Fourier transformation are such that they are *self-reciprocal* under the operation $\mathbb{F}\Psi_n = (-i)^n\Psi_n$. In this section we shall find these functions and explore their main properties. They are particularly important in physics since they happen to be the wave functions of the quantum-mechanical harmonic oscillator system. We shall prepare in this way the terrain for the introduction of the Bargmann transform (Section 9.2). The second main topic is the *repulsive* oscillator wave function basis.

7.5.1. Self-Reciprocal Functions and Operators under Fourier Transformation

In Section 7.1 we saw that the Fourier transform of a unit Gaussian bell function of width ω was another such function of width $1/\omega$ [Eq. (7.22)]. Hence a function proportional to a Gaussian of *unit* width,

$$\Psi_0(q) \coloneqq 2^{1/2}\pi^{1/4}G_1(q) = \pi^{-1/4}\exp(-q^2/2), \tag{7.156}$$

will be *self-reciprocal* under Fourier transformation: $\mathbb{F}\boldsymbol{\Psi}_0 = \boldsymbol{\Psi}_0$. We have chosen the constant $\pi^{-1/4}$ in front of the exponential so that the function will have unit norm:

$$\|\boldsymbol{\Psi}_0\|^2 = (\boldsymbol{\Psi}_0, \boldsymbol{\Psi}_0) = \int_{-\infty}^{\infty} dq\,|\Psi_0(q)|^2 = 1 \tag{7.157}$$

[compare with (7.21)]. How can we generate other self-reciprocal functions? If we had an operator $\mathbb{Z}$ such that

$$\mathbb{F}\mathbb{Z}\mathbb{F}^{-1} = \rho\mathbb{Z}, \tag{7.157a}$$

then $\mathbb{Z}\boldsymbol{\Psi}_0$ as well as any $\mathbb{Z}^n\boldsymbol{\Psi}_0$ would have the property

$$\mathbb{F}\mathbb{Z}^n\boldsymbol{\Psi}_0 = (\mathbb{F}\mathbb{Z}\mathbb{F}^{-1})^n\boldsymbol{\Psi}_0 = \rho^n\mathbb{Z}^n\boldsymbol{\Psi}_0. \tag{7.157b}$$

Moreover, as $\mathbb{F}^4 = \mathbb{1}$ [Eq. (7.26)], ρ can be only a fourth root of unity, i.e., $\rho = 1, -1, i,$ or $-i$. Most of the operators we have introduced can be expressed in terms of the operators $\mathbb{Q}$ and $\mathbb{P}$ [Eqs. (7.55) and (7.56)]: multiplication of a function by its argument and $-i$ times differentiation. Further, as these operators turn into each other under Fourier transformation [Eq. (7.57)], we can propose their most general *linear* combination:

$$\mathbb{Z} = a\mathbb{Q} + b\mathbb{P}. \tag{7.158}$$

Asking for

$$\lambda\mathbb{Z} = \mathbb{F}\mathbb{Z}\mathbb{F}^{-1} = a\mathbb{F}\mathbb{Q}\mathbb{F}^{-1} + b\mathbb{F}\mathbb{Q}\mathbb{F}^{-1} = -a\mathbb{P} + b\mathbb{Q}, \tag{7.159}$$

we obtain $b = \lambda a$ and $a = -\lambda b$. For $\lambda = 1$ or -1 this equation has only the trivial solution $a = 0 = b$. For $\lambda = i$ or $-i$, choosing $a = 2^{-1/2}$ for later convenience, we find

$$\mathbb{Z} \coloneqq 2^{-1/2}(\mathbb{Q} + i\mathbb{P}) = 2^{-1/2}\left(q + \frac{d}{dq}\right), \tag{7.160a}$$

$$\mathbb{Z}^\dagger \coloneqq 2^{-1/2}(\mathbb{Q} - i\mathbb{P}) = 2^{-1/2}\left(q - \frac{d}{dq}\right). \tag{7.160b}$$

We have written (7.160b) as the adjoint of $\mathbb{Z}$ since $\mathbb{Q}$ and $\mathbb{P}$ are self-adjoint

operators in $\mathscr{L}^2(\mathscr{R})$ and $(i\mathbb{1})^\dagger = -i\mathbb{1}$. Now, by acting on the *ground-state* function (7.156), $\mathbb{Z}$ in (7.160a) produces the zero function:

$$\mathbb{Z}\Psi_0(q) = 2^{-1/2}\pi^{-1/4}\left(q + \frac{d}{dq}\right)\exp(-q^2/2) = 0. \tag{7.161}$$

Thus, only $\mathbb{Z}^\dagger$ in (7.160b) can be used to produce other self-reciprocal functions. Since the operator $\mathbb{Z}^\dagger$ is self-reciprocal under Fourier transformation, with $\lambda = -i$, $\mathbb{Z}^\dagger\Psi_0$ will be also; $(\mathbb{Z}^\dagger)^2\Psi_0$ will correspond to $\lambda = -1$, $(\mathbb{Z}^\dagger)^3\Psi_0$ to $\lambda = i$, and $(\mathbb{Z}^\dagger)^4\Psi_0$ to $\lambda = 1$. Now, functions corresponding to different eigenvalues of unitary (or hermitian) operators are orthogonal. In fact we shall show that all $\Psi_n := c_n(\mathbb{Z}^\dagger)^n\Psi_0$ are mutually orthogonal and choose the constants c_n so that they be ortho*normal*. For this purpose we need to know some facts about the operators (7.160). Their *commutator* [see Eqs. (7.59), (7.65), and (7.66)] is

$$\begin{aligned}[\mathbb{Z}, \mathbb{Z}^\dagger] &:= \mathbb{Z}\mathbb{Z}^\dagger - \mathbb{Z}^\dagger\mathbb{Z} = \tfrac{1}{2}[\mathbb{Q} + i\mathbb{P}, \mathbb{Q} - i\mathbb{P}] \\ &= \tfrac{1}{2}([\mathbb{Q}, \mathbb{Q}] + i[\mathbb{P}, \mathbb{Q}] - i[\mathbb{Q}, \mathbb{P}] + [\mathbb{P}, \mathbb{P}]) \\ &= -i[\mathbb{Q}, \mathbb{P}] = \mathbb{1}. \end{aligned} \tag{7.162}$$

By induction, we can prove that

$$[\mathbb{Z}^m, \mathbb{Z}^\dagger] = m\mathbb{Z}^{m-1}, \tag{7.163a}$$

$$[\mathbb{Z}, (\mathbb{Z}^\dagger)^n] = n(\mathbb{Z}^\dagger)^{n-1}, \tag{7.163b}$$

$$[\mathbb{Z}^m, (\mathbb{Z}^\dagger)^n] = \sum_{k=1}^{\min(m,n)} \frac{m!n!}{(m-k)!(n-k)!k!}(\mathbb{Z}^\dagger)^{n-k}\mathbb{Z}^{m-k}. \tag{7.163c}$$

Exercise 7.45. Verify (7.163). Compare with (7.67) for $\mathbb{Q}$ and $\mathbb{P}$.

7.5.2. Orthogonality of the Generated Set

From adjunction it follows that, for $m > n$, (Ψ_n, Ψ_m) is proportional to

$$\begin{aligned}((\mathbb{Z}^\dagger)^n\Psi_0, (\mathbb{Z}^\dagger)^m\Psi_0) &= (\mathbb{Z}^m(\mathbb{Z}^\dagger)^n\Psi_0, \Psi_0) \\ &= ((\mathbb{Z}^\dagger)^n\mathbb{Z}^m\Psi_0, \Psi_0) + ([\mathbb{Z}^m, (\mathbb{Z}^\dagger)^n]\Psi_0, \Psi_0). \end{aligned} \tag{7.164}$$

Now, due to (7.161), the first term disappears, while the second, after use of (7.163c), shows that we are also left with powers of $\mathbb{Z}$ acting on Ψ_0 and hence it also vanishes. If $m < n$, we repeat the procedure on the second member of the inner product, obtaining zero again. Hence (7.164) is zero

for $m \neq n$, and all $\{\Psi_n\}_{n=0}^{\infty}$ are mutually orthogonal. When $m = n$, the last term in (7.164), for $m = k = n$, yields

$$(\Psi_n, \Psi_n) = |c_n|^2(\mathbb{Z}^n(\mathbb{Z}^\dagger)^n\Psi_0, \Psi_0) = |c_n|^2 n!\,(\Psi_0, \Psi_0). \tag{7.165a}$$

This allows us to fix the modulus of c_n as $(n!)^{-1/2}$, so that $\|\Psi_n\| = 1$ and, for all n, m:

$$(\Psi_n, \Psi_m) = \delta_{nm}. \tag{7.165b}$$

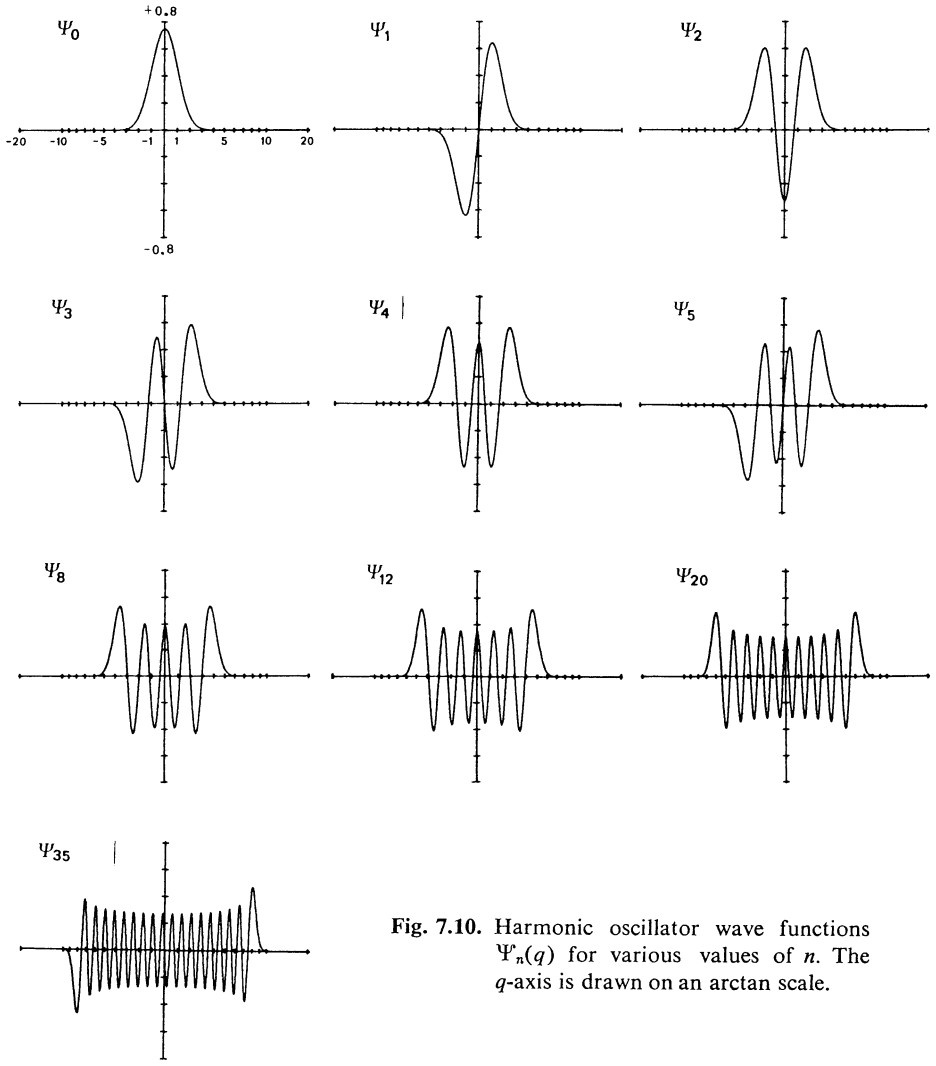


Fig. 7.10. Harmonic oscillator wave functions $\Psi_n(q)$ for various values of n. The q-axis is drawn on an arctan scale.

Table 7.3 The First Few Hermite Polynomials

$$
\begin{aligned}
H_0(q) &= 1 \\
H_1(q) &= 2q \\
H_2(q) &= 4q^2 - 2 \\
H_3(q) &= 8q^3 - 12q \\
H_4(q) &= 16q^4 - 48q^2 + 12 \\
H_5(q) &= 32q^5 - 160q^3 + 120q \\
H_6(q) &= 64q^6 - 480q^4 + 720q^2 - 120 \\
H_7(q) &= 128q^7 - 1344q^5 + 3360q^3 - 1680q \\
H_8(q) &= 256q^8 - 3584q^6 + 13{,}440q^4 - 13{,}440q^2 + 1680 \\
&\cdots
\end{aligned}
$$

By choosing c_n as real, the basis functions are thus

$$
\begin{aligned}
\Psi_n(q) &:= (n!)^{-1/2}(\mathbb{Z}^\dagger)^n \Psi_0(q) \\
&= (n!\, 2^n)^{-1/2}\left(q - \frac{d}{dq}\right)^n \Psi_0(q) \\
&= (n!\, 2^n \pi^{1/2})^{-1/2}\left(q - \frac{d}{dq}\right)^n \exp(-q^2/2) \\
&= (n!\, 2^n \pi^{1/2})^{-1/2}(-1)^n \exp(q^2/2) d^n/dq^n \exp(-q^2) \\
&=: (n!\, 2^n \pi^{1/2})^{-1/2} H_n(q) \exp(-q^2/2). \qquad (7.166)
\end{aligned}
$$

Exercise 7.46. Verify the next to last equality in (7.166). This can easily be done by induction. Show that $\Psi_n(-q) = (-1)^n \Psi_n(q)$. This is checked by noting that $\Psi_0(q)$ is even and $\mathbb{Z}^\dagger$ is of odd parity.

It is not difficult to see that $\Psi_n(q)$ has the form $\exp(-q^2/2)$ times a *polynomial of order n*, $H_n(q)$. These are the *Hermite* polynomials. In Fig. 7.10 we have plotted some $\Psi_n(q)$'s for n up to 35. The first few Hermite polynomials are given in Table 7.3. Equations (7.166) for $n = 0, 1, 2, \ldots$ thus define a denumerable orthonormal set of functions which are self-reciprocal under Fourier transformation:

$$(\mathbb{F}\Psi_n)(q) = \exp(-i\pi n/2)\Psi_n(q). \qquad (7.167)$$

7.5.3. Raising and Lowering Operators

The construction procedure we have followed is interesting in itself: From the *ground state* $\Psi_0(q)$ we have been able to obtain all other $\Psi_n(q)$ by successive application of the *raising* (or *creation*) operator $\mathbb{Z}^\dagger$. The action of this operator is to transform $\Psi_n(q)$ into $\Psi_{n+1}(q)$ as

$$\mathbb{Z}^\dagger \Psi_n = (n!)^{-1/2}(\mathbb{Z}^\dagger)^{n+1}\Psi_0 = (n+1)^{1/2}\Psi_{n+1}. \qquad (7.168)$$

The action of $\mathbb{Z}$ as defined in (7.160a) is that of a *lowering* (or *annihilation*) operator: using (7.161) and (7.163b), we find

$$\begin{aligned}\mathbb{Z}\Psi_n &= (n!)^{-1/2}\mathbb{Z}(\mathbb{Z}^\dagger)^n\Psi_0 \\ &= (n!)^{-1/2}\{(\mathbb{Z}^\dagger)^n\mathbb{Z} + [\mathbb{Z}, (\mathbb{Z}^\dagger)^n]\}\Psi_0 \\ &= (n!)^{-1/2}n(\mathbb{Z}^\dagger)^{n-1}\Psi_0 = n^{1/2}\Psi_{n-1};\end{aligned} \tag{7.169}$$

in particular, for $n = 0$ we regain (7.161).

7.5.4. The Quantum Harmonic Oscillator Hamiltonian Operator

Equations (7.168) and (7.169) can be combined as

$$\begin{aligned}\mathbb{N}\Psi_n(q) &:= \mathbb{Z}^\dagger\mathbb{Z}\Psi_n(q) = n^{1/2}\mathbb{Z}^\dagger\Psi_{n-1}(q) = n\Psi_n(q) \\ &= \frac{1}{2}\left(q - \frac{d}{dq}\right)\left(q + \frac{d}{dq}\right)\Psi_n(q) = \frac{1}{2}\left(-\frac{d^2}{dq^2} + q^2 - 1\right)\Psi_n(q)\end{aligned}$$

$$n = 0, 1, 2, \ldots. \tag{7.170}$$

We shall call $\mathbb{N}$ the *number* operator for the set $\{\Psi_n\}_{n=0}^{\infty}$. This operator is *self*-adjoint (as $[\mathbb{Z}^\dagger,\mathbb{Z}] = [\mathbb{Z}^\dagger,\mathbb{Z}]$ on $\mathscr{L}^2(\mathscr{R})$); its eigenfunctions thus ought to be orthogonal, as we showed them to be above. In quantum mechanics, the operator $\mathbb{N}$ defined here is related to

$$\mathbb{H}^h := \frac{1}{2}\left(-\frac{d^2}{dq^2} + q^2\right) = \frac{1}{2}(\mathbb{P}^2 + \mathbb{Q}^2) = \mathbb{N} + \tfrac{1}{2}\mathbb{1}, \tag{7.171}$$

which happens to be the Schrödinger Hamiltonian for the harmonic oscillator system. The eigenfunctions of the Schrödinger operator (7.171), the eigenstates of the system, are thus $\{\Psi_n(q)\}_{n=0}^{\infty}$ with eigenvalues—energies—$n + \frac{1}{2}$, $n = 0, 1, 2, \ldots$ in *natural* units. If ordinary physical units are used, this is $\hbar\omega(n + \frac{1}{2})$, where $\hbar$ is Planck's constant h divided by 2π and ω is the classical oscillator frequency. The energy being quantized in units of $\hbar\omega$, $\mathbb{Z}^\dagger$ and $\mathbb{Z}$ act as *creation* and *annihilation* operators of energy quanta for the system.

Exercise 7.47. Verify the commutation relations

$$[\mathbb{N}, \mathbb{Z}^\dagger] = \mathbb{Z}^\dagger, \qquad [\mathbb{N}, \mathbb{Z}] = -\mathbb{Z}. \tag{7.172}$$

Show that if Ψ_n is an eigenfunction of $\mathbb{N}$ corresponding to an eigenvalue n, (7.172) implies that $\mathbb{Z}^\dagger\Psi_n$ and $\mathbb{Z}\Psi_n$ will also be eigenfunctions of $\mathbb{N}$ with eigenvalues $n + 1$ and $n - 1$.

Exercise 7.48. In searching for operators with the properties (7.157) in order to generate self-reciprocal functions under Fourier transformations, we can propose *second-order* ones of the form

$$\mathbb{J} = a\mathbb{P}^2 + b(\mathbb{P}\mathbb{Q} + \mathbb{Q}\mathbb{P}) + c\mathbb{Q}^2, \qquad \mathbb{F}\mathbb{J}\mathbb{F}^{-1} = \mu\mathbb{J}. \tag{7.173}$$

Following (7.158)–(7.160), show that only $\mu^2 = 1$ yields nontrivial solutions. For $\mu = 1$, $b = 0$, and we have $a = c$, so we define

$$\mathbb{J}_0 := \tfrac{1}{4}(\mathbb{P}^2 + \mathbb{Q}^2) = \tfrac{1}{2}\mathbb{H}^h = \tfrac{1}{2}\mathbb{N} + \tfrac{1}{4}\mathbb{1}, \tag{7.174a}$$

which is, up to a chosen multiplicative constant, the operator (7.171), which neither raises nor lowers Ψ_n to any of its neighbors. For $\mu = -1$ we have two independent solutions:

$$\mathbb{J}_+ := \tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2) + \frac{i}{4}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}) = -\tfrac{1}{2}(\mathbb{Z}^\dagger)^2 =: \mathbb{J}_1 + i\mathbb{J}_2, \tag{7.174b}$$

$$\mathbb{J}_- := \tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2) - \frac{i}{4}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}) = -\tfrac{1}{2}\mathbb{Z}^2 = \mathbb{J}_+{}^\dagger =: \mathbb{J}_1 - i\mathbb{J}_2, \tag{7.174c}$$

where we have chosen a convenient set of constants for a and b. The operators $\mathbb{J}_+$ and $\mathbb{J}_-$ thus raise and lower Ψ_n by twos. Some further group-theoretical properties are obtained in Exercises 7.49 and 7.50.

Exercise 7.49. Verify that the commutation relations of the operators (7.174) are

$$[\mathbb{J}_0, \mathbb{J}_\pm] = \pm\mathbb{J}_\pm, \qquad [\mathbb{J}_+, \mathbb{J}_-] = -2\mathbb{J}_0, \tag{7.175a}$$

$$[\mathbb{J}_1, \mathbb{J}_2] = -i\mathbb{J}_0, \qquad [\mathbb{J}_0, \mathbb{J}_1] = i\mathbb{J}_2, \qquad [\mathbb{J}_2, \mathbb{J}_0] = i\mathbb{J}_1. \tag{7.175b}$$

[Equation (7.175a) or (7.175b) determines the $\mathbb{J}$'s as the generators of the isomorphic Lie algebras $sl(2, R) \simeq su(1, 1) \simeq so(2, 1) \simeq sp(2, R)$. See the book by Miller (1972) on Lie algebras and groups.] Show that, as in Exercise 7.47, if Ψ_n is an eigenfunction of $\mathbb{J}_0$ with eigenvalue $n/2$, $\mathbb{J}_\pm\Psi_n$ will also be an eigenfunction of $\mathbb{J}_0$ with eigenvalue $(n \pm 2)/2$. In acting on Ψ_0 the raising operator (7.174b) therefore generates all Ψ_n's for *even* n only—or all odd n's if we start from Ψ_1.

Exercise 7.50. Verify the identities

$$\mathbb{C} := \mathbb{J}_1{}^2 + \mathbb{J}_2{}^2 - \mathbb{J}_0{}^2 = \mathbb{J}_\pm\mathbb{J}_\mp - \mathbb{J}_0(\mathbb{J}_0 \mp \mathbb{1}) = \tfrac{3}{16}. \tag{7.176}$$

The first equality follows from (7.175) only, while the second requires the concrete realization (7.174) in terms of differential operators. Note that $[\mathbb{C}, \mathbb{J}_i] = 0$ for $i = 0, 1, 2$, defining $\mathbb{C}$ as the *Casimir* operator of the Lie algebra (7.175). Show that

$$\mathbb{J}_\pm\Psi_n = d_n{}^\pm\Psi_{n\pm2}, \qquad 4|d_n{}^+|^2 = (n+1)(n+2), \qquad 4|d_n{}^-|^2 = n(n-1), \tag{7.177}$$

by making $\|\mathbb{J}_\pm\Psi_n\|^2 = 1$ for all n, by using $\mathbb{J}_\mp = \mathbb{J}_\pm^\dagger$ in order to let all operators act on one side of the inner product, and finally by applying (7.176). Note that (7.177) checks with (7.168)–(7.169) when the relation (7.174) between $\mathbb{J}$'s and $\mathbb{Z}$'s is used.

7.5.5. Completeness of the Harmonic Oscillator Wave Functions

We now return to the study of the functions $\Psi_n(q)$ of Eq. (7.166). We note that they are all infinitely differentiable and, due to the exponential

factor, are *rapidly decreasing*, i.e., $q^m d^n \Psi_r(q)/dq^n \to 0$ for $|q| \to \infty$ and any m, n, and r. The set thus belongs to $\mathscr{C}_\downarrow^\infty$. Moreover, as we shall show, an $\mathscr{L}^2(\mathscr{R})$ function $f(q)$ which is orthogonal to all $\Psi_n(q)$'s is equivalent to the zero function. The denumerable set $\{\Psi_n(q)\}_{n=0}^\infty$ thus constitutes an *orthonormal basis* for $\mathscr{L}^2(\mathscr{R})$. To this end, we construct a *generating function* of the set:

$$\begin{aligned} G_\psi(x, q) &\coloneqq \sum_{n=0}^{\infty} (n!)^{-1/2} (x/2^{1/2})^n \Psi_n(q) \\ &= \pi^{-1/4} \exp(q^2/2) \sum_{n=0}^{\infty} (n!)^{-1} (-x/2)^n d^n/dq^n \exp(-q^2) \\ &= \pi^{-1/4} \exp(-q^2/2 + qx - x^2/4) \\ &= \exp(x^2/4) \Psi_0(q - x), \end{aligned} \tag{7.178}$$

where we have used the next to last form of Eq. (7.166) and the Taylor expansion of the Gaussian function around q. Now, if $(\mathbf{\Psi}_n, \mathbf{f}) = 0$ for all $n = 0, 1, 2, \ldots$ and $\mathbf{f} \in \mathscr{L}^2(\mathscr{R})$, then

$$0 = \big(G_\psi(x, \cdot), \mathbf{f}\big) = \exp(x^2/4) \int_{-\infty}^{\infty} dq \Psi_0(q - x) f(q), \tag{7.179}$$

which means that $(\Psi_0 * f)(x) = 0$. The Fourier transform of this restriction is $\Psi_0(y)\tilde{f}(y) = 0$, which in turn implies $\tilde{f}(y) = 0$, and hence $f(q)$ is equivalent with 0. In this sense the set $\{\mathbf{\Psi}_n\}_{n=0}^\infty \in \mathscr{C}_\downarrow^\infty \subset \mathscr{L}^2(\mathscr{R})$ is *dense* in $\mathscr{L}^2(\mathscr{R})$ and, in fact, also dense in the space of generalized functions $\mathscr{S}'$ with test functions in $\mathscr{C}_\downarrow^\infty$.

7.5.6. Harmonic Oscillator Expansions

Any vector $\mathbf{f}$ in $\mathscr{L}^2(\mathscr{R})$ or $\mathscr{S}'$ can be approximated (in the sense of the inner product with a test function in $\mathscr{C}_\downarrow^\infty$) by a linear combination of elements in $\mathscr{C}_\downarrow^\infty$ as

$$f(q) = \sum_{n=0}^{\infty} f_n^{\Psi} \Psi_n(q), \tag{7.180a}$$

where, due to the orthonormality of the basis, the generalized Fourier coefficients are

$$f_n^{\Psi} = (\mathbf{\Psi}_n, \mathbf{f}). \tag{7.180b}$$

The $\{f_n^{\Psi}\}_{n=0}^\infty$ constitute the coordinates of $\mathbf{f}$ in the $\mathbf{\Psi}$-*basis*. The original function $\mathbf{f}$ in (7.180b) and its synthesis (7.180a) can differ at most on a set of isolated points on $\mathscr{R}$. Moreover, the Parseval identity

$$(\mathbf{f}, \mathbf{g}) = \int_{-\infty}^{\infty} dq f(q)^* g(q) = \sum_{n=0}^{\infty} f_n^{\Psi *} g_n^{\Psi} \tag{7.180c}$$

also holds. The completeness of the Ψ-basis implies that, in the appropriate space of test functions,

$$\sum_{n=0}^{\infty} \Psi_n(q_1)\Psi_n(q_2) = \delta(q_1 - q_2). \tag{7.180d}$$

Expansion series in the denumerable Ψ-basis follow the same philosophy as the expansions in exponential and Bessel series discussed in Chapter 6, except that the space is here $\mathscr{L}^2(\mathscr{R})$ rather than $\mathscr{L}^2(a, b)$ and the self-adjoint operator whose eigenfunctions we are using is $\mathbb{N}$ in Eq. (7.170) rather than ∇^2 as before. For the parallel of the Dirichlet conditions for pointwise convergence of Fourier series we have to turn to the literature on orthogonal polynomial expansions. See the book by Szegő (1939, Chapter IX) and those of Alexits (1961) and Boas and Buck (1964). As in the case of Taylor series where the expansion in powers of q (around the origin) is uniformly convergent within the largest circle, with center at the origin, where the function is regular (analytic and free of singularities) and divergent outside, expansions in series of polynomials orthogonal on a segment (a, b) (i.e., *Legendre*, *Gegenbauer*, or *Jacobi* polynomials) converge inside the largest *ellipse* with foci on a and b where the expanded function is regular. For polynomials orthogonal on a half-axis (a, ∞) (i.e., *Laguerre* polynomials), this region becomes the "interior" of a parabola with focus on a, while for Hermite polynomials—and thus the present $\Psi_n(q)$ functions—the series (7.180a) will converge within any *band* centered around the real axis where the expanded function is regular. The convergence is uniform for any finite subregion of this band. If the function has a bounded discontinuity at some point q_0, the width of the band shrinks to zero and the series converges—as in the Fourier case—to the midpoint of the discontinuity.

7.5.7. Translations

We shall illustrate the use of the expansion relations (7.180a)–(7.180d) for the case of the *translated* harmonic oscillator wave function:

$$\mathbb{T}_a\Psi_n(q) = \Psi_n(q + a) = \sum_{m=0}^{\infty} T_{mn}(a)\Psi_m(q), \tag{7.181a}$$

$$T_{mn}(a) = (\Psi_m, \mathbb{T}_a\Psi_m) = (\mathbb{T}_{-a}\Psi_m, \Psi_n). \tag{7.181b}$$

In the process of finding the linear combination coefficients $T_{mn}(a)$, we shall present several useful techniques, which will be applied later on.

According to (7.180b), the solution is

$$T_{mn}(a) = \int_{-\infty}^{\infty} dq\Psi_m(q)\Psi_n(q + a). \tag{7.182}$$

This integral is surely a finite number, as the Ψ's fall off as $\exp(-q^2/2)$ for $|q| \to \infty$, yet it is not trivial to calculate. We can make use of the generating function found in (7.178) by multiplying (7.182) by powers of two dummy variables, summing over n and m, and exchanging sums and integral:

$$\begin{aligned} T(x, y) &\coloneqq \sum_{m,n=0}^{\infty} (m!\, n!)^{-1/2} (x/2^{1/2})^m (y/2^{1/2})^n T_{mn}(a) \\ &= \int_{-\infty}^{\infty} dq G_\psi(x, q) G_\psi(y, q + a) \\ &= \pi^{-1/2} \exp[-(x^2 + y^2)/4 + ay - a^2/2] \\ &\quad \times \int_{-\infty}^{\infty} dq \exp[-q^2 + q(x + y - a)] \\ &= \exp(-a^2/4) \exp[(xy + ay - ax)/2]. \end{aligned} \tag{7.183a}$$

To solve the integral we have completed squares in the exponent and used the Euler integral (7.21). The use of the generating function thus allows us to solve the integral in (7.182) by solving the simpler integral in (7.183a). If we can now find the two-variable Taylor series of $T(x, y)$ and rearrange it in the form given by the defining sum in (7.183a), we shall regain the coefficients $T_{mn}(a)$. To this end we use the well-known Taylor series of the three last exponential functions and a triple-sum rearrangement formula [Appendix C, Eq. (C.5)], writing

$$\begin{aligned} T(x, y) &= \exp(-a^2/4) \sum_{k,m,n=0}^{\infty} (k!\, m!\, n!)^{-1} 2^{-k-m-n} (-1)^m a^{n+m} x^{m+k} y^{n+k} \\ &= \exp(-a^2/4) \sum_{m,n=0}^{\infty} \sum_{k=0}^{\min(m,n)} [k!\,(m-k)!\,(n-k)!]^{-1} \\ &\quad \times 2^{-m-n+k} (-1)^{m-k} a^{m+n-2k} x^m y^n. \end{aligned} \tag{7.183b}$$

Comparison of like powers of x and y with (7.183a) thus yields

$$\begin{aligned} T_{mn}(a) &= \exp(-a^2/4) 2^{-(n+m)/2} (-1)^m (n!\, m!)^{1/2} \\ &\quad \times \sum_{k=0}^{\min(m,n)} [k!\,(m-k)!\,(n-k)!]^{-1} 2^k (-1)^k a^{m+n-2k}. \end{aligned} \tag{7.184}$$

Exercise 7.51. Verify that (7.184) fulfills $T_{mn}(0) = \delta_{mn}$ and that due to (7.69)

$$\nabla^{\psi}_{mn} \coloneqq \frac{\partial}{\partial a} T_{mn}(a)|_{a=0} = \delta_{m,n-1}(n/2)^{1/2} - \delta_{m,n+1}[(n+1)/2]^{1/2} \tag{7.185a}$$

constitutes a "half-infinite" matrix which represents ∇ in the Ψ-basis and agrees with the action of $-i\mathbb{P}$ on $\Psi_n(q)$ obtained from (7.160) and (7.168)–(7.169). Equation (7.184) is the exponentiation of (7.185a).

Exercise 7.52. By Fourier transformation, find the action of the multiplication-by-exponential operator (7.29). On the Ψ-basis functions it is represented by a half-infinite matrix whose coefficients $E^{\psi}_{mn}(a)$ are $(-i)^{m-n}$ times those of the translation operator in (7.184). From these find that matrix representing $\mathbb{Q}$:

$$Q^{\psi}_{mn} := \frac{\partial}{\partial a} E^{\psi}_{mn}(a)|_{a=0} = \delta_{m,n-1}(n/2)^{1/2} + \delta_{m,n+1}[(n+1)/2]^{1/2}. \quad (7.185b)$$

Verify that this agrees with the action of $\mathbb{Q}$ on $\Psi_n(q)$ obtained from (7.160) and (7.168)–(7.169).

Exercise 7.53. Verify that $\mathbf{Q}^{\psi} := \|Q^{\psi}_{mn}\|$ and $\mathbf{P}^{\psi} := \|-i\nabla^{\psi}_{mn}\|$, considered as half-infinite matrices whose rows and columns range over all nonnegative integers, in (7.185) satisfy the Heisenberg commutation relation (7.59b).

One case which will appear later on (as *coherent states*) is the oscillator wave-function series for the displaced Gaussian bell $\Psi_0(q+a)$. For $n=0$ the sum in (7.184) reduces to the single term $k=0$, and hence

$$T_{m0}(a) = \exp(-a^2/4)(m!)^{-1/2}(-a/2^{1/2})^m \quad (7.186a)$$

whereby

$$\Psi_0(q+a) = \exp(-a^2/4)\sum_{m=0}^{\infty}(m!)^{-1/2}(-a/2^{1/2})^m\Psi_m(q)$$
$$= \exp(-a^2/4)G_{\psi}(-a,q). \quad (7.186b)$$

In view of (7.178), this is an identity.

7.5.8. Coherent States

One rather remarkable property of the functions (7.186) is that, for all complex a, they are *eigenfunctions of the lowering operator*:

$$\mathbb{Z}\Psi_0(q+a) = (-a/2^{1/2})\Psi_0(q+a). \quad (7.187)$$

This fact is somewhat unexpected since $\mathbb{Z}$ is *not* a self-adjoint operator. Equation (7.187) holds as can easily be verified since each term in the sum is lowered by one value of m, the term $n=0$ disappearing. As the sum is infinite, however, lowering the terms by one unit still leaves us with an infinite sum.

A function *proportional* to (7.186b) can be found by acting with $\exp(a\mathbb{Z}^{\dagger})$ on $\Psi_0(q)$ and using the first equality in (7.166):

$$\Upsilon_c(q) := \exp(c\mathbb{Z}^{\dagger})\Psi_0(q) = \sum_{n=0}^{\infty}(n!)^{-1}c^n(\mathbb{Z}^{\dagger})^n\Psi_0(q)$$
$$= \sum_{n=0}^{\infty}(n!)^{-1/2}c^n\Psi_n(q) = \exp(c^2/2)\Psi_0(q-2^{1/2}c)$$
$$= G_{\psi}(2^{1/2}c,q) = \pi^{-1/4}\exp(-q^2/2 - c^2/2 + 2^{1/2}qc), \quad (7.188a)$$
$$\mathbb{Z}\Upsilon_c(q) = c\Upsilon_c(q). \quad (7.188b)$$

This is the definition of the *coherent states* in quantum optics [see, for example, the book by Klauder and Sudarshan (1968, Chapter 7) for a full account]. Mathematically, the states (7.188) do not look, perhaps, too exciting at present since they are basically displaced Gaussians. For *complex* c (7.188) will be seen to be rather useful. Physically, moreover, they happen to be the closest quantum-mechanical approximation to the classical harmonic oscillator motion and are widely employed in laser theory.

The coherent states (7.188) are not orthogonal; their inner product (overlap) can easily be calculated by the unitarity of translations and the result (7.186a):

$$\begin{aligned}(\Upsilon_c, \Upsilon_{c'}) &= \exp[(c^{*2} + c'^2)/2](\mathbb{T}_{-2^{1/2}c}\Psi_0, \mathbb{T}_{-2^{1/2}c'}\Psi_0)\\ &= \exp[(c^{*2} + c'^2)/2](\Psi_0, \mathbb{T}_{2^{1/2}c^* - 2^{1/2}c'}\Psi_0)\\ &= \exp[(c^{*2} + c'^2)/2]T_{00}(2^{1/2}c^* - 2^{1/2}c')\\ &= \exp[(c^{*2} + c'^2)/2]\exp[-(c^* - c')^2/2] = \exp(c^*c'). \quad (7.189)\end{aligned}$$

In Part IV we shall show that the set of coherent states $\{\Upsilon_c\}_{c\in\mathscr{C}}$ forms a basis for the (*Bargmann*) Hilbert space of entire analytic functions with certain growth conditions.

7.5.9. Some Properties of the Harmonic Oscillator Expansions

The expansion of an $\mathscr{L}^2(\mathscr{R})$ function in a harmonic oscillator wave-function series has several properties which have their counterparts in Fourier series and which we have collected in Table 7.4. (a) The Ψ partial-wave coefficients of a linear combination of functions are the linear combination of their partial-wave coefficients. (b) The functions of the Ψ-basis are real; hence if f_n^{ψ} are the series coefficients of $f(q)$, $f(q)^*$ will have coefficients $f_n^{\psi *}$. (c) The series coefficients for $f(-q)$ are, due to the parity of the basis functions, $(-1)^n f_n^{\psi}$. (d) The series coefficients for $df(q)/dq$ can be found from (7.185a) and are shown in Table 7.4. In this basis, therefore, unlike the Fourier case, they are *not* multiples of the series coefficients of the original functions. (e) If $\tilde{f}(q)$ is the Fourier transform of $f(q)$, due to (7.167), their Ψ partial-wave coefficients will be related as $\tilde{f}_n^{\psi} = (-i)^n f_n^{\psi}$. (f) Combining the two former results or directly from (7.185b) the Ψ coefficients of $qf(q)$ can be found in terms of those of $f(q)$ as in Table 7.4. (g) The role of ∇ under Fourier transformation is here taken by the number operator $\mathbb{N}$ in Eq. (7.170) or $\mathbb{H}^h$ in (7.171). Thus if $f(q)$ has Ψ coefficients f_n^{ψ}, those of $(-d^2/dq^2 + q^2)\cdot f(q)$ will be $(2n + 1)f_n^{\psi}$. (h) The Ψ coefficients of the product $f(q)g(q)$ are the corresponding generalized convolution of the coefficients of the factors. The finite-dimensional counterpart of this operation has been discussed in Section 3.1. Unfortunately, it is not so simple as for Fourier series or transforms.

Several miscellaneous properties of the harmonic oscillator functions follow. Some of them—mainly pertaining the Hermite polynomials—can be found in most special functions texts.

Exercise 7.54. Relationships between differentiability and convergence rate are not so easy to obtain for the Ψ-basis coordinates as for Fourier series coefficients in Section 4.4. Using similar techniques—absolute values, Schwartz inequalities, and Fourier transformation—for the operator $\mathbb{H}$ in (7.171), show that if $f(q)$ and $\tilde{f}(p)$ are such that their second derivatives are square-integrable (i.e., $\|\mathbf{f}''\| < \infty$, $\|\tilde{\mathbf{f}}''\| < \infty$), then the Ψ-basis coefficients' decrease is bounded as

$$|f_n| \leqslant (2n + 1)^{-1}(\|\mathbf{f}''\| + \|\tilde{\mathbf{f}}''\|). \tag{7.190}$$

Exercise 7.55. Prove the three-term *recursion relation* for the harmonic oscillator wave functions

$$\Psi_{n+1}(q) = [2/(n + 1)]^{1/2} q \Psi_n(q) - [n/(n + 1)]^{1/2} \Psi_{n-1}(q). \tag{7.191}$$

This can easily be found from (7.166), (7.185), or the Christoffel–Darboux formula for Hermite polynomials. It provides an economical algorithm for the numerical computation of the oscillator functions.

Exercise 7.56. Show the explicit form of the Hermite polynomials to be

$$H_n(q) = n! \sum_{m=0}^{[n/2]} \frac{(-1)^m (2q)^{n-2m}}{m!(n - 2m)!}, \tag{7.192}$$

where $[n/2]$ is the largest integer smaller or equal to $n/2$. This is most easily done using the generating function (7.178), expanding the next to last expression in powers of x, and comparing the coefficients with those of the second expression. You will come to use a double-summation exchange formula: Eq. (C.3).

Exercise 7.57. Prove the rather remarkable expression

$$\exp(-y\, d^2/dq^2) q^n = y^{n/2} H_n(q/2y^{1/2}). \tag{7.193}$$

This can be done first for $y = \frac{1}{4}$, comparing directly with (7.192) and later effecting a change of scale in q.

Exercise 7.58. Consider the variables $q_\pm := q_1 \pm q_2$, so that $\partial_{q_1} = \partial_{q_+} + \partial_{q_-}$ and $\partial_{q_2} = \partial_{q_+} - \partial_{q_-}$. On $\mathscr{C}^\infty$ functions of q_+ only, where the operator action is well defined, the following identity holds:

$$\exp(-\tfrac{1}{4}\partial_{q_+}^2) f(q_+) = \exp(-\tfrac{1}{8}\partial_{q_1}^2) \exp(-\tfrac{1}{8}\partial_{q_2}^2) f(q_+). \tag{7.194a}$$

Applying this on the Newton binomial

$$f(q_+) = q_+^{\,n} = \sum_{m=0}^{n} \binom{n}{m} q_1^{\,m} q_2^{\,n-m}, \tag{7.194b}$$

you can find by (7.192) the *addition formula* for Hermite polynomials,

$$H_n(q_1 + q_2) = 2^{-n/2} \sum_{m=0}^{n} \binom{n}{m} H_m(2^{1/2} q_1) H_{n-m}(2^{1/2} q_2), \tag{7.194c}$$

which in turn leads to

$$\Psi_n(q_1 + q_2) = \pi^{1/4}2^{-n/2}\exp[(q - y)^2/2]\sum_{m=0}^{n}\binom{n}{m}^{1/2}\Psi_m(2^{1/2}q_1)\Psi_{n-m}(2^{1/2}q_2). \tag{7.195}$$

The last equation can be verified independently by multiplying by $(x/2^{1/2})^n/(n!)^{1/2}$ and summing over n, using a double-summation exchange (Appendix C) and the generating function (7.178). See the difference from Eqs. (7.181)–(7.184).

Exercise 7.59. An upper bound for the zeros of Hermite polynomials is $(n - 1)[2/(n + 2)]^{1/2}$ [see the book by Szegő (1939, Section 6.32)]. For large n, show that this constrains $\Psi_n(q)$ to be significantly different from zero only for $q \leq (2n)^{1/2}$. The "width" of the functions $\Psi_n(q)$ in Fig. 7.10 is thus $\sim 2(2n)^{1/2}$. Show that, from the discussion in Section 2.1 and the description of phase space (Fig. 2.24), the maximum elongation in p and q of an oscillator with energy $n := E = (p^2 + q^2)/2$ is precisely $(2n)^{1/2}$.

7.5.10. Fourier Transformation Suggested as a Hyperdifferential Operator

One further consequence of the construction of the harmonic oscillator wave functions $\Psi_n(q)$ as functions which are self-reciprocal under Fourier transformation, Eq. (7.167), is that, as eigenfunctions of the operator $\mathbb{H}^h$ in (7.171),

$$(\mathbb{F}\Psi_n)(q) = \exp(-i\pi n/2)\Psi_n(q) = \exp[-\tfrac{1}{2}i\pi(\mathbb{H}^h - \tfrac{1}{2})]\Psi_n(q). \tag{7.196}$$

The last term is an exponentiated operator with the action of the Fourier transform on all elements of the Ψ-basis. As this basis is dense in the space of generalized functions, the action (7.196) will extend weakly to it. We can thus write the Fourier (*integral*) transform as the hyperdifferential operator

$$\mathbb{F} = \exp(i\pi/4)\exp[-i\pi(\mathbb{P}^2 + \mathbb{Q}^2)/4]. \tag{7.197}$$

This equality is valid if the functions acted upon are $\mathscr{C}_\downarrow^\infty$ functions. For

Table 7.4 A Function and Its Harmonic Oscillator Partial-Wave Coefficients under Some Operators and Operations

Operation	$f(q)$	f_n^Ψ
Linear combination	$af(q) + bg(q)$	$af_n^\Psi + bg_n^\Psi$
Complex conjugation	$f(q)^*$	$f_n^{\Psi *}$
Inversion	$f(-q)$	$(-1)^n f_n^\Psi$
Differentiation	$df(q)/dq$	$[(n+1)^{1/2}f_{n+1}^\Psi - n^{1/2}f_{n-1}^\Psi]/2^{1/2}$
Multiplication	$qf(q)$	$[(n+1)^{1/2}f_{n+1}^\Psi + n^{1/2}f_{n-1}^\Psi]/2^{1/2}$
	$\frac{1}{2}\left(-\frac{d^2}{dq^2} + q^2 - 1\right)f(q)$	nf_n^Ψ
Fourier transformation	$\tilde{f}(q)$	$(-i)^n f_n^\Psi$

$\mathscr{L}^2(\mathscr{R})$ or generalized functions, inner products with $\mathscr{C}_\downarrow^\infty$ test functions must be taken in order to give meaning to this expression.

In Part IV we shall give a unified description of hyperdifferential expressions such as (7.193) and (7.197).

7.5.11. The Quantum Repulsive Oscillator and Its Wave Functions

The second theme to be presented in this section on oscillator wave functions is a short analysis of the solutions of the differential equation

$$\mathbb{H}^r\chi_\lambda(q) = \lambda\chi_\lambda(q), \tag{7.198a}$$

$$\mathbb{H}^r := \frac{1}{2}(\mathbb{P}^2 - \mathbb{Q}^2) = -\frac{1}{2}\left(\frac{d^2}{dq^2} + q^2\right). \tag{7.198b}$$

Equations (7.198) resemble the harmonic oscillator equations (7.170)–(7.171) except for the sign of the $\mathbb{Q}^2$ term. The operator $\mathbb{H}^r$ is the Schrödinger Hamiltonian for the *repulsive* quantum oscillator system, whose potential energy $-q^2$ repels the particle from the origin. Some of the reasons to be interested in the solutions of (7.198) are the following: (a) They represent a neat application of Fourier transform theory, similar to the Airy function solution of (7.61)–(7.64), the free-fall (linear potential) quantum system. (b) Properties of orthogonality and completeness of the set $\{\chi_\lambda(q)\}_{\lambda\in\mathscr{R}}$, to be discussed in Section 8.2, will hinge on this derivation. (c) The repulsive oscillator, together with the linear potential, free-particle, and harmonic oscillator quantum Hamiltonians, constitutes a basis for the class of *quadratic* operators $\mathbb{H} = a\mathbb{P}^2 + b\mathbb{Q}\mathbb{P} + c\mathbb{Q}^2 + d\mathbb{P} + e\mathbb{Q} + f\mathbb{1}, a, \ldots, f \in \mathscr{C}$, whose Green's functions constitute the integral kernels of the linear canonical transforms of Part IV.

7.5.12. Finding the Repulsive Oscillator Wave Functions

Straightforward Fourier transformation of the differential equation (7.198) is not conducive to its solution since from (7.57) $\mathbb{F}\mathbb{H}^r\mathbb{F}^{-1} = -\mathbb{H}^r$, so no simplification is gained. If we could rid ourselves of the q^2 term in (7.198b) and replace it by, say, q, d/dq, or qd/dq, the Fourier method would reduce the degree of the differential equation as was done in (7.61). A change of function could achieve this: we let $\chi_\lambda(q) = \exp[\zeta(q)]\upsilon_\lambda(q)$ and, $\exp[\zeta(q)]$ being self-reproducing under d/dq, we arrange $\zeta(q)$ so that the second derivative cancels the troublesome q^2 term. Setting $\zeta(q) = cq^2$, with c as yet undetermined,

$$\mathbb{H}^r\chi_\lambda(q) = -\frac{1}{2}\exp(cq^2)\left[\frac{d^2}{dq^2} + 4cq\frac{d}{dq} + 2c + (4c^2 + 1)q^2\right]\upsilon_\lambda(q). \tag{7.199}$$

If, now, $4c^2 + 1 = 0$, i.e., $c = \sigma i/2$, $\sigma = \pm 1$, the differential equation which $v_\lambda(q)$ has to satisfy is

$$[\mathbb{P}^2 + 2\sigma\mathbb{Q}\mathbb{P} - (2\lambda + \sigma i)]v_\lambda(q) = 0, \tag{7.200}$$

which *is* amenable to simplification by Fourier transformation. Applying $\mathbb{F}$, we find

$$[\mathbb{Q}^2 - 2\sigma\mathbb{P}\mathbb{Q} - (2\lambda + \sigma i)]\tilde{v}_\lambda(p) = 0; \tag{7.201a}$$

i.e.,

$$\left[2\sigma ip\frac{d}{dp} + p^2 - (2\lambda - \sigma i)\right]\tilde{v}_\lambda(p) = 0. \tag{7.201b}$$

The solutions for this equation have the form $p^a \exp(bp^2)$ with $a = -\frac{1}{2} - i\sigma\lambda$ and $b = i\sigma/4$. Equation (7.201b) is *singular* for $p = 0$, so the solutions for $p > 0$ and $p < 0$ are uncoupled and independent. Let these be chosen as

$$\tilde{v}_\lambda{}^{\pm}(p) = (2\pi)^{-1/2} p_{\pm}^{-1/2 - i\sigma\lambda} \exp(i\sigma p^2/4) = \tilde{v}_\lambda{}^{\mp}(-p), \tag{7.202a}$$

where

$$p_+ \coloneqq \begin{cases} p, & p > 0, \\ 0, & p \leqslant 0, \end{cases} \qquad p_- \coloneqq \begin{cases} 0, & p \geqslant 0, \\ -p, & p < 0. \end{cases} \tag{7.202b}$$

We shall now set $\sigma = 1$. The $\sigma = -1$ case follows similarly. Retracing our steps through the inverse Fourier transform and the change of function involving $\exp(iq^2/2)$, we find

$$\chi_\lambda{}^{\pm}(q) = 2^{i\lambda/2}(2\pi)^{-1}\int_{-\infty}^{\infty} dp p_{\pm}^{-1/2 - i\lambda} \exp[i(p^2/4 + pq + q^2/2)] = \chi_\lambda{}^{\mp}(-q), \tag{7.203a}$$

where we have introduced a phase $2^{i\lambda/2}$ into the definition for later convenience. A change of variable $p = 2\exp(i\pi/4)z^{1/2}$, the Taylor series expansion of $\exp(ipq)$, and Euler's integral form for the gamma function (Appendix A) allow (7.203a) to be written as a series:

$$\chi_\lambda{}^{\pm}(q) = C_\lambda \exp(iq^2/2) \sum_{n=0}^{\infty} [\pm 2\exp(3i\pi/4)q]^n \Gamma(n/2 - i\lambda/2 + \tfrac{1}{4})/n!, \tag{7.203b}$$

$$C_\lambda \coloneqq \exp[i(\pi/8 - \tfrac{1}{2}\lambda \ln 2)] \cdot 2^{-3/2}\pi^{-1} \exp(\pi\lambda/4). \tag{7.203c}$$

It can also be put in terms of Whittaker's form of the *parabolic cylinder* function (see the special function tables of Erdelyi *et al.* [1968, Vol. 2, p. 119, Eq. (3)]):

$$\chi_\lambda{}^{\pm}(q) = C'_\lambda D_{i\lambda - 1/2}(\mp 2^{1/2}\exp(3i\pi/4)q), \tag{7.203d}$$

$$C'_\lambda \coloneqq \exp(i\pi/8)2^{-3/4}\pi^{-1}\exp(\pi\lambda/4)\Gamma(1/2 - i\lambda). \tag{7.203e}$$

For $\sigma = -1$, the expressions for $\chi_\lambda{}^{+}(q)$ and $\chi_\lambda{}^{-}(q)$ are interchanged. The function $\chi_\lambda^{+}(q)$ is shown in Fig. 7.11. The overall asymptotic behavior $|q| \gg 1$ is given by the exponential factor for q in (7.203a), namely $\chi_\lambda{}^{\pm}(q) \sim$

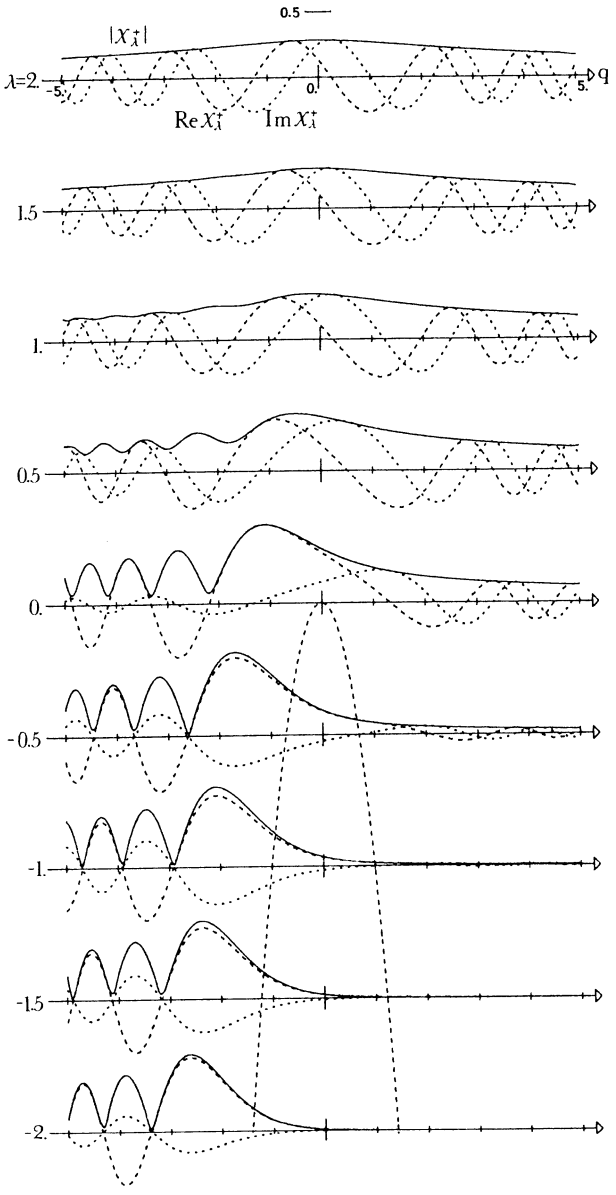


Fig. 7.11. Repulsive oscillator wave functions $\chi_\lambda{}^+(q)$ for values of λ between 2 (top) and -2 (bottom). We show the real, imaginary, and absolute values of this function by heavy dotting, light dotting, and continuous plot. The dotted parabola extending downward from $\lambda = 0$ represents the repulsive oscillator quantum potential. "Inside" this region, the quantity $q^2/2 + \lambda$ is negative, so the curvature of $\chi_\lambda{}^+(q)$ is proportional to the function; i.e., solutions are damped. "Outside" this region, $q^2/2 + \lambda$ is positive, and the solutions oscillate.

$\exp(iq^2/2)$. The function thus oscillates with strongly increasing rapidity. The repulsive functions (7.203) are neither in $\mathscr{L}^2(\mathscr{R})$ nor in $\mathscr{L}^1(\mathscr{R})$. They will be seen to constitute, nevertheless, a complete orthonormal basis—in the Dirac sense—for the Hilbert space $\mathscr{L}^2(\mathscr{R})$.

Exercise 7.60. Follow the procedure (7.198)–(7.201) in order to find the *harmonic* oscillator wave functions as solutions of (7.170)–(7.171) by the use of the Fourier transformation.

7.5.13. Alternative Path: Fourier Transformation of $q_{\pm}^{\tau}$, τ Complex

Another way to find the repulsive oscillator wave functions (7.203), which will provide an alternative form for the solutions of (7.201) equivalent to those considered from (7.202) onward, is to see the function $\tilde{v}_{\lambda}{}^{\pm}(p)$ as the product of $p_{\pm}^{-1/2-i\lambda}$ and a Gaussian of imaginary width $\exp(ip^2/4)$. The inverse Fourier transform will thus be the convolution of the inverse Fourier transforms of the factors.

Exercise 7.61. Show that the formula (7.22) which finds the Fourier transform of a Gaussian $G_{\omega}(q)$ of width ω as $\omega^{-1/2}G_{1/\omega}(p)$ holds for complex ω as well as long as $\operatorname{Re}\omega \geqslant 0$. This involves a change of variable $q' = \omega^{-1/2}q$ for complex ω which inclines the path of integration to an angle $-\frac{1}{2}\arg\omega$. See Fig. 7.12. This integral can be evaluated by complex contour integration for $|\arg\omega| < \pi/2$ and as a limit outside the integral for ω pure imaginary. For the factor under discussion,

$$\exp(ip^2/4) = 2\pi^{1/2}\exp(i\pi/4)G_{2i}(p); \tag{7.204a}$$

the inverse Fourier transform is thus

$$(\mathbb{F}^{-1}\mathbf{G}_{2i})(q) = (2i)^{-1/2}G_{1/2i}(q) = (2\pi)^{-1/2}\exp(-iq^2). \tag{7.204b}$$

We always mean $i = \exp(i\pi/2)$, lest multivaluation problems appear.

The calculation of the inverse Fourier transform of $p_{\pm}^{-1/2-i\lambda}$ is a more complicated affair. To begin the excursion, let us calculate the Fourier transforms of $q_{+}{}^{\tau}$ and $q_{-}{}^{\tau}$, where τ is a complex number and $q_{\pm}$ is defined as

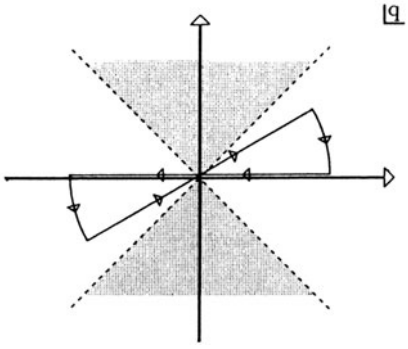


Fig. 7.12. "Bow-tie" contour deformation. Shaded areas indicate the quadrants where the Gaussian integrand diverges for $|q| \to \infty$.

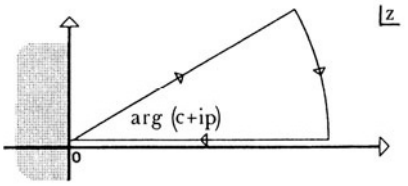


Fig. 7.13. "Sector" contour deformation. Shaded half-plane indicates asymptotic divergence.

in (7.202b). To avoid integration contours at the edges of the convergence regions, we shall first multiply the function q_+^{τ} by a decreasing exponential $\Theta_c(q) \coloneqq \exp(-cq)$ and q_-^{τ} by $\Theta_c(-q) = \exp(cq)$, $c > 0$:

$$[\mathbb{F}(q_\pm^{\tau}\Theta_c(\pm q))](p) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq(q_\pm)^{\tau}\exp[-q(\pm c + ip)]$$

$$= (2\pi)^{-1/2}(c \pm ip)^{-\tau-1}\int_0^{\infty \exp i(c \pm ip)} dzz^{\tau}\exp(-z), \quad (7.205a)$$

where we have effected a change of variables $z = q(\pm c + ip)$. The integral in (7.205a) is thus taken along a ray in the direction of $\arg(c \pm ip)$ which lies in the region of convergence of the integrand, $\operatorname{Re} z > 0$, i.e., for $c > 0$ (Fig. 7.13), and which by Cauchy's theorem equals the same integral along the positive axis. This integral can then be recognized as Euler's integral formula for the gamma function $\Gamma(\tau + 1)$ (Appendix A). For $\pm i = \exp(\pm i\pi/2)$, the transform we are looking for is the limit of (7.205a) as $c \to 0^+$, namely,

$$(\mathbb{F}q_\pm^{\tau})(p) = (2\pi)^{-1/2}\exp[\mp i(\tau + 1)\pi/2]\Gamma(\tau + 1)\lim_{c\to 0^+}(p \mp ic)^{-\tau-1}. \quad (7.205b)$$

Expressions of the type $\lim_{\varepsilon\to 0}(p \mp i\varepsilon)^{-n}$ were dealt with in Section 7.4 for integer n [Eqs. (7.140)] leading to derivatives of the Dirac δ. For complex n—call it ν—the situation is not so extreme but does require care. As the function is multivalued, consider

$$(x + iy)^{\nu} = |x + iy|^{\nu}\exp[i\nu\arg(x + iy)] \quad (7.206a)$$

where the branch cut runs along the negative x-axis. For $x > 0$ the limits $y \to 0^{\pm}$ can be taken without problem, yielding $|x|^{\nu}\exp(i\nu\arg x) = x^{\nu}$. For $x < 0$, however, we have to specify that we approach the negative axis from above or below (Fig. 7.14): If $y \to 0^+$, $\arg(x + iy) \to \pi$, while if $y \to 0^-$,

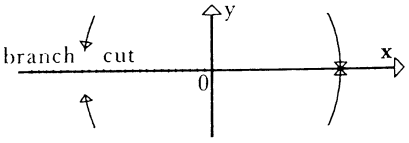


Fig. 7.14. Real limits of the complex power function. A branch cut extends along the negative real axis.

$\arg(x + iy) \to -\pi$; thus (7.206a) becomes $|x|^{\nu} \exp(\pm i\nu\pi)$. Introducing now the functions $x_{\pm}$ defined as in (7.202b),

$$\lim_{y \to 0^+} (x \mp iy)^{\nu} = x_+{}^{\nu} + x_-{}^{\nu} \exp(\mp i\nu\pi) \tag{7.206b}$$

for $\nu \neq -1, -2, \ldots$. [The analysis of (7.206) as ν becomes a negative integer can be found in Gel'fand *et al.* (1964, Vol. I, Section 4.4).] We can now put (7.206) into (7.205b) for $\nu = -\tau - 1$ and obtain the Fourier transform of the $q_{\pm}{}^{\tau}$ functions, which can be conveniently written in matrix form:

$$\mathbb{F}\begin{pmatrix} q_+{}^{\tau} \\ q_-{}^{\tau} \end{pmatrix} = (2\pi)^{-1/2}\Gamma(\tau + 1)\begin{pmatrix} -i\exp(-i\pi\tau/2) & i\exp(i\pi\tau/2) \\ i\exp(i\pi\tau/2) & -i\exp(-i\pi\tau/2) \end{pmatrix}\begin{pmatrix} p_+^{-\tau-1} \\ p_-^{-\tau-1} \end{pmatrix}. \tag{7.207}$$

From a development parallel to the above, or by inverting (7.207) for $\tau \leftrightarrow -\tau - 1$, we find

$$\mathbb{F}^{-1}\begin{pmatrix} p_+{}^{\tau} \\ p_-{}^{\tau} \end{pmatrix} = (2\pi)^{-1/2}\Gamma(\tau + 1)\begin{pmatrix} i\exp(i\pi\tau/2) & -i\exp(-i\pi\tau/2) \\ -i\exp(-i\pi\tau/2) & i\exp(i\pi\tau/2) \end{pmatrix}\begin{pmatrix} q_+^{-\tau-1} \\ q_-^{-\tau-1} \end{pmatrix}. \tag{7.208}$$

Exercise 7.62. Verify that (7.25) holds for (7.207)–(7.208), namely,

$$(\mathbb{F}^2 q_{\pm}{}^{\tau})(q') = (-q')_{\pm}{}^{\tau} = q'^{\tau}_{\mp}. \tag{7.209}$$

You will come to use the gamma function reflection formula (A.9a). The matrix forms (7.207)–(7.208) are quite handy.

Exercise 7.63. The functions $q_{\pm}{}^{\tau}$ are solutions to the differential equation

$$i\mathbb{Q}\mathbb{P}f_{\tau}(q) = q\frac{d}{dq}f_{\tau}(q) = \tau f_{\tau}(q). \tag{7.210}$$

Show that, under Fourier transformation, Eq. (7.210) behaves as expected from (7.207)–(7.208).

7.5.14. Completion of the Alternative Path

Having found Eqs. (7.207) and (7.208), which will appear later in various contexts, we return to our original aim, namely, the alternative calculation of the repulsive oscillator wave functions as the convolution of two inverse transforms, (7.204) and (7.208), with the phase defined in (7.203a),

$$\begin{aligned} \chi_{\lambda}{}^{\pm}(q) &= 2^{i\lambda/2}\exp(iq^2/2)(\mathbb{F}^{-1}\mathfrak{v}_{\lambda}{}^{\pm})(q) \\ &= 2^{1/2+i\lambda/2}\exp(i\pi/4)\exp(iq^2/2)[\mathbb{F}^{-1}(p_{\pm}^{-1/2-i\lambda}\mathbf{G}_{2i})](q) \\ &= 2^{i\lambda/2}(2\pi)^{-1/2}\exp(iq^2/2)[(\mathbb{F}^{-1}p_{\pm}^{-1/2-i\lambda}) * \mathbf{G}_{1/2i}](q). \end{aligned} \tag{7.211}$$

Equation (7.208) can be now used for $\tau = -\frac{1}{2} - i\lambda$, and, after a few simplifications, one arrives at an alternative expression for (7.203) given by

$$\chi_\lambda{}^{\pm}(q) = 2^{i\lambda/2}(2\pi)^{-3/2}\Gamma(\tfrac{1}{2} - i\lambda)\int_{-\infty}^{\infty} dq'(a_\lambda{}^{\pm}q'^{-1/2-i\lambda}_{+} + b_\lambda{}^{\pm}q'^{-1/2-i\lambda}_{-}) \times \exp[i(-q'^2 + 2qq' - q^2/2)], \tag{7.212a}$$

where

$$a_\lambda{}^{+} = i\exp(\pi\lambda/2) = b_\lambda{}^{-}, \qquad a_\lambda{}^{-} = \exp(-\pi\lambda/2) = b_\lambda{}^{+}. \tag{7.212b}$$

The repulsive oscillator functions have appeared little in the literature. The reason for this seems to have been the fact that their explicit expression is not very compact and the evaluation of integrals involving them would require the use of arduous analytical calculations. In Part IV we hope to convince the reader that integral transform techniques are available to reduce their evaluation to much simpler analysis involving only matrix algebra.

7.5.15. Fourier Transformation of the Repulsive Oscillator Wave Functions

We can bind together the two expressions for the repulsive oscillator functions (7.203) and (7.212) if we consider the problem of finding the Fourier transform of the $\chi_\lambda{}^{\pm}(q)$. Far from being just a messy calculation, this will show several interesting relations which will be used in Part IV. We remarked before that $\mathbb{F}\mathbb{H}^r\mathbb{F}^{-1} = -\mathbb{H}^r$, so we can expect that $\mathbb{F}\boldsymbol{\chi}_\lambda{}^{\pm}$ will be a linear combination of the $\boldsymbol{\chi}^{\pm}_{-\lambda}$. From Eq. (7.203) and by using various formulas for Gaussians, their Fourier transformations, and convolution,

$$\begin{aligned}(\mathbb{F}\boldsymbol{\chi}_\lambda{}^{\pm})(p) &= 2^{i\lambda/2}(2\pi)^{1/2}\exp(i\pi/4)[\mathbb{F}(\mathbf{G}_i\cdot\mathbb{F}^{-1}\tilde{\boldsymbol{\upsilon}}_\lambda{}^{\pm})](p)\\ &= 2^{i\lambda/2}(\mathbf{G}_{1/i} * \tilde{\boldsymbol{\upsilon}}_\lambda{}^{\pm})(p)\\ &= 2^{i\lambda/2}(2\pi)^{-1}\exp(i\pi/4)\int_{-\infty}^{\infty} dp'p'^{-1/2-i\lambda}_{\pm}\\ &\quad\times\exp[i(-p^2/2 + pp' - p'^2/4)].\end{aligned} \tag{7.213}$$

It will be observed that the integral, although akin to (7.203), has the same sign of the Gaussian exponentials as (7.212) for $-\lambda$. By a change of variables $q' := p'/2$, one obtains separately the two summands of this equation, which, after some cancellations and rearrangements, read, in matrix form,

$$\mathbb{F}\begin{pmatrix}\boldsymbol{\chi}_\lambda{}^{+}\\ \boldsymbol{\chi}_\lambda{}^{-}\end{pmatrix} = C'_\lambda\begin{pmatrix}-i\exp(-\pi\lambda/2) & \exp(\pi\lambda/2)\\ \exp(\pi\lambda/2) & -i\exp(-\pi\lambda/2)\end{pmatrix}\begin{pmatrix}\boldsymbol{\chi}^{+}_{-\lambda}\\ \boldsymbol{\chi}^{-}_{-\lambda}\end{pmatrix}, \tag{7.214a}$$

$$C'_\lambda = \exp(i\pi/4)(2\pi)^{-1/2}\Gamma(\tfrac{1}{2} - i\lambda). \tag{7.214b}$$

Exercise 7.64. Verify that (7.214) yields

$$(\mathbb{F}^2\boldsymbol{\chi}_\lambda{}^{\pm})(q) = \chi_\lambda{}^{\pm}(-q) = \chi_\lambda{}^{\mp}(q), \tag{7.215}$$

as was done in Exercise 7.62, thereby checking that (7.25) holds properly.

It might appear amusing that the matrix form (7.214) matches that of (7.207) for $\tau = -\frac{1}{2} - i\lambda$, that is, *the Fourier transform properties of the pair* $\chi_\lambda{}^\pm$ *are the same as those of* $q_\pm^{-1/2-i\lambda}$. This fact is neither isolated nor accidental. As will be brought out in Part IV, what happens is that the $\chi_\lambda{}^\pm(q)$ are unitary integral transforms of $q_\pm^{-1/2-i\lambda}$. The transform in question has as its kernel the exponential factor in the integral (7.203a). We have seen that this transform and the Fourier one *commute*. In fact we shall come to prove that $\chi_\lambda{}^\pm = \mathbb{F}^{-1/2} q_\pm^{-1/2-i\lambda}$. As the power functions are simpler to handle than the parabolic cylinder ones, it is more convenient to work in the transform space of functions and finally transform back the results. See Exercise 9.7.

As stated before, the repulsive oscillator functions are orthonormal in the sense of Dirac and complete in $\mathscr{L}^2(\mathscr{R})$. *Orthogonality* is easy to prove:

Exercise 7.65. Using the self-adjoint operator $\mathbb{H}^r$ and the defining equation (7.198), show that $(\chi_\lambda{}^\pm, \chi_{\lambda'}^\pm) = 0$ for $\lambda \neq \lambda'$.

Exercise 7.66. Using the Parseval formula and the fact that $\chi_\lambda{}^\pm(q)$ are the Fourier transforms of $\tilde{v}_\lambda{}^\pm(p)$, with disjoint supports, show that $(\chi_\lambda{}^\pm, \chi_{\lambda'}^\mp) = 0$.

Dirac orthonormality will be discussed in Section 8.2, while completeness must wait until Part IV. Generating functions and other properties will appear in various sections.

7.6. Uncertainty Relations

A given function and its Fourier transform exhibit a number of complementary properties. We have seen time and again that a very "peaked" function has a "broad" transform and vice versa. The precise statement of this reciprocal width relation will be given. It constitutes, when applied in quantum mechanics, the fundamental Heisenberg uncertainty relation.

7.6.1. General Discussion

The Fourier transform of a rectangle function of width ε [Eqs. (7.4) and (7.5)] is proportional to $\sin(p\varepsilon/2)/p$. The spread or width of the latter can be defined roughly as that of the central peak of the function (Fig. 7.1) between the values $-\pi$ and π of the sine argument; that is, $p = \pm 2\pi/\varepsilon$. The width of the rectangle function transform is thus $4\pi/\varepsilon$. The *product* of the widths of the two functions is then 4π—a constant independent of ε. The narrower the rectangle, the broader its transform and vice versa. As a second example, the Gaussian bell function of width ω, Eq. (7.20), has a Gaussian of width $1/\omega$

as its Fourier transform. The product of the widths defined in this way is unity.

These examples suggest that a relation of the kind width($\mathbf{f}$) × width($\tilde{\mathbf{f}}$) = constant should exist—if we can agree on a general definition of what the width of a function means. As we shall see, there are at least two working definitions. One is particularly important as it gives rise to the quantum-mechanical uncertainty relation between position and momentum measurements recognized by Heisenberg.

7.6.2. Moments

Given a function $f(q)$, we associate with it, using the language of probability theory, a positive *distribution function* $|f(q)|^2$. The rth *moment* of such a distribution is defined to be

$$\overline{q^r} \coloneqq \left[\int_{-\infty}^{\infty} dq q^r |f(q)|^2\right] \Big/ \left[\int_{-\infty}^{\infty} dq |f(q)|^2\right]. \tag{7.216}$$

The first moment $\overline{q^1}$ is the *average* of $|f(q)|^2$, which can be interpreted as the "center of gravity" of the area under the curve. If the function $f(q)$ has definite symmetry under reflections through the origin, its average $\overline{q^1}$ is zero.

Exercise 7.67. Show that if a function with zero average is displaced by a, the average of the displaced function will be a.

7.6.3. Dispersion and the Heisenberg Uncertainty Relation

The second moment $\overline{q^2}$ represents the peaking of the distribution $|f(q)|^2$ around the origin. For the Gaussian function we can use (7.23) to find its $\overline{q^2}$ as $\|\mathbb{Q}\mathbf{G}_\omega\|^2/\|\mathbf{G}_\omega\|^2 = \omega/2$. For the rectangle function of width ε, the second moment is $\varepsilon^2/12$. Second moment and "intuitive" width are thus not the same. In particular, a displaced Gaussian will have a larger second moment than its undisplaced version. It is thus convenient to define the *dispersion* Δ_f of a function $f(q)$ as the second moment of $|f(q)|^2$ with respect to its average, i.e.,

$$\begin{aligned}\Delta_f &\coloneqq \left[\int_{-\infty}^{\infty} dq(q - \overline{q^1})^2 |f(q)|^2\right] \Big/ \left[\int_{-\infty}^{\infty} dq |f(q)|^2\right] \\ &= \|(\mathbb{Q} - \overline{q^1})\mathbf{f}\|^2/\|\mathbf{f}\|^2. \end{aligned} \tag{7.217}$$

It describes the peaking of $f(q)$ independently of the location of the peak. We shall prove the main result of this section (Section 7.6), which can be stated as follows: the product of the dispersion of a function $\mathbf{f}$ and that of its Fourier transform $\tilde{\mathbf{f}}$ has a lower bound of value $\frac{1}{4}$:

$$\Delta_f \Delta_{\tilde{f}} \geqslant 1/4. \tag{7.218}$$

7.6.4. Proof of the Uncertainty Relation

It is sufficient to consider functions whose average is zero. If this is not the case, we can always translate $f(q)$ by $\overline{q^1}$ without changing its dispersion. The Fourier-transformed function $\tilde{f}(p)$ will be multiplied then by a phase $\exp(ip\overline{q^1})$ which also leaves its dispersion invariant. Assuming now that at least the first derivative of $\mathbf{f}$ is in $\mathscr{L}^2(\mathscr{R})$ and $\overline{q^1} = 0$ for $\mathbf{f}$ and $\tilde{\mathbf{f}}$, we write

$$\begin{aligned}
\|\mathbf{f}\|^4 \Delta_f \Delta_{\tilde{f}} &= \|\mathbb{Q}\mathbf{f}\|^2 \|\mathbb{Q}\tilde{\mathbf{f}}\|^2 \\
&= \|\mathbb{Q}\mathbf{f}\|^2 \|\mathbb{P}\mathbf{f}\|^2 && \text{[by (7.57)]} \\
&\geqslant |(\mathbb{Q}\mathbf{f}, \mathbb{P}\mathbf{f})|^2 && \text{(Schwartz inequality)} \\
&\geqslant \tfrac{1}{4}|(\mathbb{Q}\mathbf{f}, \mathbb{P}\mathbf{f}) - (\mathbb{P}\mathbf{f}, \mathbb{Q}\mathbf{f})|^2 && [|z|^2 \geqslant (\operatorname{Im} z)^2] \\
&= \tfrac{1}{4}|(\mathbf{f}, \mathbb{Q}\mathbb{P}\mathbf{f}) - (\mathbf{f}, \mathbb{P}\mathbb{Q}\mathbf{f})|^2 && (\mathbb{Q} \text{ and } \mathbb{P} \text{ self-adjoint}) \\
&= \tfrac{1}{4}|(\mathbf{f}, [\mathbb{Q}, \mathbb{P}]\mathbf{f})|^2 = \tfrac{1}{4}\|\mathbf{f}\|^4 && \text{[commutator (7.59)]}, \qquad (7.219)
\end{aligned}$$

which proves (7.218).

Exercise 7.68. Show that had we kept $(q - \overline{q^1})^2$ and $(p - \overline{p^1})^2$ in the derivation (7.219) the same final result would be obtained.

7.6.5. Dispersion of Coherent States and of Oscillator Wave Functions

Let us verify the uncertainty relationship for some of the examples at hand. For the Gaussian function $G_\omega(q)$ we saw that $\Delta_{G_\omega} = \omega/2$, as $\tilde{G}_\omega(p) \sim G_{1/\omega}(p)$, $\Delta_{G_\omega} \cdot \Delta_{\tilde{G}_\omega} = \frac{1}{4}$. For this function, therefore, the lower limit of the uncertainty relation (7.218) is attained. For the coherent states (7.188), essentially rescaled and translated Gaussians of unit width, the same is true:

$$\Delta_{\Upsilon_c} = \|\mathbb{Q}\boldsymbol{\Upsilon}_c\|^2 / \|\boldsymbol{\Upsilon}_c\|^2 = \tfrac{1}{2}, \qquad c \in \mathscr{C}. \qquad (7.220)$$

For the harmonic oscillator function of Section 7.5 (see Fig. 7.10), the dispersion can be calculated as follows:

$$\begin{aligned}
\Delta_{\Psi_n} &= (\boldsymbol{\Psi}_n, \mathbb{Q}^2\boldsymbol{\Psi}_n) = \tfrac{1}{2}(\boldsymbol{\Psi}_n, \mathbb{Q}^2\boldsymbol{\Psi}_n) + \tfrac{1}{2}(\tilde{\boldsymbol{\Psi}}_n, \mathbb{P}^2\tilde{\boldsymbol{\Psi}}_n) \\
&= (\boldsymbol{\Psi}_n, \mathbb{H}\boldsymbol{\Psi}_n) = n + \tfrac{1}{2}, \qquad (7.221)
\end{aligned}$$

where we have used their properties under Fourier transformation and the fact that they are eigenfunctions of the operator $\mathbb{H}$ in (7.171). The dispersion of the $\Psi_n(q)$ and their Fourier transforms is thus proportional to n. (Recall Exercise 7.59.)

7.6.6. Minimum Dispersion States

The Gaussian function can be shown to be the *only* function—up to translation, normalization, and dilatation—which attains the minimum

allowed by the uncertainty relation (7.218). For the equality in (7.218) to hold, (7.219) requires (a) that the Schwartz inequality be valid as an equality, i.e., that $\mathbb{Q}\mathbf{f}$ be parallel to $\mathbb{P}\mathbf{f}$, and (b) that $(\mathbb{Q}\mathbf{f}, \mathbb{P}\mathbf{f})$ be pure imaginary. The first requirement implies that $f(q)$ satisfies $df(q)/dq = icqf(q)$ for some constant $c \in \mathscr{C}$, which means that $f(q) = c' \exp(icq^2/2)$, $c' \in \mathscr{C}$. The second requirement then narrows the choice to $\operatorname{Re} c = 0$. Finally, if the function is to be square-integrable, $\operatorname{Im} c > 0$. We are thus left with the Gaussian bell function, and, through (complex) translations, with all coherent states.

7.6.7. Equivalent Width

We must remark that the proof of the uncertainty relation required that the first derivative of $f(q)$ be square-integrable. This bars the preceding analysis from applying to the rectangle function. In fact, the evaluation of $\Delta_{\tilde{R}}$ requires the integration of p^2 times $[\sin(\varepsilon p/2)/p]^2$ over $p \in \mathscr{R}$, which is infinity. Yet, as we argued at the beginning of this section, some form of width reciprocity *does* hold for this pair of functions. Another definition which embodies the intuitive concept of "broadness" of a function is that of *equivalent width*:

$$W_f \coloneqq \int_{-\infty}^{\infty} dq f(q)/f(0). \tag{7.222}$$

[Compare with Eqs. (4.69) for Fourier series.] The quantity (7.222) gives the equivalent width of a rectangle function which has the same area as the area under the curve $f(q)$ with height $f(0)$. The equivalent width can easily be zero or infinity if $\tilde{f}(0) = 0$ or $f(0) = 0$, so the estimate has to be made judiciously, translating $f(q)$ if necessary. The complementarity relation afforded by the definition (7.222) is

$$W_f \cdot W_{\tilde{f}} = 2\pi. \tag{7.223}$$

Equation (7.223) can be proven by noting that the numerator of each factor equals $(2\pi)^{1/2}$ times the denominator of the other. *Checking*: For the rectangle function of width ε, $W_R = \varepsilon$, while by using (7.10b), $W_{\tilde{R}} = 2\pi/\varepsilon$. For the unit Gaussian of width ω in (7.20), $W_G = (2\pi\omega)^{1/2}$.

Last, as our estimation of the "width" of the $\Psi_n(q)$ in Exercise 7.59 suggests, other definitions of width may be set up.

7.6.8. Complementarity and Operator Noncommutation

Complementarity relations between properties of a function and its Fourier transform are particularly suited to describe the observed facts in quantum mechanics. Although this is not the place to expound the general theory and supporting data, we shall try to indicate where uncertainty relations of the Heisenberg type appear by giving a few simplified rules of the

game. (a) Replace a classical observable $S(q, p)$ function of position q and its canonically conjugate momentum p by a self-adjoint operator in $\mathscr{L}^2(\mathscr{R})$, $S(\mathbb{Q}, \mathbb{P})$, usually in the *Schrödinger* representation given by (7.55)–(7.56). (b) The state of a system is described by a wave function $\psi(q)$, where $|\psi(q)|^2$ represents the probability density of finding the particle at the position q; hence $\|\Psi\| = 1$ since the probability of finding the particle in the whole of $\mathscr{R}$ is unity. (c) The momentum-space description of the state is given by $\tilde{\psi}(p)$. (d) The mean or expected value of the observable S when the system is in the state Ψ is $\bar{s} = (\Psi, \mathbb{S}\Psi)$. (e) There is a *dispersion* in the results of measurements on S given by $\Delta_\Psi(S) \coloneqq \|(\mathbb{S} - \bar{s})\Psi\|^2$. Note that if Ψ happens to be an eigenstate of $\mathbb{S}$ with eigenvalue σ, then $\bar{s} = \sigma$ and $\Delta_\Psi(S) = 0$.

It is in the last point that we establish contact with our derivation (7.219), for assume that two quantities represented by operators $\mathbb{S}$ and $\mathbb{R}$ are subject to simultaneous measurement. What quantum mechanics tells us is that the results of the two measurements cannot be simultaneously dispersionless *unless* $\mathbb{S}$ and $\mathbb{R}$ commute. The proof will clarify the statement further: by a process similar to (7.219) and by setting $\bar{s}$ and $\bar{r}$ to zero as justified by Exercise 7.68,

$$\Delta_\Psi(S) \cdot \Delta_\Psi(R) = \|\mathbb{S}\Psi\|^2 \|\mathbb{R}\Psi\|^2 \geqslant |(\mathbb{S}\Psi, \mathbb{R}\Psi)|^2 \geqslant \tfrac{1}{4}|(\Psi, [\mathbb{S}, \mathbb{R}]\Psi)|^2 \quad (7.224)$$

The product of the dispersions of the two measurements is thus bounded from below by the expectation value of $[\mathbb{S}, \mathbb{R}]$ when the system is in a state Ψ.

For measurements of position and momentum the representing operators are $\mathbb{Q}$ and $\hbar\mathbb{P}$ for which (7.59) holds. The actual value of the left-hand side depends on the state Ψ, but a lower bound is determined by their commutator expectation value, i.e., $\hbar/4$.

Other observables whose dispersion product is bounded by (7.224) are the components of three-dimensional angular momentum. There are further uncertainty relations between physical quantities such as angle–angular momentum and time–energy whose form, however close to (7.224), does *not* stem from this argument alone.

A good account of quantum mechanics and the role of uncertainty relations can be found in Messiah (1964, pp. 129–139). Some hard-core research articles on uncertainty relations other than the basic Heisenberg one have been written by Susskind and Glogower (1964), Carruthers and Nieto (1965, 1968), and Jackiw (1968).

8

Integral Transforms Related to the Fourier Transform

Fourier analysis can take different forms as we adapt it to various problems at hand. The main results of the Fourier integral theorem are used to justify continuous partial-wave analyses in terms of functions other than the oscillating exponential ones. Section 8.1 presents the bilateral and the more common unilateral Laplace transform where the expanding functions are the decreasing exponential functions $\exp(pq)$. In Section 8.2 we expand functions in terms of powers $x_{\pm}^{iq-1/2}$ (bilateral Mellin) or of powers x^q (common Mellin) as a continuous analogue of the ordinary Taylor series expansion. Section 8.3 deals with Fourier transforms of functions of N variables and applies them to the general solution of the N-dimensional elastic–diffusive equation. In particular, the three-dimensional wave and general heat equations are treated. Hankel transforms (Section 8.4) use the Bessel functions as the expanding set and arise out of N-dimensional Fourier transforms of functions of the radius. The elastic–diffusive equation solutions are completed, and the difference between odd and even dimensions is pointed out. We list, finally, several transform pairs which use cylindrical functions as their expanding set. Under the title of "other" integral transforms, in Section 8.5 we give a rough outline of the Sturm–Liouville approach. This is applied in particular to transforms using Airy functions. Other approaches lead to Hilbert and Stieltjes transforms. All sections are basically independent of one another except for Hankel transforms, which are built out of N-dimensional Fourier transforms. Those transforms which are only briefly mentioned in the text are accompanied by a bibliographical survey.

8.1. Laplace Transforms

The Laplace transform is essentially the Fourier transform on the imaginary axis of the transform argument. The direct implementation of this idea leads to the *bilateral* Laplace transform. The more commonly known version of this transform, the *unilateral* Laplace transform, is obtained for causal functions, i.e., those which are zero on the negative half-line. The Laplace transform, formulated in this way, allows in a rather natural way for the introduction of the initial conditions in the solution of certain differential equations.

8.1.1. Bilateral Laplace Transforms

Consider the Fourier transform pair, Eqs. (7.1). By setting $p =: -is$, the pair now reads

$$(\mathbb{L}_B^{-1}\mathbf{f}^{BL})(q) := f(q) = -i(2\pi)^{-1/2}\int_{-i\infty}^{i\infty} ds f^{BL}(s)\exp(qs), \tag{8.1a}$$

$$(\mathbb{L}_B\mathbf{f})(s) := f^{BL}(s) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq f(q)\exp(-qs), \tag{8.1b}$$

where we have also put $f^{BL}(s) := \tilde{f}(-is)$, thus defining $f^{BL}(s)$ as the *bilateral Laplace transform* of $f(q)$. In terms of the new transform functions, the Parseval identity appears as

$$\int_{-\infty}^{\infty} dq f(q)^* g(q) = -i\int_{-i\infty}^{i\infty} ds f^{BL}(s)^* g^{BL}(s). \tag{8.1c}$$

We note that not every function which has a Fourier transform is bound to have a Laplace transform as the integral (8.1b) may well diverge. This happens when $f(q)$ behaves asymptotically like any finite negative power of q since the exponential kernel dominates the growth of the integrand.

8.1.2. Exponential Growth

To describe the regions in the s-plane where (8.1b) converges, it is convenient to introduce definitions concerning asymptotic exponential growth. If there exist constants k', n', and c' such that for $|q| \to \infty$

$$|f(q)| < k' \exp(c'|q|^{n'}) \tag{8.2}$$

and if n and c are the minima of the n' and c' for which (8.2) holds, $f(q)$ is said to be of *order* n, *type* c, and *growth* (n, c). When we consider q real, we may examine separately the cases $q \to +\infty$ and $q \to -\infty$.

The growth of a Gaussian $G_\omega(q) \sim \exp(-q^2/2\omega)$ is thus $(2, -\mathrm{Re}(1/2\omega))$. A simple exponential function $\exp(aq)$, $a \in \mathscr{C}$, will be of growth $(1, \mathrm{Re}\, a)$ for $q > 0$ and $(1, -\mathrm{Re}\, a)$ for $q < 0$. Constants are of growth $(0, c)$. If two functions $f_1(q)$ and $f_2(q)$ are of the same order n, the type of their product is the

sum of their types: $c_1 + c_2$. If their order is different, say $n_1 > n_2$, the growth of their product is (n_1, c_1).

For the bilateral Laplace transform of a (locally integrable) function $f(q)$ to exist, it is sufficient that the integrand in (8.1b) be of growth $(n > 0, c < 0)$. Due to the factor $\exp(-qs)$ of growth $(1, \mp s)$ for $q \gtrless 0$, $s \in \mathscr{R}$, we can contemplate three cases for the growth (n_f^+, c_f^+) of $f(q)$ at $q \to +\infty$:

(a) If $n_f < 1$, the growth of the integrand will be determined by that of the exponential factor, which is $(1, -s)$.
(b) If $n_f = 1$, the integrand growth will be $(1, c_f^+ - s)$.
(c) If $n_f > 1$, the growth will be (n_f^+, c_f^+).

At $q \to -\infty$, let the growth of $f(q)$ be (n_f^-, c_f^-). In the three cases the integrand growth will be as follows:

(a′) $(1, s)$ for $n_f^- < 1$;
(b′) $(1, c_f^- + s)$ for $n_f^- = 1$;
(c′) (n_f^-, c_f^-) for $n_f^- > 1$.

The $q > 0$ part allows integration for (a) $\operatorname{Re} s > 0$, (b) $\operatorname{Re} s > c_f^+$, and (c) all s as long as $c_f^+ < 0$. The $q < 0$ part, independently, allows integration for (a′) $\operatorname{Re} s > 0$, (b′) $\operatorname{Re} s < -c_f^-$, and (c′) all s as long as $c_f^- < 0$. The bilateral Laplace transform $f^{BL}(s)$ will thus exist for some region in the complex s-plane only if both parts permit integration. Conditions (a) and (b) restrict the allowed region to a right half-plane, while (a′) and (b′) restrict it to a left half-plane (Fig. 8.1). Only if the two half-planes have a nonempty

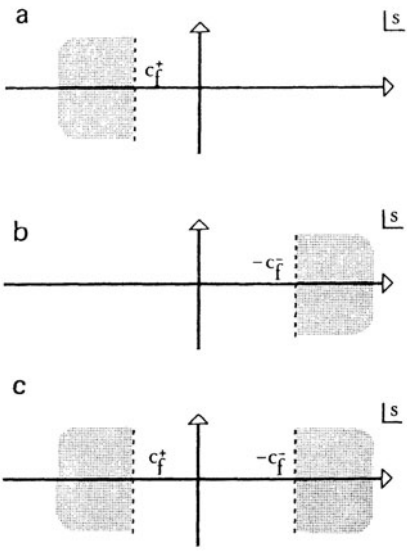


Fig. 8.1. Restrictions on the values of the complex variable s where the bilateral Laplace transform (8.1b) exists. (a) For $q > 0$; (b) for $q < 0$. Shaded areas indicate that the integral diverges. For the overlap between the two allowed regions (c), the transform exists.

overlap band will $f^{BL}(s)$ exist, and then only within this band. Cases (c) and (c′), when allowed, impose no restrictions on the s region.

8.1.3. Examples

As an example, consider $E_{\|}(q) \coloneqq \exp(c|q|)$, $c \in \mathscr{C}$. The growth of this function in both directions is (1, Re c); hence the bilateral Laplace integral (8.1b) exists, according to cases (b′) and (b), for $-\text{Re}\, c < \text{Re}\, s < \text{Re}\, c$, i.e., a vertical band in the complex s-plane centered about the imaginary axis. It is

$$E_{\|}^{BL}(s) = (2\pi)^{-1/2}\left\{\int_{-\infty}^{0} dq \exp[-q(s-c)] + \int_{0}^{\infty} dq \exp[-q(s+c)]\right\}$$
$$= (2\pi)^{-1/2}[1/(s+c) - 1/(s-c)], \qquad -\text{Re}\, c < \text{Re}\, s < \text{Re}\, c. \tag{8.3}$$

The transform function $E_{\|}^{BL}(s)$ is thus seen to have poles at $s = c$ and $s = -c$ which lie on the boundary of the existence band and determine its width. Perhaps surprisingly, the function (8.3) appears to be a well-defined function throughout the complex s-plane. Beyond the band boundaries, this *analytic continuation* of $E_{\|}^{BL}(s)$ is *not* the bilaterial Laplace transform of any function. Yet it can be used for contour integration purposes. Consider the task of finding the *inverse* transform (8.1a) of (8.3): Fig. 8.2. The integral

$$-i(2\pi)^{-1}\int_{-i\infty}^{i\infty} ds[1/(s+c) - 1/(s-c)]\exp(qs) \tag{8.4}$$

can be found for $q > 0$ by closing the integration contour counterclockwise in the Re $s < 0$ half-plane and using the familiar Cauchy and Jordan results.

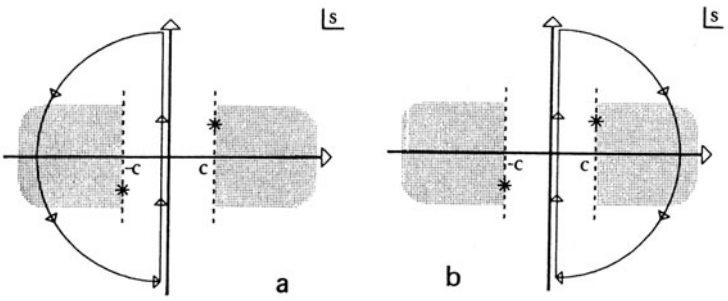


Fig. 8.2. Regions of existence of the bilateral Laplace transform (8.3) (unshaded). Asterisks indicate the locations of the poles of the function. On calculating the inverse Laplace transform (8.4), the integration can be performed for (a) $q > 0$ and (b) $q < 0$ using the analytic continuation of the function and complex contour integration techniques.

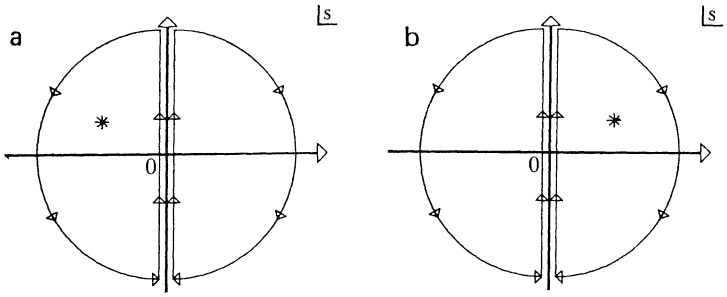


Fig. 8.3. Complex integration contours used in calculating the inverse bilateral Laplace transform in Eq. (8.6) for (a) Re $c < 0$ and (b) Re $c > 0$.

As the contour will enclose the $s = -c$ pole of residue $\exp[q(-c)]$, the result is $\exp(-qc)$. When $q < 0$, the contour may be closed in the Re $s > 0$ half-plane, the result being, as expected, $\exp(qc)$. The reconstitution of the original function for $q \in \mathscr{R}$ is thus $\exp(c|q|)$.

The convergence band in the s-plane must, however, be specified. It is part of the definition of the transform function. To illustrate this, consider the two functions

$$E_+(q) := \begin{cases} \exp(cq), & q > 0, \\ 0, & q \leqslant 0, \end{cases} \qquad E_-(q) := \begin{cases} 0, & q \geqslant 0, \\ \exp(cq), & q < 0. \end{cases} \tag{8.5}$$

Performing the integration in (8.1b), we see that

$$\begin{aligned} E_+^{BL}(s) &= (2\pi)^{-1/2}(s - c)^{-1}, && \text{Re } s > \text{Re } c; \\ E_-^{BL}(s) &= -(2\pi)^{-1/2}(s - c)^{-1}, && \text{Re } s < \text{Re } c. \end{aligned} \tag{8.6}$$

If we are asked to perform the inverse bilateral Laplace transform (8.1a) of $(2\pi)^{-1/2}(s - c)^{-1}$—without specifying the existence region—following the usual complex contour integration techniques (Fig. 8.3), we would come up with $E_+(q)$ if Re $c < 0$ or with $E_-(q)$ if Re $c > 0$.

Exercise 8.1. Show that the preceding paradox is resolved when we note that in taking the bilateral Laplace transform of $E_+(q)$ for Re $c > 0$ or that of $E_-(q)$ for Re $c < 0$ we are actually violating the conditions of the Fourier integral theorem. The inverse transform integrates them over the nonexistence region of the functions.

8.1.4. Unilateral Laplace Transforms

It might appear that the change of variables $p =: -is$ involved in defining the bilateral Laplace transform out of the Fourier transform has little new to offer us in the way of techniques for solving problems which do not yield to the Fourier methods. The "paradox" involved in (8.5)–(8.6), however,

suggests a fruitful restatement of the transform which makes it applicable to time evolution of systems by *causal* functions, i.e., functions which are zero for negative values of the argument. The study of these functions and the behavior of their Fourier transforms in the complex plane occupied Section 7.4. Some significant computational and conceptual simplifications are obtained by the Laplace transform method. It will allow us to find solutions $f(q)$ to differential equations which can exhibit exponential growth $(1, c)$ for any finite c—that is, oscillating, damped, or exponentially growing solutions—in terms of the initial conditions at $q = 0$: $f(0)$, $df(q)/dq|_{q=0}$, and/or higher derivatives according to the order of the differential equation.

Let $f(q)$ be a function of growth $(1, c)$ in the positive q direction and let $\gamma >$ Re c. Build the function

$$f_\gamma(q) := \begin{cases} \exp(-\gamma q) f(q), & q > 0, \\ f(0)/2, & q = 0, \\ 0, & q < 0, \end{cases} \tag{8.7}$$

which is absolutely integrable. Assuming the other conditions of the Fourier integral theorem hold, the Fourier transform of (8.7) is

$$\tilde{f}_\gamma(p) = (2\pi)^{-1/2} \int_0^\infty dq f(q) \exp[-q(\gamma + ip)]. \tag{8.8}$$

We now perform the change of variable $s := \gamma + ip$ and set $f^L(s) := (2\pi)^{1/2} \tilde{f}_\gamma(p)$—the constant $(2\pi)^{1/2}$ is introduced so as to conform to custom. The Fourier transform pair (7.1) thus becomes

$$(\mathbb{L}^{-1}\mathbf{f}^L)(q) := f(q) = (2\pi i)^{-1} \int_{\gamma - i\infty}^{\gamma + i\infty} ds f^L(s) \exp(qs), \qquad q > 0, \tag{8.9a}$$

$$(\mathbb{L}\mathbf{f})(s) := f^L(s) = \int_0^\infty dq f(q) \exp(-qs), \qquad \text{Re } s > \text{Re (type } f). \tag{8.9b}$$

The function $f^L(s)$ is said to be the *unilateral* Laplace transform—or simply *the* Laplace transform—of $f(q)$ and the latter the *inverse* Laplace transform of $f^L(s)$. The Parseval identity is

$$\int_0^\infty dq \exp(-2\gamma q) f(q)^* g(q) = (2\pi i)^{-1} \int_{\gamma - i\infty}^{\gamma + i\infty} ds f^L(s)^* g^L(s), \tag{8.9c}$$

where γ is larger than the types of $f(q)$ and $g(q)$.

8.1.5. On Bromwich Contours

A few remarks are in order as the following feature of (8.9) might appear puzzling: Having introduced an upper bound γ for the growth of $f(q)$ into the definition (8.7), we end up with an integration contour $\int_{\gamma - i\infty}^{\gamma + i\infty}$ which

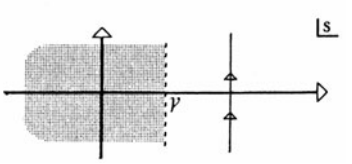


Fig. 8.4. Existence region (unshaded) for the unilateral Laplace transform and integration contour for the inverse transform.

depends on γ but of which we seem to have no clue before the integral is performed. Actually we do, as recalling one of the main results of Section 7.4 will show. Following Eq. (7.126) we proved that the Fourier transform of (8.7) is (a) an entire analytic function in the lower complex half-plane $\operatorname{Im} p < 0$ and (b) bounded by a constant C_f (as $a = 0$). As here $s = \gamma - \operatorname{Im} p + i \operatorname{Re} p$, *the function* $f^L(s)$ *will be entire analytic in the right half-plane* $\operatorname{Re} s > \gamma$. *The value of* γ *is thus a left bound for the region of analyticity of the function* $f^L(s)$. See Fig. 8.4. When we perform the inverse Laplace transform (8.9a), the integration path is such that $f^L(s)$ is analytic and bounded to its right and all singularities are confined to its left. Such integration paths are referred to as *Bromwich* contours. Clearly, for $q < 0$, the exponential factor $\exp(qs)$ in (8.9a) allows us to invoke Cauchy and Jordan and close the integration contour with a semicircle at infinity, obtaining $f(q) = 0$ for this region [Fig. 8.5(a)]. For $q > 0$ the integration requires more effort but can usually be dealt with by applying Cauchy and Jordan for poles and other techniques for branch cuts [Fig. 8.5(b)].

8.1.6. Example

Consider an example,

$$f_{n,c}(q) := \begin{cases} q^n \exp(cq), & q > 0, \\ 0, & q \leqslant 0, \end{cases} \tag{8.10}$$

which is of growth (1, Re c). The construction of its Laplace transform pro-

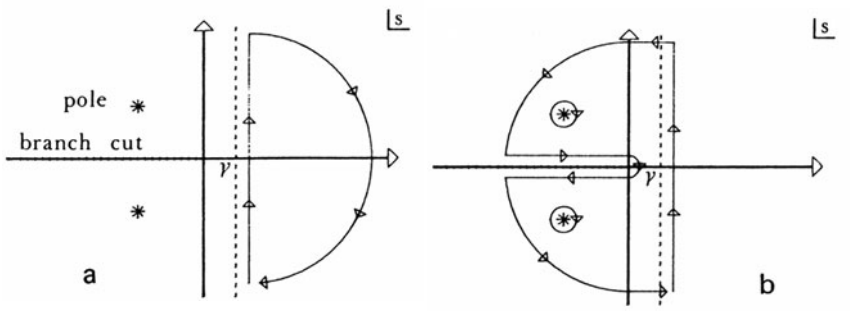


Fig. 8.5. Bromwich integration contours for the inverse unilateral transform for (a) $q < 0$ and (b) $q > 0$. A pair of conjugate poles and a branch cut have been assumed for the analytic continuation of the transform function.

ceeds by (8.7) with a choice of $\gamma > \text{Re } c$, which makes the function integrable. Its Laplace transform can be found by successive integration by parts as

$$\begin{aligned} f^L_{n,c}(s) &= \int_0^\infty dqq^n \exp[-q(s-c)] \\ &= -(s-c)^{-1}q^n \exp[-q(s-c)]|_{q=0}^{\infty} \\ &\quad + n(s-c)^{-1}\int_0^\infty dqq^{n-1}\exp[-q(s-c)] \\ &= \cdots = n!\,(s-c)^{-n}\int_0^\infty dq \exp[-q(s-c)] = n!\,(s-c)^{-n-1}, \end{aligned}$$

$$\text{Re}(s-c) = \gamma - \text{Re } c > 0, \quad (8.11)$$

i.e., it is a function with an $(n+1)$-fold pole at $s = c$. The integration (8.11) is properly valid only for Re $s >$ Re c, so the inverse Laplace transform along a vertical path at γ is inside this region, with $f^L(s)$ free of singularities to the right of it. The function $f^L(s)$, however, possesses an *analytic continuation* to the whole complex s-plane which allows its inverse transformation by means of the Cauchy and Jordan results. The former states that

$$(2\pi i)^{-1}\oint ds(s-c)^{-n-1}g(s) = (n!)^{-1}\,d^n g(s)/ds^n|_{s=c}, \quad (8.12)$$

while the latter tells us that for $q > 0$ we can set up a Bromwich contour with vanishing contribution at the infinite semicircle, so that $f(q)$ is regained as

$$\begin{aligned} (2\pi i)^{-1}\int_{\gamma-i\infty}^{\gamma+i\infty} ds[n!\,(s-c)^{-n-1}]\exp(sq) \\ = (2\pi i)^{-1}n!\oint ds(s-c)^{-n-1}\exp(sq) \\ = \frac{d^n}{ds^n}[\exp(sq)]\Big|_{s=c} = q^n\exp(cq). \end{aligned} \quad (8.13)$$

In Table 8.1 we have listed some useful Laplace transform pairs. Much more extensive tables can be found in the Bateman manuscript project (Erdelyi *et al.* (1954, Vol. I, Chapters IV and V) and in a recent table by Oberhettinger and Badii (1973).

In most applications it is the *inverse* Laplace transform of a function which yields the final solution to the problem. Thus it is the second part of the above example which should be of primary interest. It tells us that the inverse transform of a simple pole ($n = 0$) at $s = c$ is an exponential function $\exp(cq)$ times $(n!)^{-1}$. *Pairs* of poles at $c = a \pm ib$ will thus inverse-transform to oscillating functions *sin* or *cos*, depending on the relative residue signs.

Exercise 8.2. Verify the pairs of Laplace transforms of Table 8.1 where $f^L(s)$ is a function of the kind discussed above.

8.1.7. Derivatives and Boundary Conditions

The second main ingredient in the solution of differential equations by Laplace transformation is the way in which derivatives of functions transform and initial conditions appear. Assume $f(q)$ is differentiable as many times as required and that all its derivatives grow, for $q > 0$, not faster than $(1, \gamma)$ for some common γ. Then if $f^L(s)$ is the Laplace transform of $f(q)$, the transform of $f'(q) := df(q)/dq$ can be found from (8.9b) by integration by parts [in doing so we assume $f'(q)$ is continuous on $(0, \infty)$; see Exercise 8.4]:

$$\begin{aligned}(\mathbb{L}\mathbf{f}')(s) &= \int_0^\infty dq f'(q) \exp(-sq) \\ &= f(q) \exp(-sq)|_{q=0}^{\infty} + s \int_0^\infty dq f(q) \exp(-sq) \\ &= -f(0) + s(\mathbb{L}\mathbf{f})(s). \end{aligned} \tag{8.14}$$

The important thing about (8.14) is that $(\mathbb{L}\mathbf{f}')(s)$ is $s(\mathbb{L}\mathbf{f})(s)$—a result obtainable by Fourier transformation alone—*plus* the boundary value $f(0)$ of the transforming function. The second derivative is as easy to calculate and yields

$$(\mathbb{L}\mathbf{f}'')(s) = -f'(0) - sf(0) + s^2(\mathbb{L}\mathbf{f})(s). \tag{8.15}$$

The case for higher derivatives is included in Table 8.2: The boundary values and derivatives up to the order of differentiation minus one appear. For many differential equations this is all that is needed to determine the solution uniquely.

8.1.8. The Driven, Damped Oscillator

As an example where the boundary conditions appear, let us draw upon our old driven, damped harmonic oscillator system whose equation of motion is

$$\left(M \frac{d^2}{dq^2} + c \frac{d}{dq} + k\right) f(q) = F(q) \tag{8.16}$$

[see Eqs. (2.1) and (7.111), except that here we do not need to restrict c to positive values]. Using (8.14) and (8.15), we find the Laplace transform of (8.16) to be

$$M[-f'(0) - sf(0) + s^2 f^L(s)] + c[-f(0) + sf^L(s)] + kf^L(s) = F^L(s). \tag{8.17}$$

From here we can easily solve for $f^L(s)$:

$$\begin{aligned} f^L(s) &= (Ms^2 + cs + k)^{-1}\{F^L(s) + [Mf'(0) + (Ms + c)f(0)]\} \\ &:= f_F{}^L(s) + f_B{}^L(s). \end{aligned} \tag{8.18}$$

The structure of (8.18) is rather transparent: it contains a "stationary" term $f_F{}^L(s)$ due to the driving force transform $F^L(s)$ plus a transient response to the boundary conditions $f_B{}^L(s)$. The latter is immediately invertible: the two poles of the denominator are located by factoring the expression

$$Ms^2 + cs + k = M(s - s_+)(s - s_-). \tag{8.19a}$$

$$s_\pm := -\Gamma \pm ip_e, \qquad \Gamma := c/2M, \qquad p_e := (p_0{}^2 - \Gamma^2)^{1/2}, \qquad p_0 := (k/M)^{1/2}, \tag{8.19b}$$

where we have used the same variables as in (7.113). The inverse Laplace transform of $f_B^L(s)$ is zero for $q < 0$ since the integration path follows any abscissa $\gamma > \Gamma$. For $q > 0$ the integral can be found by closing the Bromwich contour around the denominator roots:

$$\begin{aligned} f_B(q) &= (2\pi i)^{-1} \int_{\gamma - i\infty}^{\gamma + i\infty} ds[(s - s_+)(s - s_-)]^{-1}[f'(0) + (s + c/M)f(0)] \\ &= -(s_- - s_+)^{-1}[f'(0) + (s_- + c/M)f(0)] \exp(s_- q) \\ &\quad - (s_+ - s_-)^{-1}[f'(0) + (s_+ + c/M)f(0)] \exp(s_+ q) \\ &= \exp(-\Gamma t)\{f(0)[\cos(p_e q) + \Gamma \sin(p_e q)/p_e] + f'(0) \sin(p_e q)/p_e\} \\ &= f(0)[cG(q) + M\dot{G}(q)] + Mf'(0)G(q), \end{aligned} \tag{8.20}$$

where

$$G(q) := \begin{cases} \exp(-\Gamma q) \sin(p_e q)/Mp_e, & q > 0, \\ 0, & q \leqslant 0, \end{cases} \tag{8.21}$$

is the Green's function of the system and $\dot{G}(q)$ its derivative. In obtaining this result we have used (8.13) with $n = 0$ and $s_\pm$ for c and collected terms. The transient response is identical to the corresponding results we have previously obtained from (2.10)–(2.13) and (7.115)–(7.122).

As to the stationary solution term $f_F{}^L(s)$ we see that it is $F^L(s)$ multiplied by the reciprocal of (8.19). Our intuition should tell us that the inverse Laplace transform of this product is a convolution—Laplace version—of the inverse transforms of the factors. In fact, it is exactly (7.117), namely,

$$f_F(q) = \int_0^q dq' F(q')G(q - q'), \tag{8.22}$$

with the understanding that the driving force $F(q)$ is, as are all functions, subject to unilateral Laplace transformation, zero up to $q = 0$.

Exercise 8.3. Starting from the relation between product and convolution under Fourier transformation, show that the unilateral Laplace version of this correspondence is as given in Table 8.2. Note that the abscissa of the integration path must be *larger* than the type of the factors.

Exercise 8.4. Show that if the function $f'(q)$ in (8.14) is discontinuous at some point d, its Laplace transform has an extra term involving the discontinuity of the function at that point, as shown in Table 8.2. Examine the case where there is more than one such point.

Exercise 8.5. Prove the rest of the entries in Table 8.2.

The Laplace transform has been used to solve Eq. (8.16) once more. In terms of directness and ease, the Laplace methods seems to be preferable to the Fourier transform, as the latter does not allow for growing functions without requiring Dirac δ's. The "cutting" process of Section 7.4 for negative q's also involves some effort. For these reasons, the unilateral Laplace transform has found wide acceptance as a tool in engineering and electronic computation. Texts centering on this method include (among many others) those of Gardner and Barnes (1942), Doetsch (1950, 1955, and 1961), and Craig (1964). Most books dealing with Fourier transforms will also have a chapter on Laplace transforms. The considerable mathematical interest of the latter has merited a few volumes by itself, such as the treatise by Widder (1941), Smith (1966), and Kuhfittig (1978). It is with some misgivings that we close this section having presented only the barest essentials of the subject. Function vector space concepts such as orthogonality and completeness of a basis, however, seem to be easier to develop in terms of Fourier—and similar *unitary*—transforms.

Table 8.1 Some Useful Laplace Transform Pairs

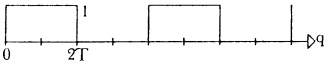
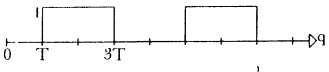
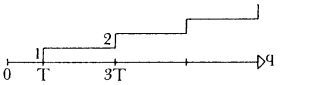
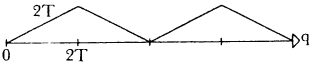
$f(q)$	$f^L(s)$	Domain
$\exp(cq)$	$(s - c)^{-1}$	$\operatorname{Re} s > c$
$\sin cq$	$c/(s^2 + c^2)$	$\operatorname{Re} s > 0$
$\cos cq$	$s/(s^2 + c^2)$	$\operatorname{Re} s > 0$
$\Theta(q - a), a > 0$	$s^{-1} \exp(-as)$	$\operatorname{Re} s > 0$
	$\{s[1 + \exp(-2Ts)]\}^{-1}$	$\operatorname{Re} s > 0$
	$(s \cosh Ts)^{-1}$	$\operatorname{Re} s > 0$
	$(s \sinh Ts)^{-1}$	$\operatorname{Re} s > 0$
	$s^{-2} \tanh Ts$	$\operatorname{Re} s > 0$
$q^n \exp(cq)$	$n!\,(s - c)^{-n-1}$	$\operatorname{Re} s > c$
$\exp(-q^2/2a^2)$	$a(\pi/2)^{1/2} \exp(a^2s^2/2) \operatorname{erfc}(2^{-1/2}as)$	All $s \in \mathscr{C}$
$J_\mu(cq), \mu > -1$	$(s^2 + c^2)^{-1/2} c^{-\mu}[(s^2 + a^2)^{1/2} - s]^\mu$	$\operatorname{Re} s > 0$

Table 8.2 Laplace Transform under Various Operators and Operations

Relation	$f(q)$	$f^L(s)$
Linear combination	$af(q) + bg(q)$	$af^L(s) + bg^L(s)$
Translation	$f(q - a)$	$\exp(-as)\left[f^L(s) + \int_{-a}^{0} dq' f(q') \exp(-sq')\right]$
	$\exp(aq)f(q)$	$f^L(s - a)$
Dilatation	$f(q/c)$, $c > 0$	$cf^L(cs)$
Multiplication	$f(q)g(q)$	$(2\pi i)^{-1} \int_{\gamma - i\infty}^{\gamma + i\infty} ds' f^L(s') g^L(s - s')$, $\gamma >$ type f, g
Convolution	$\int_0^q dq' f(q') g(q - q')$	$f^L(s) g^L(s)$
Differentiation	$\frac{d^n}{dq^n} f(q)$, continuous	$s^n f^L(s) - \sum_{m=1}^{n} s^{m-1} f^{(n-m)}(0)$
	$\frac{d}{dq} f(q)$, discontinuous at $q = d$	$sf^L(s) - f(0) + \exp(-dq)[f(d^-) - f(d^+)]$
	$(-q)^n f(q)$	$\frac{d^n}{ds^n} f^L(s)$
Integration	$\int_0^q dq' f(q')$	$s^{-1} f^L(s)$
	$-q^{-1} f(q)$	$\int_0^s ds' f(s')$

8.2. Mellin Transforms

Mellin transforms are closely related to Fourier transforms and constitute a "continuous analogue" of Taylor series. As was the case with Laplace transforms, there are at least two versions of this transform, a bilateral and a unilateral one. The first will help us to establish Dirac orthonormality and completeness relations for the repulsive oscillator wave functions. The second is useful for several of its properties involving convolution transformation of differential equations into difference relations and the appearance of gamma functions.

8.2.1. Positive, Negative, and Bilateral Mellin Transforms

Consider the direct and inverse Fourier transform equations (7.1) for functions $g(q)$ and $\tilde{g}(p)$ and make the change of variables $q =: \ln x$, so that $\exp(\pm ipq) = x^{\pm ip}$, mapping the real line q onto the positive half-line x. As $dq = dx/x$, it is convenient to attach a factor $x^{-1/2}$ to the kernel x^{ip} and a

factor $x^{-1/2}$ to $g(\ln x)$, denoting the new function by $f(x)$. After this has been done, the Fourier transform pair is

$$f(x) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} d\lambda f_+{}^M(\lambda) x^{i\lambda - 1/2}, \qquad x \in (0, \infty), \tag{8.23a}$$

$$f_+{}^M(\lambda) = (2\pi)^{-1/2} \int_0^{\infty} dx f(x) x^{-i\lambda - 1/2}, \qquad \lambda \in \mathscr{R}, \tag{8.23b}$$

where, in addition, we have changed the dummy variable p by λ and $\tilde{g}(p)$ by $f_+{}^M(\lambda)$. The function $f_+{}^M(\lambda)$ will be called the *positive Mellin transform* of $f(x)$. Effecting the same changes of variable and notation, the Parseval identity (7.1c) becomes

$$\int_0^{\infty} dx f(x)^* g(x) = \int_{-\infty}^{\infty} d\lambda f_+{}^M(\lambda)^* g_+{}^M(\lambda). \tag{8.23c}$$

The transform pair (8.23a)–(8.23b) is somewhat lopsided, since the function $f(x)$ is allowed to have only a positive argument. Negative values of x can be admitted only if, to begin with, we had introduced a change of variables $q =: \ln(-x)$, $x < 0$. By following through with the same substitutions, this leads to

$$f(x) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} d\lambda f_-{}^M(\lambda)(-x)^{i\lambda - 1/2}, \qquad x \in (-\infty, 0), \tag{8.24a}$$

$$f_-{}^M(\lambda) = (2\pi)^{-1/2} \int_{-\infty}^{0} dx f(x)(-x)^{-i\lambda - 1/2}, \qquad \lambda \in \mathscr{R}, \tag{8.24b}$$

and the Parseval identity

$$\int_{-\infty}^{0} dx f(x)^* g(x) = \int_{-\infty}^{\infty} d\lambda f_-{}^M(\lambda)^* g_-{}^M(\lambda). \tag{8.24c}$$

Correspondingly, $f_-{}^M(\lambda)$ will be called the *negative Mellin transform* of $f(x)$. As, clearly, the positive and negative halves of $f(x)$ are in general unrelated, the two transforms $f_+{}^M(\lambda)$ and $f_-{}^M(\lambda)$ are independent. If we introduce the positive—and negative—x-function (7.202b),

$$x_+ := \begin{cases} x, & x > 0, \\ 0, & x \leqslant 0, \end{cases} \qquad x_- := \begin{cases} 0, & x \geqslant 0, \\ -x, & x < 0, \end{cases} \tag{8.25}$$

we can *join* (8.23) and (8.24) for $x \in \mathscr{R}$ as

$$(\mathbb{M}_B^{-1}\mathbf{f}^{BM})(x) := f(x) = (2\pi)^{-1/2} \sum_{\sigma = \pm} \int_{-\infty}^{\infty} d\lambda f_\sigma^{BM}(\lambda) x_\sigma^{i\lambda - 1/2}, \tag{8.26a}$$

$$(\mathbb{M}_B\mathbf{f})_\sigma(\lambda) := f_\sigma^{BM}(\lambda) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dx f(x) x_\sigma^{-i\lambda - 1/2}, \tag{8.26b}$$

$$\int_{-\infty}^{\infty} dx f(x)^* g(x) = \sum_{\sigma = \pm} \int_{-\infty}^{\infty} d\lambda f_\sigma^{BM}(\lambda)^* g_\sigma^{BM}(\lambda). \tag{8.26c}$$

The *pair* of functions $\{f_\sigma^{BM}(\lambda)\}_{\sigma=\pm}$, $\lambda \in \mathscr{R}$, are called the *bilateral* Mellin transform of $f(x)$, $x \in \mathscr{R}$. We must stress that the two component functions $f_\pm^{BM}(\lambda)$ are needed to reconstitute $f(x)$ for $x \in \mathscr{R}$. The latter is the inverse bilateral Mellin transform of the pair $f_\pm^{BM}(\lambda)$.

8.2.2. Orthogonality and Completeness of $x_\pm^{i\lambda-1/2}$

The bilateral Mellin synthesis (8.26a) can be seen as the continuous analogue of the Taylor expansion. Whereas the latter sums over the positive integer powers of x, the former involves integration of powers along a line in the complex plane. This is represented schematically in Fig. 8.6. Actually, pairs of series and transforms occur in several other instances, as will be mentioned in Section 8.5. Last, as we have only performed a change of variable and function in passing from the Fourier transform to the bilateral Mellin transform (8.26), the powerful results of the former can be translated to the latter *verbatim*.

One of the results of Section 7.3 was to justify that if one of the functions of an integral transform pair was introduced in the other and the integrals exchanged, a representation of the Dirac δ by a divergent integral was obtained. Following this procedure for the bilateral Mellin transform, substituting (8.26a) into (8.26b), we obtain the *orthogonality* relation for the set of functions $\{(2\pi)^{-1/2}x_\sigma^{-i\lambda-1/2}\}_{\sigma=\pm,\lambda\in\mathscr{R}}$ as

$$(2\pi)^{-1}\int_{-\infty}^{\infty} dx x_\sigma^{i\lambda-1/2}x_{\sigma'}^{-i\lambda'-1/2} = \delta(\lambda-\lambda')\delta_{\sigma,\sigma'}, \tag{8.27}$$

where $\delta_{\sigma,\sigma'}$ is the ordinary Kronecker δ in the indices σ and σ' and $\delta(\lambda-\lambda')$ the Dirac δ in the index λ. Similarly, by substituting (8.26b) into (8.26a) and exchanging integrals, the *completeness* relation

$$(2\pi)^{-1}\sum_{\sigma=\pm}\int_{-\infty}^{\infty} d\lambda x_\sigma^{i\lambda-1/2}x_\sigma'^{-i\lambda-1/2} = \delta(x-x') \tag{8.28}$$

is obtained. The set of functions $\{(2\pi)^{-1/2} - x_\sigma^{i\lambda-1/2}\}_{\sigma=\pm,\lambda\in\mathscr{R}}$ thus constitutes a generalized (Dirac) orthonormal basis for $\mathscr{L}^2(\mathscr{R})$. Equations (8.27)–(8.28) are valid for the positive or negative Mellin transforms separately if we disregard the index σ and restrict integration and δ's to positive or negative values of x.

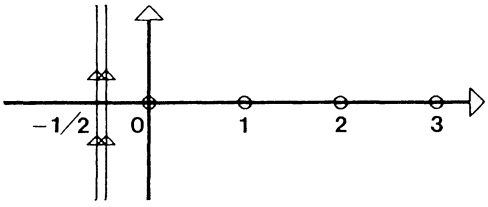


Fig. 8.6. The bilateral Mellin transform (double integration contour at $-\frac{1}{2}+i\lambda$) as a continuous analogue of the Taylor series (circles on the integer points).

Exercise 8.6. Derive the orthogonality relation (8.27) from (7.93) for $n = 0$, $q = \lambda - \lambda'$, and $p = \ln(\pm x)$ for the supports of $x_\pm$. Similarly, derive the completeness relation (8.28) from (7.93) for $n = 0$, $p = \lambda$, $q = \ln(\pm x)$, $q' = \ln(\pm x')$ in the appropriate ranges. You will be faced with a δ in $\ln x - \ln x'$ for which (7.96) can be used.

8.2.3. Completeness of the Repulsive Oscillator Wave Functions

The results (8.27) and (8.28) lead us neatly to the orthogonality and completeness relation for the repulsive oscillator wave functions presented in Section 7.5. The $\tilde{v}_\lambda{}^\pm(p)$ functions in Eqs. (7.202), which were instrumental in the solution of the problem, are (for $\sigma = 1$) $p_\pm^{-i\lambda-1/2}$ times the phase $\exp(ip^2/4)$, which is independent of λ. Now multiplication of the set in (8.27)–(8.28) by a purely x-dependent phase leaves the *inner product* (8.27) invariant: the phase of the first function cancels the phase of the second. Similarly, when multiplied by $\exp(ix^2/4)\exp(-ix'^2/4)$ on both sides the λ-integral (8.28) yields completeness for the $\tilde{v}_\lambda{}^\pm(p)$, as the left-hand side is nonzero only for $x = x'$. Since the Fourier transform is unitary—and for the full explanation of *this* fact we have to rely on more general results—it will map a Dirac basis of $\mathscr{L}^2(\mathscr{R})$ onto another such basis. Thus the set of functions $v_\lambda{}^\pm(q)$ constitutes a Dirac basis of $\mathscr{L}^2(\mathscr{R})$ as well. Finally, multiplication by the λ-independent phase factor $\exp(iq^2/2)$ and the q-independent one $2^{i\lambda/2}$ validates the set $\{\chi_\lambda{}^\sigma(q)\}_{\sigma=\pm,\lambda\in\mathscr{R}}$ in (7.203) as a Dirac generalized basis, orthogonal and complete in $\mathscr{L}^2(\mathscr{R})$.

8.2.4. Unilateral Mellin Transforms

As with Laplace transforms, there are at least two versions of the Mellin transform, the bilateral one sketched above and the more usual *Mellin–Laplace*, or simply *the* Mellin, transform. We shall now detail the construction of the latter and mention some of its properties and areas of application. We start again from the Fourier transform pair (7.1) for $g(q)$ and $\tilde{g}(p)$, assuming that for some nonempty range of γ, $\exp(\gamma q)g(q)$ is integrable (this may be true only for $\gamma = 0$). We set $r := \gamma + ip$ and $u := \exp(-q) > 0$, following through with the changes in differentials and integration ranges. Finally, we introduce the functions $f(u) := (2\pi)^{-1/2}\exp(\gamma q)g(q)$ and $f^M(r) := \tilde{g}(p)$, obtaining for them the relation

$$(\mathbb{M}^{-1}\mathbf{f}^M)(u) := f(u) = (2\pi i)^{-1}\int_{\gamma-i\infty}^{\gamma+i\infty} dr f^M(r)u^{-r}, \tag{8.29a}$$

$$(\mathbb{M}\mathbf{f})(r) := f^M(r) = \int_0^\infty du f(u)u^{r-1} \tag{8.29b}$$

and the Parseval formula

$$\int_0^\infty du f(u)^* g(u)u^{2\gamma-1} = (2\pi i)^{-1}\int_{\gamma-i\infty}^{\gamma+i\infty} dr f^M(r)^* g^M(r). \tag{8.29c}$$

8.2.5. Example

Working out an example will clarify some points. Consider

$$F_{n,-c}(u) \coloneqq u^n \exp(-cu), \qquad c \in \mathscr{C},\ \mathrm{Re}\, c > 0,\ u > 0, \tag{8.30a}$$

which represents an exponentially damped oscillating function. As the integral (8.29b) over $(0, \infty)$ is convergent for $\mathrm{Re}(r + n) > 0$, the Mellin transform over this region is

$$\begin{aligned} F^M_{n,-c}(r) &= \int_0^\infty du \exp(-cu) u^{r+n-1} \\ &= c^{-r-n} \int_0^\infty du' \exp(-u') u'^{r+n-1} = c^{-r-n}\Gamma(r+n), \\ &\qquad \mathrm{Re}(r+n) > 0. \end{aligned} \tag{8.30b}$$

In changing variables for $\mathrm{Im}\, c \neq 0$ the integration contour is made along a ray in the complex u'-plane and shifted back as in Fig. 7.13 by the use of the Cauchy and Jordan results. The remaining integral is the gamma function (see Appendix A) for $\mathrm{Re}(r + n) > 0$, and this by analytic continuation defines $F^M_{n,c}(r)$ for all complex $r + n \neq 0, -1, -2, \ldots$. One of the useful characteristics of the Mellin transform is that, as we saw, exponential functions are transformed into gamma functions, whose difference relations [i.e., those relating $\Gamma(z)$ with $\Gamma(z \pm n)$] are well known. Compare this with the Laplace transform of the same example, Eq. (8.11), which is a function with an $(n + 1)$th-order pole at c. The original function in the Fourier transform pair giving rise to (8.30a) is $\sim \exp[-(\gamma + n)q - c\exp(-q)]$ for any $\gamma > -n$ which is integrable on $q \in \mathscr{R}$. The Bromwich contour yielding the inverse Mellin transform of (8.30b) is thus along a vertical path in the complex r-plane crossing the real axis at γ, to the right of all the poles of the function, as in Fig. 8.7. The inverse transform of (8.30b) can thus be found, for $u > 0$, as

$$\begin{aligned} &(2\pi i)^{-1} \int_{\gamma - i\infty}^{\gamma + i\infty} dr \Gamma(r+n)(uc)^{-r} c^{-n} \\ &\quad = (2\pi i)^{-1} c^{-n} \sum_{m=-n}^{-\infty} \oint_{Cm} dr \Gamma(r+n)(uc)^{-r} \\ &\quad = c^{-n} \sum_{m=-n}^{-\infty} [\mathrm{Res}\, \Gamma(r+n)|_{r=m}](uc)^{-m} \\ &\quad = c^{-n} \sum_{k=0}^{\infty} (-1)^k (uc)^{n+k}/k! = u^n \exp(-cu) = F_{n,-c}(u). \end{aligned} \tag{8.30c}$$

In the process, we have used the Cauchy–Jordan results to reduce the Bromwich contour to a series of contours C_m enclosing the integrand poles a $-n, -n - 1, \ldots$ and the residue formula for the gamma function at these

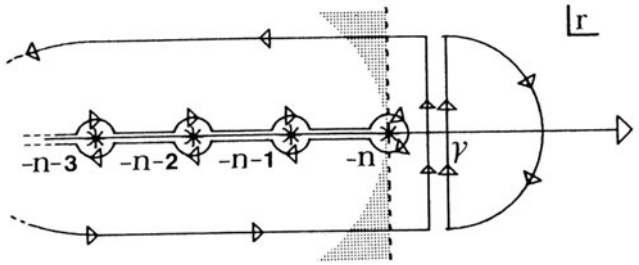


Fig. 8.7. Integration contour for Eq. (8.30c).

points [see Eq. (A.7)]. The exponential series is thus regained, and the correct original function follows. Several functions and their Mellin transforms are listed in Table 8.3. Extensive tables of Mellin transforms can be found in the Bateman manuscript project [see Erdelyi *et al.* (1954, Chapters VI and VII)].

Exercise 8.7. Check that for $u > 0$ the Bromwich contour cannot be closed through a right semicircle. Explore the situation for complex u.

The convergence requirements of the Mellin integral (8.29b) may fail to be met by many functions of interest. The inconvenient growth of a function $g(q)$ for $q \to -\infty$ ($u \to \infty$) was cured by the introduction of a factor $\exp(\gamma q)$. A similar procedure could solve growth problems for $q \to +\infty$ ($u \to 0$) with a factor $\exp(\gamma' q)$. The simultaneous correction of divergences at both ends, however, may be impossible. The Mellin transform (8.29b) can then be broken up into two Mellin transforms of functions with support on $(0, 1)$ and $[1, \infty)$ and appropriate half-planes γ and γ'. Such a procedure is followed in Morse and Feshbach (1953, p. 976). For the following results, we shall simply assume that a nonvanishing common band of convergence in the complex r-plane exists for all functions involved.

8.2.6. Further Properties

As with Fourier transforms, the properties of differentiation, multiplication by a power of the argument, and translation under Mellin transformation point toward the possible applications of this transform. Consider the Mellin transform of the derivative of a function $f'(u) := df(u)/du$ and its subsequent integration by parts:

$$(\mathbb{M}f')(r) = \int_0^\infty du[df(u)/du]u^{r-1}$$

$$= f(u)u^{r-1}\Big|_0^\infty - (r-1)\int_0^\infty duf(u)u^{r-2}. \tag{8.31}$$

If, now, within a band in the r-plane the integrand vanishes at the interval ends, the constant term in (8.31) will be zero, and Eq. (8.31) will equal

$-(r-1)(\mathbb{M}\mathbf{f})(r-1)$. This can easily be generalized for the nth derivative using the operator $\nabla^n = d^n/du^n$:

$$(\mathbb{M}\nabla^n\mathbf{f})(r) = -\sum_{p=1}^{n}(-1)^p(r-1)(r-2)\cdots(r-p)f^{(n-p)}(u)u^{r-p}\Big|_{u=0}^{\infty} + (-1)^n(r-1)(r-2)\cdots(r-n)(\mathbb{M}\mathbf{f})(r-n). \tag{8.32a}$$

If all boundary values are zero, this reduces to

$$(\mathbb{M}\nabla^n\mathbf{f})(r) = (-1)^n[\Gamma(r)/\Gamma(r-n)](\mathbb{M}\mathbf{f})(r-n). \tag{8.32b}$$

We see that differentiation of the original function becomes essentially a *translation* of the transform's argument. Using integration by parts, Eqs. (8.32) can be validated for antiderivatives as well, for negative values of n. The integration constants must be set to zero. Pure translation of the transform's argument [i.e., without multiplication by $(r-p)$-factors] can be achieved by multiplying $f(u)$ by u^n. Using the multiplication by argument operator $\mathbb{Q}$ introduced in (7.55), we can write

$$(\mathbb{M}\mathbb{Q}^n\mathbf{f})(r) = (\mathbb{M}\mathbf{f})(r+n). \tag{8.33}$$

Equations (8.32) and (8.33) are of course valid for real or complex n within the convergence band of the Mellin integral for the function in question. They can be combined as in, say,

$$(\mathbb{M}\mathbb{Q}^m\nabla^n\mathbf{f})(r) = (\mathbb{M}\nabla^n\mathbf{f})(r+m) = (-1)^n[\Gamma(r+m)/\Gamma(r+m-n)](\mathbb{M}\mathbf{f})(r+m-n), \tag{8.34a}$$

$$(\mathbb{M}\nabla^n\mathbb{Q}^m\mathbf{f})(r) = (-1)^n[\Gamma(r)/\Gamma(r-n)](\mathbb{M}\mathbb{Q}^m\mathbf{f})(r-n) = (-1)^n[\Gamma(r)/\Gamma(r-n)](\mathbb{M}\mathbf{f})(r+m-n). \tag{8.34b}$$

Further properties of operator and operations under Mellin transformation can be found in Table 8.3.

Exercise 8.8. Note that as (8.34), for $m = 1 = n$, is valid for an arbitrary function with appropriate growth conditions, one can deduce from here that $[\nabla, \mathbb{Q}] := \nabla\mathbb{Q} - \mathbb{Q}\nabla = \mathbb{1}$ on any function in this space. Similarly, verify by algebraic manipulations on multinomials that (7.67) holds.

The peculiar relationship under Mellin transformation among differentiation, multiplication by powers of the argument, and translations should not be surprising as that is precisely the behavior of x^r as a function of r under these operations.

8.2.7. Applications and References

One of the areas of application of the Mellin transform concerns the solution of the Laplace equation $\nabla^2 f(\mathbf{u}) = 0$ in two or more dimensions with

certain boundary conditions. When ∇ is written in polar coordinates (u, ϕ) [see Eq. (6.16)] and is multiplied by u^2, it is

$$(u^2\,\partial^2/\partial u^2 + u\,\partial/\partial u + \partial^2/\partial\phi^2)f(u, \phi) = 0. \tag{8.35}$$

Mellin transformation of (8.35) with respect to the radial variable u leads, by (8.34a), to

$$(r^2 + \partial^2/\partial\phi^2)f^M(r, \phi) = 0, \tag{8.36}$$

whose solutions are of the form

$$f^M(r, \phi) = a(r)\cos r\phi + b(r)\sin r\phi. \tag{8.37}$$

The boundary conditions one can impose on $f(u, \phi)$ in order to fix $a(r)$ and $b(r)$ are, for instance, $f(u, \phi)$ as a function of u for two given values of ϕ, say ϕ_a and ϕ_b. These can represent, for instance, the electrostatic potential between two fixed, charged, nonconducting plates forming a wedge between ϕ_a and ϕ_b, the stress or the stationary temperature distribution between two such walls with fixed temperature. This problem, with a variety of boundary conditions, has been solved by Tranter (1948) and Lemon (1962). Essentially, the Mellin transforms of the boundary conditions are equated to (8.37) for $\phi = \phi_a$ and ϕ_b, respectively. The ensuing solutions are examined, for instance, in the books by Colombo (1959) and Sneddon (1972, Chapter 4).

Exercise 8.9. Examine more closely the conditions under which the Mellin transformation from (8.35) to (8.36) holds. Assume $f(u, \phi)$ behaves like u^{γ_1} for $u \to 0$ and u^{γ_2} for $u \to \infty$. Show that (8.36) holds for $-\gamma_1 < u < -\gamma_2$.

Exercise 8.10. Note that once the functions $a(r)$ and $b(r)$ in (8.37) have been found, the function (8.37) still has to be subject to an inverse Mellin transform. As the two functions in (8.37) contain the boundary data, one needs to know the inverse transform of a *product* of two functions. Prove the *convolution* formulas in Table 8.3.

Table 8.3 Mellin Transform under Various Operators and Operations

Relation	$f(u)$	$f^M(r)$
Linear combination	$af(u) + bg(u)$	$af^M(r) + bg^M(r)$
Translation	$u^n f(u)$	$f^M(r + n)$
	$d^m f(u)/du^m$	$(-1)^m[\Gamma(r)/\Gamma(r - m)]f^m(r - m)$
Differentiation	$(\ln u)^k f(u)$	$d^k f^M(r)/dr^k$
Dilatation	$f(au)$, $a > 0$	$a^r f^M(r)$
	$b^{-1}f(u^{1/b})$	$f^M(br)$
Multiplication	$f(u)g(u)$	$(2\pi i)^{-1}\int_{\gamma-i\infty}^{\gamma+i\infty} dr' f^M(r')g^M(r - r')$
Convolution	$\int_0^\infty u'^{-1}\,du' f(u/u')g(u')$	$f^M(r)g^M(r)$

Table 8.4 Some Useful Mellin Transform Pairs

$f(u)$	$f^M(r)$	Domain
$u^n \exp(-cu)$, Re $c > 0$	$c^{-r-n}\Gamma(r+n)$	Re $(r+n) > 0$
$(1+u^n)^{-m}$	$\Gamma(r/n)\Gamma(m-r/n)/n\Gamma(m)$	$0 <$ Re $r < mn$
$\exp(-u^2/2\omega)$	$(2\omega)^{r/2}\frac{1}{2}\Gamma(r/2)$	$0 <$ Re r
$\cos au$	$a^{-r}\Gamma(r)\cos(\pi r/2)$	$0 <$ Re $r < 1$
$\sin au$	$a^{-r}\Gamma(r)\sin(\pi r/2)$	$0 <$ Re $r < 1$
$\dfrac{1+u\cos\phi}{1-2u\cos\phi+u^2}$, $\lvert\phi\rvert < \pi$	$\pi\cos r\phi/\sin r\pi$	$0 <$ Re $r < 1$
$\dfrac{u\sin\phi}{1-2u\cos\phi+u^2}$, $\lvert\phi\rvert < \pi$	$\pi\sin r\phi/\sin r\pi$	$0 <$ Re $r < 1$
$u^{-\nu}J_\nu(au)$	$\dfrac{(a/2)^{\nu-r}\Gamma(r/2)}{2\Gamma(\nu-r/2+1)}$	$0 <$ Re $r < 1$

8.3. N-Dimensional Fourier Transforms

A straightforward generalization of the results for the Fourier transformation of functions of one variable is the consideration of functions of N variables and their corresponding N-fold Fourier transformation. Most results from the one-dimensional case can be "vectorized" by inspection.

8.3.1. Extension from One to N Dimensions

Consider a function $f(\mathbf{q})$ of the vector variable $\mathbf{q} = (q_1, q_2, \ldots, q_N)$. As a function of q_1 we can apply the Fourier transformation (7.1b)—assuming all necessary conditions are satisfied—and obtain a function $\tilde{f}^{[1]}(p_1, q_2, \ldots, q_N)$. This function in turn can be subject to the same transformation with respect to the variable q_2 and so on, obtaining finally

$$(\mathbb{F}_{(N)}^{-1}\tilde{\mathbf{f}})(\mathbf{q}) \coloneqq f(\mathbf{q}) = (2\pi)^{-N/2}\int_{\mathscr{R}^N} d^N\mathbf{p}\tilde{f}(\mathbf{p})\exp(i\mathbf{p}\cdot\mathbf{q}), \tag{8.38a}$$

$$(\mathbb{F}_{(N)}\mathbf{f})(\mathbf{p}) \coloneqq \tilde{f}(\mathbf{p}) = (2\pi)^{-N/2}\int_{\mathscr{R}^N} d^N\mathbf{q}f(\mathbf{q})\exp(-i\mathbf{p}\cdot\mathbf{q}), \tag{8.38b}$$

where

$$\int_{\mathscr{R}^N} d^N\mathbf{q}\cdots \coloneqq \int_{-\infty}^{\infty} dq_1\int_{-\infty}^{\infty} dq_2\cdots\int_{-\infty}^{\infty} dq_N\cdots, \tag{8.38c}$$

and similarly for integration over $\mathbf{p}$-space. We have also used the familiar inner (or *scalar*) product notation $\mathbf{p}\cdot\mathbf{q} \coloneqq p_1q_1 + p_2q_2 + \cdots + p_Nq_N$ in

order to avoid confusion with the earlier sesquilinear product $(\mathbf{p}, \mathbf{q})$ in Part I. If $\mathbf{p}$ and $\mathbf{q}$ are represented as column vectors, $\mathbf{p}\cdot\mathbf{q} = \mathbf{p}^T\mathbf{q}$, where $\mathbf{x}^T$ is the transpose of vector (or matrix) $\mathbf{x}$. The Parseval identity is

$$(\mathbf{f}, \mathbf{g})_N := \int_{\mathscr{R}^N} d^N\mathbf{q} f(\mathbf{q})^* g(\mathbf{q}) = \int_{\mathscr{R}^N} d^N\mathbf{p} \tilde{f}(\mathbf{p})^* \tilde{g}(\mathbf{p}) = (\tilde{\mathbf{f}}, \tilde{\mathbf{g}})_N. \quad (8.38d)$$

8.3.2. Linear Transformations of the Underlying Space

The properties of the N-dimensional Fourier transform under linear combination, convolution, translation, and differentiation are perfectly parallel to those of the one-dimensional transform in Chapter 7, except for some factors or exponents involving the value of N which are easy to ascertain. In Table 8.5 we have collected these results. Most can be found by inspection, "vectorizing" the corresponding one-dimensional expressions: replacing q, p, and qp by $\mathbf{q}$, $\mathbf{p}$, and $\mathbf{q}\cdot\mathbf{p}$; $\int_{-\infty}^{\infty} dq$ by $\int_{\mathscr{R}^N} d^N\mathbf{q}$; factors of $(2\pi)^{-1/2}$ by $(2\pi)^{-N/2}$; etc. For dilatations, however, we have a nontrivial generalization: general linear transformations in $\mathbf{q}$-space and corresponding ones in $\mathbf{p}$-space. To obtain them, assume $f(\mathbf{q})$ and its Fourier transform $\tilde{f}(\mathbf{p})$ are known. We wish to find, in terms of these, the transform of

$$(\mathbb{D}_\mathbf{A}\mathbf{f})(\mathbf{q}) = |\det \mathbf{A}|^{-1/2} f(\mathbf{A}^{-1}\mathbf{q}), \quad (8.39)$$

where $\mathbb{D}_\mathbf{A}$ is an operator which carries the action of the $N \times N$ matrix $\mathbf{A}$, which we assume to be real and nonsingular ($\det \mathbf{A} \neq 0$). Equation (8.39) is the natural generalization of Eq. (7.34). A change of variable $\mathbf{q}' := \mathbf{A}^{-1}\mathbf{q}$ yields

$$\begin{aligned}(\mathbb{F}_{(N)}\mathbb{D}_\mathbf{A}\mathbf{f})(\mathbf{p}) &= |\det \mathbf{A}|^{-1/2}(2\pi)^{-N/2} \int_{\mathscr{R}^N} d^N\mathbf{q} f(\mathbf{A}^{-1}\mathbf{q}) \exp(-i\mathbf{p}\cdot\mathbf{q}) \\ &= |\det \mathbf{A}|^{1/2}(2\pi)^{-N/2} \int_{\mathscr{R}^N} d^N\mathbf{q}' f(\mathbf{q}') \exp(-i\mathbf{p}\cdot\mathbf{A}\mathbf{q}') \\ &= |\det \mathbf{A}|^{1/2}(\mathbb{F}\mathbf{f})(\mathbf{A}^T\mathbf{p}) = (\mathbb{D}_{\mathbf{A}^{T-1}}\mathbb{F}_{(N)}\mathbf{f})(\mathbf{p}) \quad (8.40)\end{aligned}$$

since $\mathbf{p}^T\mathbf{A}\mathbf{q}' = (\mathbf{A}^T\mathbf{p})^T\mathbf{q}'$ and $d^N\mathbf{q} = \det \mathbf{A}\, d^N\mathbf{q}'$ is the transformation Jacobian. When $\det \mathbf{A} < 0$, i.e., as in a reflection through the origin of an odd number of coordinate axes, an odd number of integrations will have the usual bound order inverted. A reversal of these integration limits will cancel the sign of $\det \mathbf{A}$ and yield an absolute valued factor $|\det \mathbf{A}|$.

Exercise 8.11. Show that the dilatation operator $\mathbb{D}_\mathbf{A}$ is *unitary*, i.e., $(\mathbb{D}_\mathbf{A}\mathbf{f}, \mathbb{D}_\mathbf{A}\mathbf{g})_N = (\mathbf{f}, \mathbf{g})_N$ for all $\mathbf{f}$ and $\mathbf{g}$ for which the inner product is finite. This parallels Exercise 7.9–10.

Exercise 8.12. Verify that $\mathbb{D}_{\mathbf{A}}\mathbb{D}_{\mathbf{B}} = \mathbb{D}_{\mathbf{AB}}$ applied to any function $f(\mathbf{q})$. This generalizes Exercise 7.9.

Exercise 8.13. Find the N-dimensional convolution forms of Table 8.5.

Exercise 8.14. Define the multiplication-by-q_j operator as $\mathbb{Q}_j$ and the differentiation operator $\mathbb{P}_k := -i\partial/\partial q_k$ as generalizations of (7.55) and (7.56). Show that

$$\mathbb{F}_{(N)}\mathbb{P}_j\mathbb{F}_{(N)}^{-1} = \mathbb{Q}_j, \qquad \mathbb{F}_{(N)}\mathbb{Q}_k\mathbb{F}_{(N)}^{-1} = -\mathbb{P}_k. \tag{8.41}$$

Clearly, also

$$[\mathbb{Q}_j, \mathbb{P}_k] := \mathbb{Q}_j\mathbb{P}_k - \mathbb{P}_k\mathbb{Q}_j = i\mathbb{1}, \tag{8.42}$$

as in (7.59).

Exercise 8.15. Define the N-dimensional *dispersion* of a function $f(\mathbf{q})$ as

$$\Delta_f^{(N)} := \left[\int_{\mathscr{R}^N} d^N\mathbf{q}|f(\mathbf{q})|^2(\mathbf{q} - \overline{\mathbf{q}^1})^2\right] \Big/ \left[\int_{\mathscr{R}^N} d^N\mathbf{q}|f(\mathbf{q})|^2\right], \tag{8.43}$$

where $\overline{\mathbf{q}^1}$ is the vector *average* (or first moment) of $f(\mathbf{q})$, the analogue of (7.216) for $r = 1$ and vector $\mathbf{q}$. From (8.41) and (8.42), show that the uncertainty relation (7.218) becomes

$$\Delta_f^{(N)}\Delta_{\tilde{f}}^{(N)} \geqslant N/4. \tag{8.44}$$

What happens with the equivalent width relation (7.223)?

The relation between linear transformations in $\mathbf{q}$- and $\mathbf{p}$-spaces embodied in Eq. (8.40) has a very important particular case: if the transformation matrix $\mathbf{A}$ is an *orthogonal* matrix [i.e., an angle-preserving transformation so that

$$(\mathbf{A}\mathbf{q}_1)\cdot\mathbf{A}\mathbf{q}_2 = \mathbf{q}_1{}^T\mathbf{A}^T\mathbf{A}\mathbf{q}_2 = \mathbf{q}_1{}^T\mathbf{q}_2 = \mathbf{q}_1\cdot\mathbf{q}_2$$

for every $\mathbf{q}_1, \mathbf{q}_2 \in \mathscr{R}^N$], then $\mathbf{A}^T = \mathbf{A}^{-1}$, $\det \mathbf{A} = \pm 1$, and the transformations in $\mathbf{q}$- and $\mathbf{p}$-space are the *same*. In terms of operators this means that, for $\mathbf{A}$ orthogonal, $\mathbb{D}_{\mathbf{A}}$ and $\mathbb{F}_{(N)}$ *commute*. In the $N = 1$ case, the analogue of an orthogonal matrix is multiplication by ± 1, and in Section 7.2 we saw that parity was preserved under Fourier transformations. For $N > 1$ the statement follows that the properties of a function under rotation and inversion are preserved under $\mathbb{F}_{(N)}$. In its full generality, the specification of "properties under rotation" requires group theory. (In three dimensions, knowledge of spherical harmonics is required, while for $N = 2$, Fourier series is all one needs. This case will be developed in Section 8.4.) One property, *invariance*, is nevertheless easy to state: a function $f(\mathbf{q})$, $\mathbf{q} \in \mathscr{R}^N$, is invariant under orthogonal transformations if $f(\mathbf{q}) = f(\mathbf{A}^{-1}\mathbf{q})$ for all orthogonal $\mathbf{A}$. This means that the function can depend only on the norm $q := (\mathbf{q}\cdot\mathbf{q})^{1/2}$. Under Fourier transformation this property becomes $\tilde{f}(\mathbf{p}) = \tilde{f}(\mathbf{A}^{-1}\mathbf{p})$, so $\tilde{f}$ in turn can also only depend on $p := (\mathbf{p}\cdot\mathbf{p})^{1/2}$.

8.3.3. The Diffusive–Elastic Medium with Sources

We shall illustrate the use of the N-dimensional Fourier transform in finding the general form for the solution of the elastic, diffusive medium with sources in N dimensions, governed by

$$\nabla^2 f(\mathbf{q}, t) + F(\mathbf{q}, t) = c^{-2} \frac{\partial^2}{\partial t^2} f(\mathbf{q}, t) + a^{-2} \frac{\partial}{\partial t} f(\mathbf{q}, t), \tag{8.45}$$

with initial conditions $f(\mathbf{q}, t_0)$ and $\dot{f}(\mathbf{q}, t_0) \coloneqq \partial f(\mathbf{q}, t)/\partial t|_{t=t_0}$ at some "initial" time t_0. Expression (8.45) resembles in part the diffusion equation, Eq. (5.1), with diffusion constant a, and in part the wave equation (5.15) with propagation velocity c. The sum of the two terms on the right-hand side states that the acceleration of the observable f due to its curvature at $\mathbf{q}$ is *diminished* by the velocity-dependent term, which has the effect of a viscous braking force. Further, the source term $F(\mathbf{q}, t)$ acts as a driving force in the regions of $(\mathbf{q}, t)$-space where it applies. The limits $c \to \infty$ and $a \to \infty$ lead, respectively, to the simple heat and wave equations in N dimensions.

Assuming $f(\mathbf{q}, t)$ and its derivatives are square-integrable in $\mathscr{R}^N$, we can apply the N-dimensional Fourier transform to (8.45), obtaining

$$-p^2 \tilde{f}(\mathbf{p}, t) + \tilde{F}(\mathbf{p}, t) = c^{-2} \frac{\partial^2}{\partial t^2} \tilde{f}(\mathbf{p}, t) + a^{-2} \frac{\partial}{\partial t} \tilde{f}(\mathbf{p}, t), \tag{8.46}$$

with initial conditions $\tilde{f}(\mathbf{p}, t_0) \coloneqq [\mathbb{F}_{(N)}\mathbf{f}(\cdot, t_0)](\mathbf{p})$ and $\dot{\tilde{f}}(\mathbf{p}, t_0)$. In this equation the most difficult part, the N-dimensional Laplacian operator, has been converted into a factor of $-p^2$ as with one-dimensional problems. Equation (8.46) is thus a second-order ordinary differential equation in time, which has been solved in Section 7.3 [Eq. (7.111)] using Fourier transforms and again in Section 8.1 [Eq. (8.16)] using Laplace techniques. By treating p^2 as a parameter and establishing the correspondence between $\{c^{-2}, a^{-2}, p^2, t\}$ and $\{M, c, k, q\}$, the solution to (8.46) is

$$\tilde{f}(\mathbf{p}, t) = \tilde{f}_F(\mathbf{p}, t) + \tilde{f}_B(\mathbf{p}, t). \tag{8.47}$$

The *transient* term solution to the homogeneous equation (8.46) (with the $\tilde{F}$ term absent) is given in terms of the boundary conditions at time t_0 as

$$\begin{aligned} \tilde{f}_B(\mathbf{p}, t) = {} & \tilde{f}(\mathbf{p}, t_0)[a^{-2}\tilde{G}(\mathbf{p}, t - t_0) + c^{-2}\dot{\tilde{G}}(\mathbf{p}, t - t_0)] \\ & + \dot{\tilde{f}}(\mathbf{p}, t_0)\tilde{G}(\mathbf{p}, t - t_0). \end{aligned} \tag{8.48}$$

The function $\tilde{G}(\mathbf{p}, t - t_0)$ can be copied from the simple oscillator Green's function [Eq. (2.11a), (2.11b), (2.12), (2.13a), (2.13b), (7.116), or (8.21), exchanging symbols as before and ω_e for p_e] as

$$\tilde{G}(\mathbf{p}, t) = \begin{cases} c^2 \exp(-\Gamma t) \sin \omega_e t/\omega_e, & t > 0, \\ 0, & t \leqslant 0, \end{cases} \tag{8.49a}$$

$$\Gamma \coloneqq c^2/2a^2, \qquad \omega_e \coloneqq (c^2 p^2 - \Gamma^2)^{1/2}. \tag{8.49b}$$

The time derivative of (8.49) is $\dot{\tilde{G}}(\mathbf{p}, t)$. The tilde has been kept for (8.49) as its $\mathbb{F}_{(N)}^{-1}$ transform will be the Green's function for the equation (8.45) we are solving.

The *stationary* solution to (8.46) due to the source $\tilde{F}(\mathbf{p}, t)$ is given by the *convolution*—with respect to t—of the source function with (8.49) [see (7.117) or (8.22) with the proper symbol exchange], i.e.,

$$\tilde{f}_F(\mathbf{p}, t) = (\tilde{F} \overset{t}{*} \tilde{G})(\mathbf{p}, t) = \int_{t_0}^{t} dt' \tilde{F}(\mathbf{p}, t') \tilde{G}(\mathbf{p}, t - t'). \tag{8.50}$$

We assume the source to start operating not earlier than the initial time t_0.

Equation (8.45), whose solution we are seeking, now requires that we apply $\mathbb{F}_{(N)}^{-1}$ to (8.47)–(8.50). The transient term (8.48) is the product of functions of $\mathbf{p}$; hence its inverse transform will be a convolution over $\mathbf{q}$ of the factors. As the initial conditions are assumed to be given, the key lies in finding

$$\begin{aligned} G_N(\mathbf{q}, t) &\coloneqq [\mathbb{F}_{(N)}^{-1} \tilde{G}(\cdot, t)](\mathbf{q}) \\ &= (2\pi)^{-N/2} c^2 \exp(-\Gamma t) \int_{\mathscr{R}^N} d^N\mathbf{p} (c^2 p^2 - \Gamma^2)^{-1/2} \\ &\quad \times \sin[(c^2 p^2 - \Gamma^2)^{1/2} t] \exp(i\mathbf{p}\cdot\mathbf{q}). \end{aligned} \tag{8.51}$$

Once this Green's function—and its time derivative—is found, the transient term will be given by

$$\begin{aligned} f_B(\mathbf{q}, t) &= (2\pi)^{-N/2} \{ f(\cdot, t_0) \overset{q}{*} [a^{-2} G_N(\cdot, t - t_0) + c^{-2} \dot{G}_N(\cdot, t - t_0)] \}(\mathbf{q}) \\ &\quad + (2\pi)^{-N/2} c^{-2} [\dot{f}(\cdot, t_0) \overset{q}{*} G_N(\cdot, t - t_0)](\mathbf{q}). \end{aligned} \tag{8.52a}$$

The stationary solution will be a *double* convolution—with respect to $\mathbf{q}$ and t—of the source with the Green's function:

$$\begin{aligned} f_F(\mathbf{q}, t) &= (2\pi)^{-N/2} (F \ast\ast G_N)(\mathbf{q}, t) \\ &= (2\pi)^{-N/2} \int_{t_0}^{t} dt' \int_{\mathscr{R}^N} d^N\mathbf{q}' F(\mathbf{q}', t') G_N(\mathbf{q} - \mathbf{q}', t - t'). \end{aligned} \tag{8.52b}$$

The most general solution will be, finally, (8.52a) plus (8.52b).

8.3.4. Wave Equation in Three Dimensions

As before, it will simplify matters to look for the *fundamental* solutions to the equation of motion, that is, those solutions or their time derivatives which at $t = t_0$ are Dirac δ's in $\mathbf{q}$, as these are found in terms of the Green's function $G_N(\mathbf{q}, t - t_0)$ and its time derivative. In this section we shall examine two limiting cases of interest: the wave equation in three dimensions, obtained in the limit $a \to \infty$, and the diffusion equation in N dimensions,

which is the limit $c \to \infty$. The wave equation for two and N dimensions and the general solution of (8.45) will be found in Section 8.4. We shall attach the indices w for wave and h for heat to the Green's functions in order to avoid confusion.

The wave equation in three dimensions simplifies the problem of finding the Green's function (8.51) since for $a \to \infty$, $\Gamma \to 0$. We are left with the calculation of the three-dimensional inverse Fourier transform of $\tilde{G}^w(\mathbf{p}, t) = c \sin(cpt)/p$. By introducing the well-known spherical coordinates

$$\begin{aligned} p_1 &= p \sin\theta \sin\varphi, & p &\in [0, \infty), \\ p_2 &= p \sin\theta \cos\varphi, & \theta &\in [0, \pi], \\ p_3 &= p \cos\theta, & \varphi &\in [0, 2\pi), \end{aligned} \tag{8.53}$$

and setting the $\theta = 0$ direction along the vector $\mathbf{q}$ so that $\mathbf{p}\cdot\mathbf{q} = pq\cos\theta$, the volume integrals (8.38) become

$$\int_{\mathscr{R}^3} d^3\mathbf{p} \cdots = \int_0^\infty p^2\, dp \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi \cdots. \tag{8.54}$$

We thus calculate

$$\begin{aligned} G_3{}^w(\mathbf{q}, t) &= (2\pi)^{-3/2} c \int_0^\infty p\, dp \sin(cpt) \int_0^\pi \sin\theta\, d\theta \exp(-ipq\cos\theta) \int_0^{2\pi} d\varphi \\ &= (2\pi)^{-1/2} c \int_0^\infty p\, dp \sin(cpt) \int_{-1}^1 du \exp(-ipqu) \qquad (u := \cos\theta) \\ &= (2\pi)^{-1/2}(2c/q) \int_0^\infty dp \sin(cpt) \sin pq \\ &= (2\pi)^{-1/2}(c/q) \int_0^\infty dp\{\cos[p(q - ct)] - \cos[p(q + ct)]\} \\ &= (2\pi)^{1/2}(c/2q)[\delta(q - ct) - \delta(q + ct)] \qquad \text{[Eq. (7.93)]} \\ &= (2\pi)^{1/2} c\delta(\mathbf{q}^2 - c^2t^2) \qquad \text{[Eq. (7.94b)].} \end{aligned} \tag{8.55}$$

Similarly, we find

$$\dot{G}_3{}^w(\mathbf{q}, t) = -(2\pi)^{1/2}(2c^2/q)[\delta'(q - ct) + \delta'(q + ct)]. \tag{8.56}$$

The general solution to initial conditions is thus found from (8.48) (for $a \to \infty$), (8.55), and (8.56) for $t > t_0$, and by remembering that $q \geqslant 0$,

$$\begin{aligned} f_B(\mathbf{q}, t) = &-(4\pi)^{-1} \int_{\mathscr{R}^3} d^3\mathbf{q}' f(\mathbf{q}', t_0) |\mathbf{q} - \mathbf{q}'|^{-1} \delta'(|\mathbf{q} - \mathbf{q}'| - c(t - t_0)) \\ &+ (4\pi c)^{-1} \int_{\mathscr{R}^3} d^3\mathbf{q}' \dot{f}(\mathbf{q}', t_0) |\mathbf{q} - \mathbf{q}'|^{-1} \delta(|\mathbf{q} - \mathbf{q}'| - c(t - t_0)). \end{aligned} \tag{8.57}$$

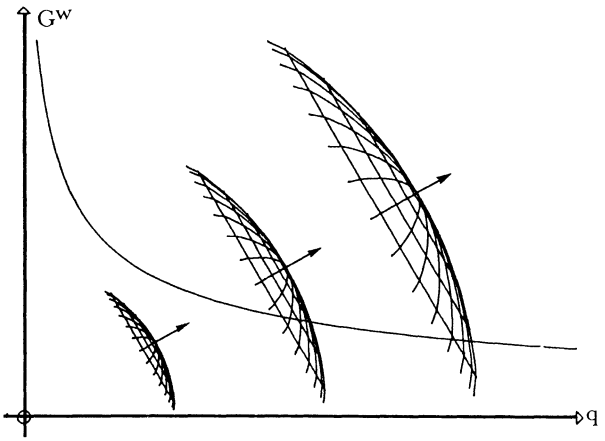


Fig. 8.8. The fundamental solutions $G_3^w(\mathbf{q}, t)$ of the three-dimensional wave equation are expanding spherical singularity shells modulated by a radial geometric factor of q^{-1} (continuous line).

It should be observed that wave propagation in three-dimensional elastic media has the following properties:

(a) The *causality principle* is obeyed due to the appearance of the δ's and the restriction $t > t_0$: if a disturbance is localized at a point $\mathbf{q}_0$ at time t_0, no information is available at a point $\mathbf{q}_1$ as long as $|\mathbf{q}_0 - \mathbf{q}_1| > c(t - t_0)$. [Just for the record, it should be noted that (8.55) and (8.56) possess *advanced* solutions for $t < t_0$ besides the *retarded* ones for $t > t_0$ which were kept in (8.57); the former are usually considered nonexistent based on the present lack of solid experimental evidence. Yet see Puthoff and Targ (1976, Sections IV and V and the references within).]

(b) *Reciprocity* holds. The effect of a disturbance at $\mathbf{q}_0$ on $\mathbf{q}_1$ is the same as that of a disturbance at $\mathbf{q}_1$ on $\mathbf{q}_0$ if their proper time ordering is respected. This is a consequence of our assumption that space is homogeneous and isotropic—Eq. (8.45) involves only ∇^2—and is reflected in the fact that the Green's function (8.57) is a function of $|\mathbf{q} - \mathbf{q}'|$ only.

(c) A point (singular) disturbance at t_0 propagates as an expanding spherical singularity shell of radius $c(t - t_0)$ modulated by a *geometric* factor $|\mathbf{q}|^{-1}$. See Fig. 8.8. This factor gives rise to the familiar "inverse-square" law for isotropic illumination, the latter being proportional to the square of the disturbance amplitude.

(d) There is no backwave; once the expanding singularity shell described above passes over a point, the medium again remains at rest.

Exercise 8.16. Consider the case of $N = 1$ dimension. This only simplifies the necessary inverse Fourier transformation. The Green's functions obtained

will be identical to (5.27) found for the case of elastic media with fixed ends. Except for the lifting of this restriction, all conclusions of Section 5.2 continue to hold. Note carefully that the three-dimensional Green's functions (8.55)–(8.56) are $-q^{-1}\partial/\partial q$ times the one-dimensional Green's functions (5.27a)–(5.27b). This fact will be generalized in Section 8.4.

Exercise 8.17. Consider the *energy* in a three-dimensional elastic vibrating medium. This can be found along lines parallel to (5.40)–(5.42), except that integration proceeds over $\mathscr{R}^3$. Show that the *partial energy* of each constituent wave $E_{\mathbf{p}} := p^2|\tilde{f}(\mathbf{p}, t)|^2 + c^{-2}|\dot{\tilde{f}}(\mathbf{p}, t)|^2$ is separately conserved. As the medium is governed by a linear equation, there will be no energy exchange between different partial waves. The wave equation thus has a continuous infinity of conservation laws, one for each value of $\mathbf{p}$.

Exercise 8.18. Propose solutions to the three-dimensional wave equation of the form $(2\pi)^{-3/2}\exp[i(\mathbf{p}\cdot\mathbf{q} + pct)]$. Expand a general solution in terms of these and the partial-wave coefficients in terms of the initial conditions. Thus reconstitute Eq. (8.57). [See the article by Halevi (1973).]

Exercise 8.19. Show the transitivity of time evolution. Compare with Exercises 5.10 and 5.17.

8.3.5. The Diffusion Equation in N Dimensions

A second family of cases where Eq. (8.45) yields to an easy solution is the limit $c \to \infty$, when the medium becomes purely diffusive. Although $\Gamma \to \infty$ and $\omega_e \simeq i(\Gamma - a^2p^2)$, the limit of (8.49a) is well defined. It is $\tilde{G}_N{}^h(\mathbf{p}, t) = a^2\exp(-a^2\mathbf{p}^2t)$. The inverse $\mathbb{F}_N$ transform of $\tilde{G}_N{}^h(\mathbf{p}, t)$ is easy to find in Cartesian coordinates, the function being the product of Gaussians of width $(2a^2t)^{-1}$ in each of the coordinates. By Eq. (7.22) we find, in N dimensions,

$$\begin{aligned} G_N{}^h(\mathbf{q}, t) &= a^2\prod_{k=1}^{N}(\pi/a^2t)^{1/2}[\mathbb{F}^{-1}\mathbf{G}_{(2a^2t)^{-1}}](q_k) \\ &= a^2(2a^2t)^{-N/2}\exp(-\mathbf{q}^2/4a^2t). \end{aligned} \tag{8.58}$$

The general transient solution thus becomes, from (8.52a),

$$f_B(\mathbf{q}, t) = (4\pi a^2t)^{-N/2}\int_{\mathscr{R}^N} d^N\mathbf{q}'f(\mathbf{q}', t_0)\exp[-(\mathbf{q} - \mathbf{q}')^2/4a^2(t - t_0)], \tag{8.59}$$

leaving out the initial velocity as a boundary condition for $f_B(\mathbf{q}, t)$. The differential equation is now of first order in time. The fundamental solutions are spreading Gaussians of width $2a^2(t - t_0)$ with a decreasing maximum of $(4\pi a^2t)^{-N/2}$. See Fig. 8.9. One can see that the temperature maximum drops faster for higher dimensions: heat simply has more directions in which to escape.

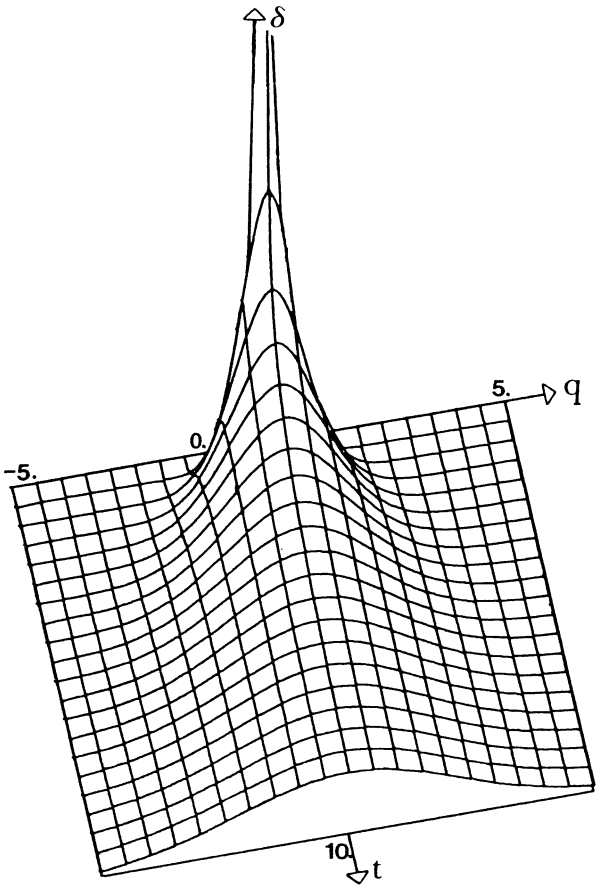


Fig. 8.9. The fundamental solution $G_1^h(q, t)$ of the one-dimensional diffusion equation (for $a = \frac{1}{2}$). The initial condition given by a Dirac δ at $q = 0$ develops in time as a spreading Gaussian.

It is interesting to compare the Green's function for a one-dimensional heat flow in an unbounded medium (Fig. 8.9) with the heat flow in a *ring* discussed in Section 5.1 (the Green's function is shown in Fig. 4.13, reading time development upward). Exercise 8.20 indicates some further developments.

Exercise 8.20. Solve the N-dimensional homogeneous diffusion equation (8.45) ($c \to \infty$) by proposing separable solutions in all coordinates. Choosing the boundary conditions, you should arrive at (8.59).

Exercise 8.21. Prove that total heat is conserved. Compare with Exercise 5.1.

Table 8.5 A Function and Its N-Dimensional Fourier Transform under Various Operators and Operations[a]

Operation	$f(\mathbf{q})$	$\tilde{f}(\mathbf{p})$
Translation	$f(\mathbf{q}+\mathbf{y})$	$\exp(i\mathbf{p}\cdot\mathbf{y})\tilde{f}(\mathbf{p})$
	$\exp(-i\mathbf{q}\cdot\mathbf{x})f(\mathbf{q})$	$\tilde{f}(\mathbf{p}+\mathbf{x})$
Linear transformation	$f(\mathbf{Aq})$	$\lvert\det\mathbf{A}\rvert^{-1}\tilde{f}(\mathbf{A}^{T-1}\mathbf{p})$
Multiplication	$f(\mathbf{q})g(\mathbf{q})$	$(2\pi)^{-N/2}(\tilde{f}*\tilde{g})(\mathbf{p})$
Convolution	$(f*g)(\mathbf{q})$	$(2\pi)^{N/2}\tilde{f}(\mathbf{p})\tilde{g}(\mathbf{p})$
Differentiation	$\nabla f(\mathbf{q})$	$i\mathbf{p}\tilde{f}(\mathbf{p})$
	$-i\mathbf{q}f(\mathbf{q})$	$\nabla\tilde{f}(\mathbf{p})$

[a] Compare with Table 7.1 for the $N = 1$ case.

Exercise 8.22. Prove the transitivity of the time evolution given by (8.59). This is the analogue of Eq. (5.11) or (5.14). Equation (7.50) should come in very handy.

The description of the wave and diffusion phenomena as well as some generalizations such as the *telegraph* equation can be found in several theoretical physics texts. Notably, Courant and Hilbert (1962) dedicate several sections of Vol. 2 to these problems, using several solution methods in Chapters III and VI.

8.4. Hankel Transforms

If a system "looks the same" from any direction in space, we say that it is invariant under rotations or isotropic. This is the case, for instance, of gravitational attraction between point masses. It is also true of many potentials in spinless quantum mechanics. The isotropy of the system implies that the governing equations of motion depend only on rotationally invariant quantities such as functions of $q := |\mathbf{q}| = (\mathbf{q}\cdot\mathbf{q})^{1/2}$ or derivatives as ∇^2. This was the case of the N-dimensional elastic–diffusive medium described by Eq. (8.45), which was not only isotropic but *homogeneous*: invariant under translations (only ∇^2 appears). The Fourier transform of an isotropic differential equation is itself isotropic, and thus the Green's function is a function of q only. Of course, initial conditions need not be isotropic. Only the laws of motion are. This brings us to examine more closely the N-dimensional Fourier transform of functions of the radial variable q only and, later, that of eigenfunctions of the rotation operators. Parametrizing N-dimensional space conveniently in spherical coordinates, we shall reduce the N-fold $\mathbb{F}_{(N)}$ integration to a single integral defining the Hankel transform.

8.4.1. Spherical Coordinates in N Dimensions

The problem of introducing spherical coordinates into N-dimensional space can be tackled by guiding ourselves with the two- and three-dimensional cases [Eqs. (6.14) and (8.53)]. Consider a vector of length q along the Nth coordinate $\mathbf{v}_N \coloneqq \{0, \ldots, 0, q\}$. (To save space we write column vectors as row vectors between braces.) We transform this vector by a rotation by an angle θ_{N-1} in the N–$(N-1)$ coordinate plane. The vector is then transformed into $\mathbf{v}_{N-1} \coloneqq \{0, \ldots, 0, q \sin \theta_{N-1}, q \cos \theta_{N-1}\}$. If $N = 2$, this is all we need to do. If $N > 2$, we now rotate $\mathbf{v}_{N-1}$ into the next higher subspace, through an angle θ_{N-2} in the $(N-1)$–$(N-2)$-plane, obtaining

$$\mathbf{v}_{N-2} \coloneqq \{0, \ldots, 0, q \sin \theta_{N-1} \sin \theta_{N-2}, q \sin \theta_{N-1} \cos \theta_{N-2}, q \cos \theta_{N-1}\}.$$

If $N = 3$, this is all. [See Eqs. (8.53).] If $N > 3$, we rotate through an angle θ_{N-3} in the $(N-2)$–$(N-3)$-plane and continue in this way, piling sines and cosines of the new angles on the components of the vector $\mathbf{v}_{N-k}$. Once a cosine is added to a component, it receives no new factors. The last rotation through θ_1 is in the 2–1 plane. The components of $\mathbf{v}_1$ are then, finally,

$$\begin{aligned}
q_1 &= q \sin \theta_{N-1} \sin \theta_{N-2} \cdots \sin \theta_2 \sin \theta_1, \\
q_2 &= q \sin \theta_{N-1} \sin \theta_{N-2} \cdots \sin \theta_2 \cos \theta_1, \\
q_3 &= q \sin \theta_{N-1} \sin \theta_{N-2} \cdots \cos \theta_2, \\
&\cdots \\
q_k &= q \sin \theta_{N-1} \cdots \sin \theta_k \cos \theta_{k-1}, \\
&\cdots \\
q_{N-1} &= q \sin \theta_{N-1} \cos \theta_{N-2}, \\
q_N &= q \cos \theta_{N-1}.
\end{aligned} \tag{8.60a}$$

If we let $\theta_{N-1} \in [0, \pi]$, then $q_N \in [-q, q]$, while the component q_{N-1} will take values in $[-q, q]$ when θ_{N-2} is also allowed to range over $[0, \pi]$—and similarly for θ_{N-3}, etc., up to θ_2. Last, θ_1 must range in $[0, 2\pi)$ if q_1 is to take positive as well as negative values. Hence, the angle ranges in (8.60a) are appropriately described by

$$\theta_1 \in [0, 2\pi), \qquad \theta_k \in [0, \pi], \qquad k = 2, 3, \ldots, N-1, q \in [0, \infty). \tag{8.60b}$$

For *any* N-dimensional vector $\mathbf{q}$ of components $\{q_1, q_2, \ldots, q_N\}$ we can find values of q and θ_k, $k = 1, 2, \ldots, N-1$, to parametrize its components. To find θ_k we construct

$$r_k \coloneqq (q_1^2 + q_2^2 + \cdots + q_k^2)^{1/2} = q \sin \theta_{N-1} \cdots \sin \theta_k = r_{k+1} \sin \theta_k, \tag{8.61a}$$

$$q_{k+1} = r_{k+1} \cos \theta_k, \tag{8.61b}$$

thus finding θ_k as $\arctan(r_k/q_{k+1})$ for $k = 1, 2, \ldots, N-1$, $r_1 = q_1$, and

$r_N = q$. Equations (8.60) thus serve to *define* spherical coordinates for N-space. We can find the *volume element* $d^N\mathbf{q}$ from Eqs. (8.61), since for fixed k they tell us that the two-dimensional vector $\{r_k, q_{k+1}\}$ is represented in polar coordinates as having radius r_{k+1} and angle θ_k as in (6.14b). Thus

$$dr_k\, dq_{k+1} = r_{k+1}\, dr_{k+1}\, d\theta_k, \qquad k = 1, 2, \ldots, N-1. \tag{8.62a}$$

Hence, recursively,

$$\begin{aligned} d^N\mathbf{q} &= dq_N\, dq_{N-1} \cdots dq_3\, dq_2\, dq_1 \\ &= dq_N \cdots dq_3 r_2\, dr_2\, d\theta_1 \\ &= dq_N \cdots dq_4 r_2 r_3\, dr_3\, d\theta_2\, d\theta_1 = \cdots \\ &= r_2 r_3 \cdots r_N\, dr_N\, d\theta_{N-1} \cdots d\theta_2\, d\theta_1 \\ &= q^{N-1}\, dq \sin^{N-2}\theta_{N-1}\, d\theta_{N-1} \cdots \sin^{N-k-1}\theta_{N-k}\, d\theta_{N-k} \cdots d\theta_1. \end{aligned} \tag{8.62b}$$

This allows us to calculate the $(N-1)$-dimensional surface of the sphere S_{N-1} in N dimensions as

$$\begin{aligned} |S_{N-1}| &= \int_0^\pi \sin^{N-2}\theta_{N-1}\, d\theta_{N-1} \cdots \int_0^\pi \sin\theta_2\, d\theta_2 \int_0^{2\pi} d\theta_1 \\ &= \{\pi^{1/2}\Gamma((N-1)/2)/\Gamma(N/2)\}|S_{N-2}|, \end{aligned} \tag{8.63a}$$

where we have used the Wallis integral for $\sin^m\theta$. Since $|S_1| = 2\pi$,

$$|S_{N-1}| = 2\pi^{N/2}/\Gamma(N/2). \tag{8.63b}$$

We verify that $|S_2| = 4\pi$ is the 2-surface of the usual sphere in three dimensions.

8.4.2. Reduction of the Fourier to the Hankel Transform

We can now tackle the problem of finding the N-dimensional Fourier transform of a function $f(q)$ of the radial variable q. Choosing the $\theta_{N-1} = 0$ axis along the direction of $\mathbf{p}$ so that $\mathbf{p}\cdot\mathbf{q} = pq\cos\theta_{N-1}$, we must perform

$$\begin{aligned} \tilde{f}(p) &= (2\pi)^{-N/2} \int_{\mathscr{R}^N} d^N\mathbf{q} f(q) \exp(-ipq\cos\theta_{N-1}) \\ &= (2\pi)^{-N/2}|S_{N-2}| \int_0^\infty q^{N-1}\, dq f(q) \int_0^\pi \sin^{N-2}\theta_{N-1}\, d\theta_{N-1} \\ &\quad \times \exp(-ipq\cos\theta_{N-1}). \end{aligned} \tag{8.64}$$

The integrations over the angles $\theta_{N-2}, \ldots, \theta_1$ have yielded $|S_{N-2}|$ as given by (8.63), and we are left with a single integral over θ_{N-1} of the type

$$\int_0^\pi \sin^{2\mu}\theta\, d\theta \exp(\pm iz\cos\theta) = \pi^{1/2}\Gamma(\mu + 1/2)(z/2)^{-\mu}J_\mu(z). \tag{8.65}$$

The Bessel function (Appendix B) thus enters into the picture. Substituting (8.65) into (8.64) and canceling the Γ-functions, we find

$$\tilde{f}(p) = p^{-N/2+1} \int_0^\infty q^{N/2}\, dq f(q) J_{N/2-1}(pq) =: (\mathbb{H}^B_{N/2-1}\mathbf{f})(p), \quad (8.66a)$$

which is defined as the *Hankel–Bochner* transform of order $N/2 - 1$ of $f(q)$. The inverse transform follows with only a change of sign in the $\exp(-i\mathbf{p}\cdot\mathbf{q})$ factor, rendered innocuous by the double sign in (8.65), so that

$$f(q) = q^{-N/2+1} \int_0^\infty p^{N/2}\, dp \tilde{f}(p) J_{N/2-1}(pq) =: (\mathbb{H}^{B^{-1}}_{N/2-1}\tilde{\mathbf{f}})(q). \quad (8.66b)$$

Notice that the transform kernels of $\mathbb{H}_\mu{}^B$ and $\mathbb{H}_\mu^{B^{-1}}$ are the same, and hence $\mathbb{H}_\mu^{B^2} = \mathbb{1}$. [Compare with the property of the Fourier transform, where $\mathbb{F}^2 = \mathbb{I}_0$; see Eq. (7.25).] This is to be expected, as from the $\mathbb{F}_{(N)}$ point of view we are dealing with rotationally invariant functions. These functions are *even* in each of the Cartesian coordinates, and thus $\mathbb{I}_0$ is equivalent to $\mathbb{1}$ in their subspace.

A Parseval formula holds for the Hankel–Bochner transforms (8.66a)–(8.66b):

$$(\mathbf{f}, \mathbf{g})_N = \int_{\mathscr{R}^N} d^N\mathbf{q} f(q)^* g(q) = |S_{N-1}| \int_0^\infty q^{N-1}\, dq f(q)^* g(q)$$

$$= (\tilde{\mathbf{f}}, \tilde{\mathbf{g}})_N = |S_{N-1}| \int_0^\infty p^{N-1}\, dp \tilde{f}(p)^* \tilde{g}(p). \quad (8.67)$$

Exercise 8.23. Examine the Hankel–Bochner transform (8.66) for $N = 1$ dimension. Show that we are dealing with *even* functions and the *cosine* Fourier transform, as $J_{-1/2}(z) = (2/\pi z)^{1/2} \cos z$.

Exercise 8.24. Examine the Hankel–Bochner transform for $N = 3$ dimensions. This has already been used in Section 8.3. In fact, it reduces to the *sine* Fourier transform as $J_{1/2}(z) = (2/\pi z)^{1/2} \sin z$.

Exercise 8.25. Find the Hankel–Bochner transform of degree μ of $f(cr)$ in terms of that of $f(r)$.

8.4.3. Recursion Relations

There is a relation between Hankel–Bochner transforms of orders μ and $\mu + m$, m an integer. This comes from a recursion relation for Bessel

functions, which can be found directly from (8.66a) and (8.65) for $\mu = N/2 - 1$:

$$\begin{aligned}
-\frac{1}{p}\frac{d}{dp}(\mathbb{H}_\mu{}^B\mathbf{f})(p) &= (2\pi)^{-\mu-1}|S_{2\mu}|\int_0^\infty q^{2\mu+1}\,dqf(q) \\
&\quad\times\int_0^\pi \sin^{2\mu}\theta\,d\theta(ip^{-1}q\cos\theta)\exp(-ipq\cos\theta) \\
&= (2\pi)^{-\mu-1}|S_{2\mu}|\int_0^\infty q^{2\mu+1}\,dqf(q)(ip^{-1}q)(2\mu+1)^{-1} \\
&\quad\times\left[\sin^{2\mu+1}\theta\exp(-ipq\cos\theta)|_{\theta=0}^{\pi}\right. \\
&\quad\left.-ipq\int_0^\pi \sin^{2\mu+2}\theta\,d\theta\exp(-ipq\cos\theta)\right] \\
&= (\mathbb{H}_{\mu+1}^B\mathbf{f})(p), \qquad (8.68)
\end{aligned}$$

where we have used integration by parts and the recursion (8.63a). It follows that

$$(-p^{-1}\,d/dp)^m(\mathbb{H}_\mu{}^B\mathbf{f})(p) = (\mathbb{H}_{\mu+m}^B\mathbf{f})(p), \qquad (8.69)$$

which relates the Hankel–Bochner transforms of orders differing by an integer.

8.4.4. Odd- and Even-Dimensional Wave Equations

As the Hankel–Bochner transform of degree $\mu = N/2 - 1$ of a function $f(q)$ is the N-dimensional Fourier transform of the function $f(q)$ of radius q, we can immediately put Eq. (8.69) to work on the problem—stated in Section 8.3—of finding the Green's function for the N-dimensional wave equation. This will show some of the characteristics of the solutions for general N. From (8.51) with $\Gamma = 0$ and $\tilde{G}^w(\mathbf{p}, t) = c\sin cpt/p$, we have

$$\begin{aligned}
G_N{}^w(\mathbf{q}, t) &= [\mathbb{F}_{(N)}\tilde{\mathbf{G}}^w(\cdot, t)](\mathbf{q}) = [\mathbb{H}_{N/2-1}^B\tilde{\mathbf{G}}^w(\cdot, t)](q) \\
&= (-q^{-1}\,\partial/\partial q)^m[\mathbb{H}_{(N-2m)/2-1}^B\tilde{\mathbf{G}}^w(\cdot, t)](q) \\
&= (-q^{-1}\,\partial/\partial q)^m G_{N-2m}^w(q, t) = [-2\,\partial/\partial(q^2)]^m G_{N-2m}^w(q, t). \qquad (8.70)
\end{aligned}$$

In (8.55) and (8.56) we have calculated $G_3{}^w(\mathbf{q}, t)$, and so we have the expressions for odd dimension $2n + 3$. Keeping only the retarded solution, we have

$$\begin{aligned}
G_{2n+3}^w(q, t) &= (-q^{-1}\,\partial/\partial q)^n G_3{}^w(q, t) \\
&= c(\pi/2)^{1/2}(-q^{-1}\,\partial/\partial q)^n[q^{-1}\delta(q - ct)], \qquad (8.71a) \\
\dot{G}_{2n+3}^w(q, t) &= -c^2(\pi/2)^{1/2}(-q^{-1}\,\partial/\partial q)^n[q^{-1}\delta'(q - ct)], \qquad (8.71b)
\end{aligned}$$

which represents an expanding singularity shell. It exhibits (a) causality,

(b) reciprocity, (c) a leading modulation factor q^{-n}, and (d) no backwave or wake.

Exercise 8.26. Verify that (8.71) correctly relates the results for one- and three-dimensional spaces. See again Exercise 8.16.

To find the wave equation Green's function in an even number of dimensions we can produce a two-dimensional world out of a three-dimensional one by assuming that all relevant objects are cylinders along the q_3-axis, that is, the initial conditions are independent of q_3. In doing this, the integral over q_3 in the convolution (8.57) can be performed on the Green's function alone, i.e.,

$$H_2{}^w(\mathbf{q}\{q_1, q_2\}, t) \coloneqq \int_{-\infty}^{\infty} dq_3 G_3{}^w(\mathbf{q}\{q_1, q_2, q_3\}, t). \tag{8.72a}$$

We can perform this in Cartesian coordinates for the retarded part of (8.55):

$$\begin{aligned} &H_2{}^w(\mathbf{q}\{q_1, q_2\}, t) \\ &\quad = c(\pi/2)^{1/2} \int_{-\infty}^{\infty} dq_3 (q_1{}^2 + q_2{}^2 + q_3{}^2)^{-1/2} \delta\big((q_1{}^2 + q_2{}^2 + q_3{}^2)^{1/2} - ct\big) \\ &\quad = c(\pi/2)^{1/2} \int_{-\infty}^{\infty} dq_3 (q_1{}^2 + q_2{}^2 + q_3{}^2)^{-1/2} ct (c^2t^2 - q_1{}^2 - q_2{}^2)^{-1/2} \\ &\qquad \times \{\delta\big(q_3 - (c^2t^2 - q_1{}^2 - q_2{}^2)^{1/2}\big) + \delta\big(q_3 + (c^2t^2 - q_1{}^2 - q_2{}^2)^{1/2}\big)\}, \end{aligned} \tag{8.72b}$$

where in the last equality we have used the expression (7.96) for a $\delta[F(q)]$ in terms of $\delta(q - a_i)$, a_i being the roots of $F(q)$; namely,

$$a_{1,2} = \pm(c^2t^2 - q_1{}^2 - q_2{}^2)^{1/2}$$

when $q_1{}^2 + q_2{}^2 < c^2t^2$. No roots exist for $q_1{}^2 + q_2{}^2 > c^2t^2$. Thus in a two-dimensional space,

$$G_2{}^w(\mathbf{q}, t) = c(c^2t^2 - q^2)^{-1/2}\Theta(ct - q) = G_2{}^w(q, t), \tag{8.73}$$

where we have introduced the Heaviside step function Θ, Eq. (7.89), and divided by $(2\pi)^{1/2}$, since the two-dimensional Green's function will be present in convolutions (8.52) with factors $(2\pi)^{-1}$ instead of $(2\pi)^{-3/2}$ as for three dimensions. As $\Theta'(q) = \delta(q)$ and $\Theta(0) \coloneqq 1/2$, from (8.73) we find

$$\begin{aligned} \dot{G}_2{}^w(q, t) &= -c^3t(c^2t^2 - q^2)^{-3/2}\Theta(ct - q) + c^2(c^2t^2 - q^2)^{-1}\delta(q - ct) \\ &= [2c\delta(q - ct) - c^2t(c^2t^2 - q^2)^{-1}]G_2{}^w(q, t). \end{aligned} \tag{8.74}$$

Equations (8.73) and (8.74), as well as the Green's functions for a higher, even number of dimensions obtained by (8.71), fulfill the properties (a), (b),

and (c), as do the solutions of the wave equation in other dimensions. As to property (d), the behavior is different. The disturbance, if originally localized, will develop a trailing wake, because of the non-δ form of $G_2^w(q, t)$, which *smears* any initial condition out of its original sharpness. This trailing wake, backwave or reverberation is a characteristic of all even-dimensional spaces. A stone thrown in a pond does not quite reproduce, thus, the behavior of waves in three-dimensional space.

8.4.5. General Solution of the Diffusive–Elastic Equation

For the Green's function of the N-dimensional general elastic–diffusive medium, we have to calculate, as in (8.70), the inverse Hankel transform of (8.49), namely,

$$\begin{aligned} G_N(\mathbf{q}, t) &= \big(\mathbb{F}_{(N)}\tilde{G}(\cdot, t)\big)(\mathbf{q}) = \big(\mathbb{H}^B_{N/2-1}\tilde{G}(\cdot, t)\big)(q) \\ &= c^2 q^{-N/2+1} \exp(-\Gamma t) \int_0^\infty dp p^{N/2}(c^2p^2 - \Gamma^2)^{1/2} \\ &\quad \times \sin[t(c^2p^2 - \Gamma^2)^{1/2}] J_{N/2-1}(pq). \end{aligned} \tag{8.75}$$

This is a rather difficult integral to do "by hand." It appears in the literature, however, as a particular case of the discontinuous Sonine integrals. [See Watson (1922, Section 13.47). In the tables of Hankel transforms by Oberhettinger (1973), it can be found by Eq. 6.43-II.] The result is

$$\begin{aligned} G_N(q, t) &= c(\pi/2)^{1/2}[\Gamma c^{-1}(c^2t^2 - q^2)^{-1/2}]^{(N-1)/2} \\ &\quad \times \exp(-\Gamma t) I_{-(N-1)/2}\big(\Gamma c^{-1}(c^2t^2 - q^2)^{1/2}\big)\Theta(ct - q), \\ &\qquad\qquad q \neq ct, \end{aligned} \tag{8.76}$$

where $I_\nu(z)$ is the *modified Bessel function* (see Appendix B) and Θ the usual Heaviside step. This function has been plotted for various values of parameters and variables in Fig. 8.10. The Green's function (8.76) includes δ terms at $q = ct$ for $N > 2$. These can be obtained for odd N using (8.68) and the fact that $G_1(q, t)$ is simply discontinuous at the advancing edge of the wave. For N even, one starts from $G_2(q, t)$.

Exercise 8.27. Consider the diffusion equation limit $c \to \infty$ of the Green's function (8.76), recalling that $I_\nu(z) \sim (2\pi z)^{-1/2} \exp(z)$ as $z \to \infty$. Verify that Eq. (8.58) is correctly reproduced.

Exercise 8.28. Consider the wave equation limit $a \to \infty$ of (8.76) using $I_\nu(z) \sim (z/2)^\nu/\Gamma(\nu + 1)$ for $\nu \neq -1, -2, \ldots$ as $z \to 0$. This verifies only the even-dimensional cases. Show that for $N = 2$, (8.73) is correctly given. For N odd and larger than 1, the result is zero since (8.76) holds for $q \neq ct$.

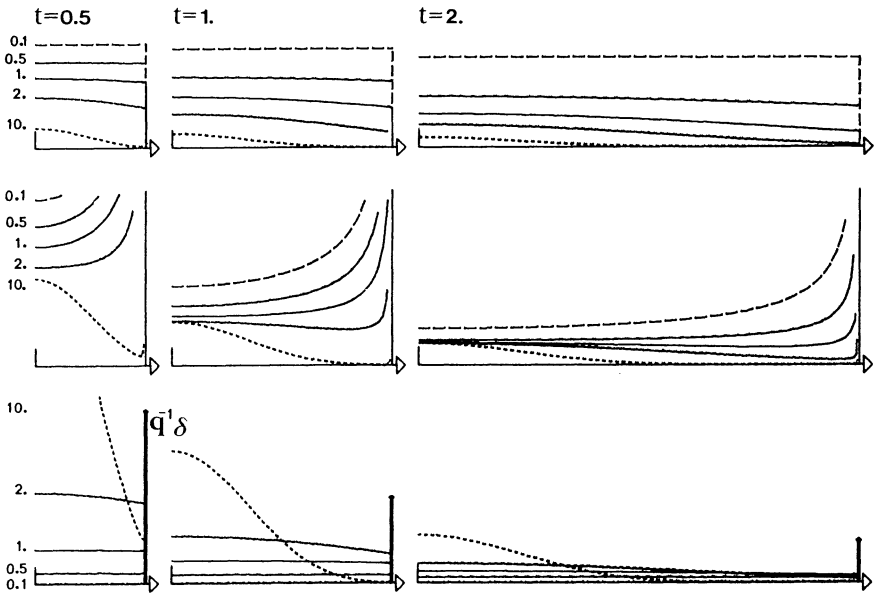


Fig. 8.10. Green's functions for elastic–diffusive media in one, two, and three dimensions (top, middle, and bottom rows). With advancing time ($t = 0.5$, 1, and 2 in the first, second, and third columns), the disturbance spreads up to $q = ct$ and is zero from there on. In each graph we have plotted the function for values of $\Gamma = 0.1$, 0.5, 1, 2, and 10 with different dottings. The first value corresponds nearly to the "wave" limit and the last value to the "diffusive" one. [Note that a change of scale is still needed: Eqs. (8.52).] The two- and three-dimensional cases have a singular edge: a $(c^2t^2 - q^2)^{-1/2}$ factor for two dimensions and a $q^{-1}\delta(q - ct)$ summand for three.

Exercise 8.29. Show that the Laplacian operator in N dimensions, Eq. (6.2), can be written in spherical coordinates (8.60) as

$$\nabla^2_{(N)} = r_N^{-N+1} \frac{\partial}{\partial r_N} r_N^{N-1} \frac{\partial}{\partial r_N} + r_N^{-2} \Lambda^2_{(N-1)}, \tag{8.77a}$$

where $r_N := q$, the radial coordinate in N-space, and $\Lambda^2_{(N-1)}$ is the *Laplacian on* S_{N-1},

$$\Lambda^2_{(k)} = \sin^{-k+2}\theta_{k-1} \frac{\partial}{\partial \theta_{k-1}} \sin^{k-2}\theta_{k-1} \frac{\partial}{\partial \theta_{k-1}} + \sin^{-2}\theta_{k-1} \Lambda^2_{(k-1)}, \tag{8.77b}$$

$$\Lambda^2_{(2)} = \partial^2/\partial\theta_1^2. \tag{8.77c}$$

This can be done recursively. For $N = 2$, Eqs. (8.77) match Eq. (6.16). If (8.77a)–(8.77b) are valid for $N = k$, $\nabla^2_{(k)}$ involving second derivatives with respect to $q_1, q_2, \ldots, q_k$, then they also hold for $\nabla^2_{(k+1)} = \partial^2/\partial q_{k+1}^2 + \nabla^2_{(k)}$. Use the recursiveness provided by Eqs. (8.61), the two dimensional case for the (r_k, q_{k+1})-plane, and $r_k^{-1}\,\partial/\partial r_k = r_{k+1}^{-1}\,\partial/\partial r_{k+1} + r_{k+1}^{-2} \cot\theta_k\,\partial/\partial\theta_k$.

8.4.6. Hankel Transforms and Definite Symmetry under Rotations

Another context in which Hankel transforms arise is in finding the Fourier transforms of functions with *definite transformation properties* under rotations. This term merits some explanation. (In Section 4.3 we used the synonymous characterization of *definite symmetry* under translations on a circle.) We examine functions, or *sets* of functions, which transform among themselves under rotations. Their characterization is aided if we ask them to be eigenfunctions of a rotationally invariant self-adjoint operator, as then they will constitute complete and orthogonal sets of functions on the angle variables. In two dimensions the procedure can be implemented in terms of Fourier techniques. If we choose functions $f_m(\mathbf{q}) \coloneqq f(q)\exp(im\theta_q)$, where q and θ_q are the radial and angular parameters of $\mathbf{q}$, then a rotation by α will transform $f_m(\mathbf{q})$ into a multiple of itself: $\mathbb{T}_\alpha f_m(\mathbf{q}) = \exp(im\alpha)f_m(\mathbf{q})$. As $\mathbb{T}_{2\pi} = \mathbb{1}$, m can only be an integer. The rotation-invariant self-adjoint operator $-i\,\partial/\partial\theta_q$ can be used to label $f_m(\mathbf{q})$, and these, we know from the theory of Fourier series, are orthogonal and complete in their inner product on $\theta_q \in (-\pi, \pi]$. Every function $f_m(\mathbf{q})$ (fixed m) will thus have the same, definite, rotation property *and so will its Fourier transform*. Consider now the two-dimensional Fourier transform of the set $\{f_m(\mathbf{q})\}$, $\{\tilde{f}_m(\mathbf{p})\}$ for fixed m and $\mathbf{f} \in \mathscr{L}^2(\mathscr{R}^2)$. Using the Bessel generating function (B.4) for $t = i\exp(i\theta)$, we can write the $\mathbb{F}_{(2)}$ kernel function as

$$\exp(\pm i\mathbf{p}\cdot\mathbf{q}) = \exp(\pm ipq\cos\theta) = \sum_{n=-\infty}^{\infty} (\pm i)^n J_n(pq)\exp(in\theta). \quad (8.78)$$

If $\mathbf{q}$ and $\mathbf{p}$ have polar coordinates q, θ_q and p, θ_p, $\mathbf{p}\cdot\mathbf{q} = pq\cos(\theta_p - \theta_q)$, and thus, for $\theta \coloneqq \theta_p - \theta_q$, we can use the expansion (8.78) in finding

$$\begin{aligned}
\tilde{f}_m(\mathbf{p}) &= \tilde{f}(p)\exp(im\theta_p) \\
&= (2\pi)^{-1}\int_0^\infty q\,dq\int_0^{2\pi} d\theta_q f(q)\exp(im\theta_q) \\
&\quad \times \sum_{n\in\mathscr{Z}} (-i)^n J_n(pq)\exp[in(\theta_p - \theta_q)] \\
&= \int_0^\infty q\,dq f(q)\sum_{n\in\mathscr{Z}} (-i)^n J_n(pq)\exp(in\theta_p) \\
&\quad \times (2\pi)^{-1}\int_0^{2\pi} d\theta_q \exp[i(m-n)\theta_q] \\
&= \int_0^\infty q\,dq f(q)(-i)^m J_m(pq)\exp(im\theta_p). \qquad (8.79)
\end{aligned}$$

That is,

$$\tilde{f}(p) = (-i)^m \int_0^\infty q\, dq f(q) J_m(pq), \tag{8.80a}$$

$$f(q) = i^m \int_0^\infty p\, dp \tilde{f}(p) J_m(pq) \tag{8.80b}$$

relate the "radial parts" of $f_m(\mathbf{q})$ and its $\mathbb{F}_{(2)}$ transform $\tilde{f}_m(\mathbf{p})$. For $m = 0$ (*invariance* under rotations) we recover the Hankel–Bochner transform (8.66) (of degree zero) for $N = 2$. For $m \neq 0$ (8.80) yields one transform for every m which differs from (8.66) for $m = N/2 - 1$ only in the powers of p and q in the integrand.

In N-dimensional space, the same kind of conclusion follows, except that the analogue of (8.78) is

$$\exp(\pm i\mathbf{p}\cdot\mathbf{q}) = (2\pi)^{N/2}(pq)^{1-N/2} \sum_{k=0}^{\infty} \exp(\pm i\pi k/2) \times J_{N/2+k-1}(pq) \sum_M Y_k^M(\Omega_q)^* Y_k^M(\Omega_p), \tag{8.81}$$

where Ω_q and Ω_p are the collective labels for the angular variables of $\mathbf{q}$ and $\mathbf{p}$ in Eqs. (8.60) and $Y_k^M(\Omega)$ are the *spherical harmonics* of rank k in N-space, M being a collective label for $N > 3$. [See, for instance, the book by Vilenkin (1968, Chapters IV and IX).] In N-space, definite transformation properties mean that we are dealing with functions of the kind $f_k^M(\mathbf{q}) = f(q) Y_k^M(\Omega_q)$. The spherical harmonics are orthogonal and complete on the space $\mathcal{L}^2(S_{N-1})$, so an analogue of the reduction (8.79) leads to

$$\tilde{f}(p) = p^{1-N/2} \exp(-i\pi k/2) \int_0^\infty q^{N/2}\, dq f(q) J_{N/2+k-1}(pq), \tag{8.82a}$$

$$f(q) = q^{1-N/2} \exp(i\pi k/2) \int_0^\infty p^{N/2}\, dp \tilde{f}(p) J_{N/2+k-1}(pq) \tag{8.82b}$$

for the radial parts of $f_k^M(\mathbf{q})$ and its $\mathbb{F}_{(N)}$ transform. Again, for $k = 0$ (*invariance*), we recover the Hankel–Bochner transform (8.66).

For the same value of the Bessel function index, (8.80), (8.82), and (8.66) differ only by powers of q and p. These can be easily absorbed into the definition of the function to be transformed. It has thus been found convenient to abstract the transform of the radial part from the number of dimensions of the original space and define *the Hankel* transform pair of order μ as

$$(\mathbb{H}_\mu \mathbf{f})(p) \coloneqq f^{H\mu}(p) = \int_0^\infty dq f(q)(pq)^{1/2} J_\mu(pq), \tag{8.83a}$$

$$(\mathbb{H}_\mu^{-1} \mathbf{f}^{H\mu})(q) \coloneqq f(q) = \int_0^\infty dp f^{H\mu}(p)(pq)^{1/2} J_\mu(pq). \tag{8.83b}$$

This is the form appearing in the Oberhettinger tables (1973) and has the advantage of symmetry in having the kernel a function of pq only.

Most authors call (8.83) *the* Hankel transform, while our original pair (8.66) is referred to as the Bochner transform. The Hankel transform occupies a part of the books by Sneddon (1951, Chapter 2; 1972, Chapter 5). For further material on this and related transforms, the reader is referred to the specialized literature. On convolution there are articles by Griffith (1957, 1958) and Haimo (1965); the latter deals in detail with applications. Extensive tables of Hankel transforms can be found in the Bateman manuscript project (Erdelyi *et al.*, 1954, Chapter VIII) and the tables by Oberhettinger (1973).

8.4.7. Other Integral Transforms with Cylindrical Function Kernels

Neumann transforms of order μ replace the Bessel function kernel in the Hankel transform by a Neumann function $(pq)^{1/2}N_\nu(pq)$. [See Griffith (1958) and the Bateman manuscript project (Erdelyi *et al.*, 1954, Chapters IX and XI) for Y and $\mathbf{H}$ transforms.] The inverse transform contains a *Struve* function kernel $(pq)^{1/2}\mathbf{H}_\mu(pq)$. A generalization of these involving *Lommel* functions can be found in the Oberhettinger tables (1973, Chapter VI).

Weber transforms of order μ are defined when

$$q[J_\mu(pq)N_\mu(pa) - J_\mu(pa)N_\mu(pq)],$$

the annular membrane determinant function in Eq. (6.37), is used as an integration kernel on (a, ∞). The inverse transform divides the direct kernel by $J_\mu(ap)^2 + N_\mu(ap)^2$ and integrates p on $(0, \infty)$. See the original paper by Titchmarsh (1923) and one by Griffith (1956).

The *Meijer–Bessel* or *Meijer K* transform of order μ makes use of the kernel $(pq)^{1/2}K_\mu(pq)$ containing the *Macdonald* function. The inverse transform integrates with a modified Bessel function $(pq)^{1/2}I_\mu(pq)$ over a Bromwich contour. Several Indian mathematicians have published articles on this subject (Verma, 1959; Saxena, 1959; and Sharma, 1963, 1965). The Bateman manuscript project [Erdelyi *et al.* (1954)] devotes Chapter X to giving a table of these. This is actually a particular case of the *Meijer transform*, introduced by Meijer (1940) as a generalization of the Laplace transform whose transform kernels are $\exp(\mp pq)/2\cdot(pq)^{\mp k-1/2}$ times the *Whittaker* functions $W_{k-1/2,m}(pq)$ for the direct and $M_{k-1/2,m}(pq)$ for the inverse transform. Both k and m are free parameters. Vilenkin (1968, Chapter VIII) gives many group-theoretical and special-function relations for integrals with Whittaker function kernels.

Kontorovich and Lebedev (1938) introduced a particular integral transform for the solution of problems in diffraction. It involves as a transform kernel a Macdonald function of imaginary index $K_{iq}(p)$ over $q \in (0, \infty)$

and for the inverse transform the kernel $2\pi^{-2}\sinh(\pi q)K_{iq}(p)/p$, also over $p \in (0, \infty)$. Its relation with some of the Neumann series (Section 6.4) is akin to the relation of the Mellin transform with the Taylor series in Fig. 8.6. The conditions for validity of the transform pair were further explored by Lebedev (1947), and the transform was generalized (Lebedev, 1949a, 1949b). A transform table appears in the Bateman manuscript project (Erdelyi *et al.*, 1954, Chapter XII) and in Oberhettinger (1973, Chapter VI). Sneddon (1972, Chapter 6) treats this transform in some detail and applies it to the study of harmonic functions in cylindrical coordinates.

8.5. Other Integral Transforms

For the most part, integral transforms can be seen as the continuous analogue of series expansions. The underlying unity is that the expanding functions in the series and the integral kernel in transforms are usually eigenfunctions of a given operator, self-adjoint in some domain. In this section, after some rather soft-focus remarks on the Sturm–Liouville point of view, we shall examine a few examples as well as other transforms which, unnamed, have appeared before or which are common in the current literature.

8.5.1. The Sturm–Liouville Problem and Integral Transforms

Assume $\mathbb{H}$ is an operator which is self-adjoint in the (Hilbert) space of functions $\mathscr{L}^2(\mathscr{Q})$, where $\mathscr{Q} \subseteq \mathscr{R}$ with some properly chosen boundary conditions. Assume, further, that we know its eigenfunctions, labeled uniquely by a (possibly collective) index $p \in \mathscr{P} \subseteq (\mathscr{R}, \mathscr{Z})$,

$$\mathbb{H}\Psi_p(q) = \lambda(p)\Psi_p(q), \qquad q \in \mathscr{Q}, \tag{8.84}$$

and its spectrum $\mathscr{L} = \lambda(\mathscr{P}) \subseteq \mathscr{R}$. The set of functions $\{\Psi_p(q)\}_{p\in\mathscr{P}}$ can be shown under certain restrictions to constitute a generalized (Dirac) basis, orthogonal and complete for $\mathscr{L}^2(\mathscr{Q})$. This is the generalized Sturm–Liouville problem, similar to the one sketched in Section 6.4. The spectrum, being a continuous set, however, is indicative of a considerably more delicate mathematical theory. The overall (simplified) features are not too difficult to state roughly: the orthogonal basis functions can be normalized so that Dirac orthonormality holds,

$$(\Psi_p, \Psi_{p'}) = \int_{\mathscr{Q}} dq\Psi_p(q)^*\Psi_{p'}(q) = \delta(p - p'), \tag{8.85a}$$

and completeness holds,

$$\int_{\mathscr{P}} dp\Psi_p(q)^*\Psi_p(q') = \delta(q - q'). \tag{8.85b}$$

Although (8.85a) tells us that the $\Psi_p(q)$ do *not* belong to $\mathscr{L}^2(\mathscr{Q})$, they do nevertheless form a generalized *basis* for that space so that for any $f(q) \in \mathscr{L}^2(\mathscr{Q})$ we can define its *transform* function,

$$f^T(p) := \int_{\mathscr{Q}} dq \Psi_p(q)^* f(q), \tag{8.86a}$$

and be assured that the inverse transform or synthesis reproduces (generally *in the norm*) the original function as

$$f(q) = \int_{\mathscr{P}} dp \Psi_p(q) f^T(p). \tag{8.86b}$$

This suggests seeing the integral transform—*passive* point of view; recall Section 1.3—as a change of basis, where $f(q)$ and $f^T(p)$ are the coordinates of the same vector $\mathbf{f} \in \mathscr{L}^2(\mathscr{Q})$ in two bases, the latter in the $\{\mathbf{\Psi}_p\}_{p\in\mathscr{P}}$-basis as $(\mathbf{\Psi}_p, \mathbf{f}) = f^T(p)$ and the former in the basis of Dirac δ's, $\{\boldsymbol{\delta}_q\}_{q\in\mathscr{Q}}$, where $(\boldsymbol{\delta}_q, \mathbf{f}) = f(q)$. Equation (8.86b) can be formally "proven" by multiplying (8.86a) by $\Psi_p(q')$, integrating over $p \in \mathscr{P}$, exchanging integrals, and using (8.85b). Equivalently, multiplication of (8.86b) by $\Psi_{p'}(q)$, integration over $q \in \mathscr{Q}$, and use of (8.85a) yield (8.86a). As a consequence of (8.84)–(8.86), the generalized Parseval relation,

$$(\mathbf{f}, \mathbf{g})_{\mathscr{Q}} = \int_{\mathscr{Q}} dq f(q)^* g(q) = \int_{\mathscr{P}} dp f^T(p)^* g^T(p), \tag{8.86c}$$

will also hold.

8.5.2. Fourier, Mellin, and Repulsive Oscillator Transforms

The Fourier transform (7.1) can be seen as stemming from the eigenbasis expansion of a defining operator $\mathbb{P} := -id/dq$, self-adjoint on $\mathscr{Q} = \mathscr{R}$ [see Eqs. (7.55) and (7.56)]. Its eigenfunctions are $(2\pi)^{-1/2} \exp(ipq)$, $p \in \mathscr{P} = \mathscr{R}$, and the spectrum is $\mathscr{L} = \mathscr{R}$. The set is an orthogonal and complete basis for $\mathscr{L}^2(\mathscr{R})$. The defining operator can also be taken to be $\mathbb{P}^2/2$, whose eigenfunctions are the same as above but whose spectrum is $\mathscr{L} = \mathscr{R}^+$ *twice* [as $\mathscr{P} = (\mathscr{R}^+, \pm)$]. The latter has the advantage of defining, equivalently, the sine and cosine Fourier transforms: These are eigenfunctions of $\mathbb{P}^2/2$ but not of $\mathbb{P}$.

The Mellin bilateral transform (8.26) can be built by looking for the eigenfunctions of the operator $\frac{1}{2}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q})$, namely, $(2\pi)^{-1/2} q_{\pm}^{ip-1/2}$. Here $\mathscr{L} = \mathscr{R}$, but $\mathscr{P} = (\mathscr{R}, \pm)$, i.e., the spectrum covers $\mathscr{R}$ *twice*. Orthogonality and completeness (8.86) are given the forms (8.27) and (8.28).

We also have the transform defined by the repulsive oscillator Schrödinger Hamiltonian $\frac{1}{2}(\mathbb{P}^2 - \mathbb{Q}^2)$, which is closely related to the Mellin transform. The eigenfunctions of this operator are the $\chi_p{}^{\pm}(q)$ found in (7.203).

They can serve to define a *repulsive* oscillator transform with the characteristics (8.84)–(8.86).

Exercise 8.30. Show that if the defining operator is $\mathbb{P}^2 - (\mu^2 - \frac{1}{4})\mathbb{Q}^{-2}$, self-adjoint on $\mathscr{L}^2(\mathscr{R}^+)$, the resulting transform is the Hankel transform of order μ given by (8.83).

8.5.3. Airy Transforms

Usually, a solid link with the Fourier transform—for which the eigenbasis properties are well established—will prove the orthogonality and completeness for a given transform basis function set. This was the path we followed for Mellin, repulsive oscillator, and Hankel transforms.

One more transform can easily be presented by this method. Consider the operator and corresponding eigenvalue equation

$$\mathbb{H}^l\Psi_\lambda^l(q) := (\tfrac{1}{2}\mathbb{P}^2 + \mathbb{Q})\Psi_\lambda^l(q) = \lambda\Psi_\lambda^l(q). \tag{8.87}$$

This equation happens to be the (time-independent) Schrödinger equation for the free-fall or linear potential. It was solved for $\lambda = 0$, in (7.61)–(7.64), in terms of the Airy function. Actually that is almost all we need since $\Psi_\lambda^l(q) = \Psi_0^l(q - \lambda)$ is the solution of (8.87) in terms of the $\lambda = 0$ solution, as can be ascertained by collecting all terms on the left-hand side and changing variables. We can thus write the solution to (8.87) in terms of (7.64) with a translated argument, viz.,

$$\Psi_\lambda^l(q) = 2^{1/3}\,\mathrm{Ai}[2^{1/3}(q - \lambda)] \tag{8.88}$$

[having chosen $c = (2\pi)^{-1/2}$]. Moreover, we can easily show that the set (8.88), for $\lambda \in \mathscr{R}$, is orthogonal and complete. Indeed, the Fourier transform of (8.88) is given by (7.63), multiplied by an exponential factor due to translation [Eq. (7.28)]:

$$\tilde{\Psi}_\lambda^l(p) = (2\pi)^{-1/2}\exp(-i\lambda p)\exp(ip^3/6). \tag{8.89}$$

Now, *this* set of functions *is* orthogonal and complete for $p \in \mathscr{R}$ and $\lambda \in \mathscr{R}$. The last λ-independent exponential factor does not alter this property, as can be shown by an argument parallel to that leading from the completeness of the bilateral Mellin basis to the completeness of the repulsive oscillator wave functions in Section 8.2. The inverse Fourier transform of (8.89), namely (8.88), will thus have the claimed property. Equation (8.88) defines the integral kernel of a transform which we can call *Airy's* transform.

An integral transform (8.84)–(8.86), in the *active* point of view (recall Section 1.3), is quite obviously associated with a *linear operator*—that is, if $f^T(p)$ and $g^T(p)$ are the transforms of $f(q)$ and $g(q)$, then $af^T(p) + bg^T(p)$ will be the transform of $af(q) + bg(q)$ for $a, b \in \mathscr{C}$—and thus we can define a linear operator $(\mathbb{T}\mathbf{f})(p) := f^T(p)$.

Most of the transforms we have examined thus far are *unitary* (those of Fourier, bilateral Mellin, Hankel, repulsive oscillator, and Airy but *not* those of Laplace or ordinary Mellin). As the corresponding Parseval identities suggest, the mapping afforded by $\mathbb{T}$ is *isometric*. The fact that $\mathscr{L}^2(\mathscr{R})$ can be shown to be mapped onto itself under Fourier and Airy transforms makes the transform operators *unitary* [since $\mathscr{L}^2(\mathscr{R})$ is a *Hilbert* space]. The Hankel transforms achieve the same for the (Hilbert) space $\mathscr{L}^2(\mathscr{R}^+)$. The bilateral Mellin and repulsive oscillator transforms are also unitary, although they map $\mathscr{L}^2(\mathscr{R})$ onto $\mathscr{L}_+{}^2(\mathscr{R}) \oplus \mathscr{L}_-{}^2(\mathscr{R})$ for the two values of the dichotomic index. Finally, the harmonic oscillator functions also provide a unitary mapping (7.180) of $\mathscr{L}^2(\mathscr{R})$ onto l^2, the (Hilbert) space of square-summable sequences.

8.5.4. Gauss–Weierstrass Transforms

Not all integral transforms are unitary though. When we look at the time evolution of systems governed by linear differential equations, linear mappings of functions through integral kernels become abundant. Consider the simple heat diffusion in one dimension described by the Green's function in (8.58) with initial conditions $f(q)$ at time $t = 0$ and $a^2 = 1/2$. Its time evolution is given by

$$(\mathbb{G}_t{}^h\mathbf{f})(q) := f^{G(t)}(q) = (2\pi t)^{-1/2} \int_{-\infty}^{\infty} dq' f(q') \exp[-(q - q')^2/2t]. \quad (8.90)$$

This is a linear mapping of a large function space [containing $\mathscr{L}^2(\mathscr{R})$] *into* $\mathscr{C}_\downarrow{}^\infty$, which has been called the *Gauss* or *Weierstrass* transform at time t. Although the "total heat" $\int dq f^{G(t)}(q)$ is constant, the usual inner product $(\mathbf{f}, \mathbf{f})$ is *not*. Hence $\mathbb{G}_t{}^h$ is not a unitary transform in the usual sense. Nevertheless, in Part IV we shall see that if an appropriate inner product is given, (8.90) *can* be turned into a unitary transform. The transform (8.90) and its *inversion* have an important bearing on the theory of heat diffusion. This was initially studied by Doetsch (1936) and Tricomi (1936, 1938). Since then, it has been the subject of several articles by Hartmann and Wintner (1950), Blackman (1952), Widder (1956, 1964), Rooney (1957, 1958, 1963), Bilodeau (1961), and Nessel (1965). There is one recent book on the heat equation by Widder (1975).

8.5.5. Complex Extensions and Analytic Continuations

A subject which will be more extensively developed in Part IV is the set of integral transforms obtained from the time evolution of *four* types of Schrödinger equations: (a) the harmonic oscillator, (b) the free particle, (c) the repulsive oscillator, and (d) the linear potential. The Green's functions

for these cases all have the general form $\exp[i(Aq^2 + Bqp + Cp^2)]$ for A, B, and C complex. This will define (the semigroup of) *complex canonical transforms*. They are all unitary in the appropriate Hilbert spaces.

Wave equations describing diffusive–elastic systems also provide integral transforms on *pairs* of functions representing elongation and velocity. They can be made unitary (thus far) only in the case when no diffusion is present. The inner product to appear in the Parseval identity is the sesquilinear form associated with the total energy of the system.

Integral transforms between pairs of functions can arise also as *analytic continuations* of series. This rather cryptic remark applies to the case of the *Mehler–Fok* transform, which can be seen as a Sturm–Liouville problem or as an analytically continued version of the Legendre transform mentioned in Section 6.4. The latter expands functions as series of Legendre polynomials $P_n(x)$. By complex contour integration techniques (usually referred to as the *Sommerfeld–Watson transform*), the series sum is replaced by an *integral* with a kernel $(2\nu + 1)P_\nu(x)/\sin \pi\nu$ over ν along a vertical path in the complex ν-plane at $\rho + i\sigma$ for fixed $\rho > -\frac{1}{2}$ and over $\sigma \in \mathscr{R}$ as shown in Fig. 8.6. This transform is used in high-energy elementary particle physics for relativistic scattering amplitude expansions in the direct and crossed channel [see the review article by Kalnins *et al.* (1975, Section III-B and the references within)]. Application of this transform to the diffraction and reflection by a wedge has been made by Oberhettinger (1954, 1958). This transform has a family of group-theoretical generalizations related by relativistic partial-wave expansions. They have been amply discussed by Vilenkin (1968, Chapter X). Sneddon (1972) dedicates Chapter 7 in his book to the study of the Mehler–Fok transform and its applications.

8.5.6. Hilbert Transforms

Sturm–Liouville theory need not be involved in all transforms. In Section 7.4 we saw that the real and imaginary parts of the Fourier transform of a causal function were related by (7.146) (for $a = 0$) as

$$f_R(p) = \pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}f_I(p'), \tag{8.91a}$$

$$f_I(p) = -\pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}f_R(p'), \tag{8.91b}$$

where $\mathscr{P}$ stands for the integral's principal value and the tildes have been dropped. Equations (8.91) define $f_I(p)$ as the *Hilbert* transform of $f_R(p)$. As the definition of the Hilbert transform is closely related to analyticity, it has served, for instance, in constructing a generalized *phasor* formalism as for

alternating-current theory, which is applicable to general frequency-modulated signals. A given real signal $\sigma(t)$ and its Hilbert transform $\tau(t)$ are merged into an *analytic* complex signal $\sigma(t) + i\tau(t) =: \rho(t) \exp[i\omega(t)t]$, where $\rho(t)$ is the signal *envelope* and $\omega(t)$ the *instantaneous frequency*. As an example, we can recall the repulsive oscillator wave functions $\chi_\lambda{}^{\pm}(q)$ in Eqs. (7.203), shown in Fig. 7.11. As $\chi_\lambda{}^{+}(q)$ is the inverse Fourier transform of a function having support on the positive half-axis, it follows that Im $\chi_\lambda{}^{+}(q)$ is the Hilbert transform of Re $\chi_\lambda{}^{+}(q)$. Figure 7.11 shows the envelope of the former to be $|\chi_\lambda{}^{+}(q)|$. A sound mathematical treatment of the Hilbert transform can be seen in Titchmarsh's Fourier classic (1937, Chapter V) or, if available, in Cotler's dissertation (1953). Further work on the application of the Hilbert transform to the theory of causal filters can be seen in the article by Urkowitz (1962) and the books by Bracewell (1965, Chapter 11) and Sneddon (1972, Section 3-21). Tables of Hilbert transforms can be found in the Bateman manuscript project (Erdelyi *et al.*, 1954, Chapter XV).

8.5.7. Stieltjes Transforms

The *Stieltjes* transform is defined as the square of the unilateral Laplace transform:

$$f^s(q) = (\mathbb{L}^2\mathbf{f})(q) = \int_0^\infty dq'' \exp(-qq'') \int_0^\infty dq' f(q') \exp(-q''q')$$

$$= \int_0^\infty dq'(q + q')^{-1} f(q'). \tag{8.92a}$$

The original function is regained as

$$f(q) = (2\pi i)^{-1} \lim_{\varepsilon \to 0^+} [f^s(-q - i\varepsilon) - f^s(-q + i\varepsilon)], \tag{8.92b}$$

as can be ascertained by noting that (8.92a) is related to the Cauchy representation (7.136) by a change of sign in the argument and a factor of $2\pi i$. If $f(q)$ is continuous at q, (8.92b) follows from Eq. (7.137d). If $f(q)$ is discontinuous, one has to substitute as usual, $\lim_{\varepsilon \to 0^+}[f(q + \varepsilon) + f(q - \varepsilon)]/2$ for the left-hand side of (8.92b). The Stieltjes transform arose from the Stieljes moment problem (Titchmarsh, 1937, Section 11.9). It has been investigated thoroughly by Widder (1937, 1938) and occupies Chapter VIII of his 1941 book. Several generalizations of the Stieljes transform involve higher powers of the denominator in (8.92a) [in Widder's book (1941)], a hypergeometric function (Varma, 1951), or a Whittaker function (Arya, 1963). Tables of Stieltjes transforms can be found in the Bateman manuscript project (Erdelyi *et al.*, 1954, Chapter XIV).

8.5.8. Convolution Transforms

Integral transforms or various general types have been further considered in the literature. One class involves the *convolution transform*, which is of the general form

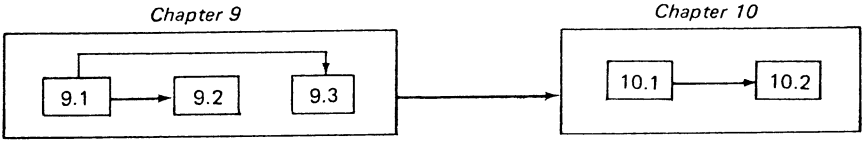
$$f^G(p) = \int_{-\infty}^{\infty} dq f(q) G(p - q), \tag{8.93}$$

where G is a rather general function including, for instance, the diffusion transform kernel. Various properties of the construct (8.93), the possibility of inversion, and its relation to hyperdifferential operators have been the subject of the book by Hirschmann and Widder (1955). Browsing through the list of references in Widder's books, one discovers many other transforms associated with as many other names. It will serve us to close the list here and reserve Part IV for the presentation of canonical transforms.

Part IV

Canonical Transforms

The aim of this part is to introduce a class of integral transforms which include, as particular cases, most of those which were discussed in Part III. It is a parametrized continuum of transforms which share several basic properties and which can be subject to *composition*. In fact, they constitute a *Lie semigroup*. For the benefit of the general reader we shall present these developments independently with a minimum of explicit use of Lie theory. Chapter 9 is devoted to the construction of the integral transform set, and Chapter 10 applies this tool to the deeper study of the diffusion equation and a class of Schrödinger equations. The ease and generality of the method, we hope, will spur the interested reader to acquaint himself with the growing research literature on the subject.



9

Construction and Properties of Canonical Transforms

In this chapter we present a class of integral transforms which we shall call canonical transforms. These constitute a parametrized continuum of transforms which include the Fourier, Laplace, Gauss–Weierstrass, and Bargmann transforms as particular cases. As these have arisen quite recently, we shall include brief historical sketches of the developments which led to their recognition and refer the interested reader to the research literature for a more rigorous treatment. Section 9.1 deals with *real* linear canonical transforms, while Section 9.2 enlarges the set to *complex* ones. The former appeared a couple of times before Moshinsky and Quesne (1974) called attention to their significance in connection with canonical transformations in quantum mechanics. A particular case of the latter was developed by Segal (1963) and Bargmann (1961) in order to formalize Fok's boson calculus (1928). Section 9.3 shows that canonical transforms have a hyperdifferential operator realization in addition to the usual integral form. Several examples and exercises show the economy of concepts and computation introduced by this new technique.

9.1. Real Linear Canonical Transforms

There are several ways to introduce the subject matter of this chapter. We have chosen here the approach which constructs canonical transforms as those unitary transformations which map the operators $\mathbb{Q}$ and $\mathbb{P}$ of Section 7.2 into real linear combinations of themselves. One finds several instances in the mathematical physics literature where this problem has been tackled. Infeld and Plebañski (1955) and, later and independently, Moshinsky and

Quesne (1971a, 1971b) have constructed unitary transformation operators in quantum-mechanical phase space in a group-theoretical context, as have Itzykson (1969) and Bargmann (1970). We present here the integral transform aspects of this construction.

9.1.1. Posing the Operator Problem

One of the main properties of the Fourier transform is that the operator $\mathbb{Q}$ of multiplication by the argument [i.e., $(\mathbb{Q}\mathbf{f})(q) = qf(q)$, Eq. (7.55)] is transformed into the operator $\mathbb{P}$ of differentiation [i.e., $(\mathbb{P}\mathbf{f})(q) = -idf(q)/dq$, Eq. (7.56)] and vice versa with a minus sign [Eqs. (7.57)]. Such transformation properties are remindful of a rotation by $\pi/2$ in a "$\mathbb{Q}$–$\mathbb{P}$ phase-space" plane. This is actually the case, without quotation marks, in the Schrödinger quantum-mechanics formalism. On a purely mathematical basis, however, we propose to investigate linear operators $\mathbb{C}$ which turn $\mathbb{Q}$ and $\mathbb{P}$ into linear combinations of each other,

$$\mathbb{Q}' \coloneqq \mathbb{C}\mathbb{Q}\mathbb{C}^{-1} = d\mathbb{Q} - b\mathbb{P}, \tag{9.1a}$$

$$\mathbb{P}' \coloneqq \mathbb{C}\mathbb{P}\mathbb{C}^{-1} = -c\mathbb{Q} + a\mathbb{P}, \tag{9.1b}$$

where the constants a, b, c, and d are real—in this section. There is one restriction: the *commutator* of (9.1a) and (9.1b) [defined as in (7.59b) and using (7.65)] is

$$\begin{aligned}[\mathbb{Q}', \mathbb{P}'] &= [d\mathbb{Q} - b\mathbb{P}, -c\mathbb{Q} + a\mathbb{P}] = i(ad - bc)\mathbb{1} \\ &= \mathbb{C}[\mathbb{Q}, \mathbb{P}]\mathbb{C}^{-1} = i\mathbb{1}.\end{aligned} \tag{9.2}$$

The four parameters must therefore relate by

$$ad - bc = 1. \tag{9.3a}$$

The Fourier transform, we see immediately, corresponds to the particular case $a = 0 = d$, $b = 1 = -c$. The identity transformation corresponds to $a = 1 = d$, $b = 0 = c$. We shall label the transform operator as $\mathbb{C}_M$ by the unimodular *matrix*

$$\mathbf{M} \coloneqq \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad \det \mathbf{M} = 1. \tag{9.3b}$$

This operator $\mathbb{C}_M$ can be made to act on an appropriate space of functions $\mathscr{B}_1$. The action is *linear*, i.e.,

$$\mathbb{C}_M(c_1\mathbf{f} + c_2\mathbf{g}) = c_1\mathbb{C}_M\mathbf{f} + c_2\mathbb{C}_M\mathbf{g}, \qquad c_1, c_2 \in \mathscr{C}, \mathbf{f}, \mathbf{g} \in \mathscr{B}_1, \tag{9.4}$$

and, due to (9.1), it has the following property: if the $\mathbb{C}_M$ transform of $f(q)$ is $f^M(q') = (\mathbb{C}_M\mathbf{f})(q')$, then the $\mathbb{C}_M$ transform of $qf(q)$ will be

$$\begin{aligned}(\mathbb{C}_M\mathbb{Q}\mathbf{f})(q') &= (\mathbb{C}_M\mathbb{Q}\mathbb{C}_M^{-1}\mathbf{f}^M)(q') = \big((d\mathbb{Q} - b\mathbb{P})\mathbf{f}^M\big)(q') \\ &= dq'f^M(q') + ib\,df^M(q')/dq'.\end{aligned} \tag{9.4a}$$

Similarly, the $\mathbb{C}_M$ transform of $(\mathbb{P}\mathbf{f})(q) = -i\,df(q)/dq$ is

$$(\mathbb{C}_M\mathbb{P}\mathbf{f})(q') = (\mathbb{C}_M\mathbb{P}\mathbb{C}_M^{-1}\mathbf{f}^M(q') = \big((-c\mathbb{Q} + a\mathbb{P})f^M\big)(q')$$
$$= -cq'f^M(q') - ia\,df^M(q')/dq'. \tag{9.4b}$$

9.1.2. Integral Transform and Kernel

As a concrete realization of the linear operator $\mathbb{C}_M$ we can propose an *integral transform* with a *kernel* $C_M(q', q)$:

$$f^M(q') = (\mathbb{C}_M\mathbf{f})(q') := \int_{\mathscr{R}} dq f(q)C_M(q', q), \tag{9.5}$$

where the integration takes place over the full real line $\mathscr{R}$. Linearity is automatically satisfied by the integral form, while conditions (9.4) will determine the kernel function $C_M(q', q)$ up to an arbitrary multiplicative constant. The extreme members of (9.4a) and (9.4b) with (9.5) are

$$\int_{\mathscr{R}} dq\cdot qf(q)C_M(q', q) = \left(dq' + ib\frac{d}{dq'}\right)\int_{\mathscr{R}} dqf(q)C_M(q', q), \tag{9.6a}$$

$$\int_{\mathscr{R}} dq[-i\,df(q)/dq]C_M(q', q) = -\left(cq' + ia\frac{d}{dq'}\right)\int_{\mathscr{R}} dqf(q)C_M(q', q). \tag{9.6b}$$

A sufficient condition for (9.6) to hold is that $C_M(q', q)$ satisfy the following differential equations:

$$qC_M(q', q) = \left(dq' + ib\frac{\partial}{\partial q'}\right)C_M(q', q), \tag{9.7a}$$

$$i\frac{\partial}{\partial q}C_M(q', q) = -\left(cq' + ia\frac{\partial}{\partial q'}\right)C_M(q', q), \tag{9.7b}$$

where the second one was obtained by integration by parts of the first integral in (9.6b) under the assumption that

$$f(q)C_M(q', q)|_{q=-\infty}^{\infty} = 0. \tag{9.7c}$$

This will help in the selection of the space $\mathscr{B}_1$ to which $f(q)$ can belong.

Proposing a solution of the kind $\exp(Aq^2 + Bq'q + Cq'^2)$, we find upon replacement that $A = ia/2b$, $B = -i/b$, $C = i\,d/2b$. The integral kernel is thus

$$C_M(q', q) = \theta_M \exp[i(aq^2 - 2q'q + dq'^2)/2b]. \tag{9.8a}$$

The choice of the multiplicative constant

$$\theta_M = (2\pi b)^{-1/2}\exp(-i\pi/4) \tag{9.8b}$$

will be seen to be convenient later on.

For real parameters, the behavior of the kernel (9.8) is that of a function which oscillates strongly for large $|q|$ and $|q'|$ but whose modulus is fixed at $(2\pi|b|)^{-1/2}$. (The limit $b \to 0$ is interesting but will be deferred until later in this section.) The validity of the assumed boundary condition (9.7c) can be seen to be the same as for ordinary Fourier transforms. We shall thus let $\mathscr{B}_1$ be $\mathscr{L}^2(\mathscr{R})$.

9.1.3. Inversion

The inversion of the $\mathbb{C}_M$ transform (9.5) with *real* parameters is easily accomplished with the help of the Fourier transform. We shall show that

$$(\mathbb{C}_M^{-1}\mathbf{f}^M)(q) = \lim_{\varepsilon \to 0} \tfrac{1}{2}[f(q+\varepsilon) + f(q-\varepsilon)] = \lim_{L\to\infty} \int_{-L}^{L} dq' f^M(q') C_M(q', q)^*. \tag{9.9}$$

If we substitute (9.5) and (9.8) into (9.9) and use the Fourier integral theorem (7.3), we obtain

$$\begin{aligned}
&\lim_{L\to\infty} \int_{-L}^{L} dq' \left[\int_{\mathscr{R}} dq'' f(q'') C_M(q', q'') \right] C_M(q', q)^* \\
&\quad = \lim_{L\to\infty} \int_{-L}^{L} dq' \int_{\mathscr{R}} dq'' f(q'')(2\pi|b|)^{-1} \\
&\qquad \times \exp[i(aq''^2 - 2q'q'' + dq'^2 - aq^2 + 2q'q - dq'^2)/2b] \\
&\quad = (2\pi|b|)^{-1} \exp(-iaq^2/2b) \lim_{L\to\infty} \int_{-L}^{L} dq' \int_{\mathscr{R}} dq'' \\
&\qquad \times \exp(iaq''^2/2b) f(q'') \exp[iq'(q - q'')/b].
\end{aligned} \tag{9.10}$$

The last step leads to (9.9) by a simple change of variables for q'.

Exercise 9.1. Prove the *Parseval* identity for real linear canonical transforms

$$\int_{\mathscr{R}} dq f(q)^* g(q) = \int_{\mathscr{R}} dq' f^M(q')^* g^M(q'). \tag{9.11}$$

The second integral is meant to be taken as $\lim_{L\to\infty} \int_{-L}^{L}$. Note carefully that (9.11)—and (9.9)—are valid strictly for *real* parameters.

The function $\mathbf{f}^M = \mathbb{C}_M\mathbf{f}$ given by (9.5) is the real linear canonical $\mathbb{C}_M$ transform of $\mathbf{f}$. For each matrix $\mathbf{M}$ we have a corresponding transform. This class of transforms has been called *Moshinsky–Quesne* (1971a, 1971b, 1974) transforms since they were recognized as such at the Solvay conference in Brussels (1970) and in their contiguous 1971 papers. [In attributing names of living authors to their mathematical constructs, care and tact must be used. Thus it should be noted that as a group-theoretical problem similar formulas

in a related but not identical context were derived by Infeld and Plebañski [1955, Eqs. (3.4)], Bargmann (1970, Section 3), and Kalnins and Miller (1974), Section 3. This representation has been called the *metaplectic* representation by Weil (1963); it is presented, for instance, by Burdet *et al.* (1978, Section 5).]

We have stated before that the Fourier transform is a *unitary* mapping of $\mathscr{L}^2(\mathscr{R})$ onto itself. This property holds for all real linear canonical transforms with the inner product defined—as usual—by

$$(\mathbf{f}, \mathbf{g})_1 := \int_{\mathscr{R}} dq f(q)^* g(q). \tag{9.12}$$

We would not bother to write (9.12) again were it not for the fact that a more general inner product will appear in Section 9.2, when the matrix parameters (9.3) are allowed to go complex. Thence the index "1" in (9.12).

9.1.4. Composition of Transforms

As we have a three-parameter continuum of canonical transforms, we may ask about the possibilities of *composition* of the elements of the set. Assume $\mathbb{Q}$ and $\mathbb{P}$ are transformed into $\mathbb{Q}'$ and $\mathbb{P}'$ by $\mathbb{C}_{M_1}$ as in (9.1) and that the latter are in turn transformed into $\mathbb{Q}''$ and $\mathbb{P}''$ by $\mathbb{C}_{M_2}$ by a similar action. The relation between the double-primed and the original operators is then

$$\begin{aligned}\mathbb{Q}'' &= \mathbb{C}_{M_2}\mathbb{Q}'\mathbb{C}_{M_2}^{-1} = \mathbb{C}_{M_2}\mathbb{C}_{M_1}\mathbb{Q}(\mathbb{C}_{M_2}\mathbb{C}_{M_1})^{-1} \\ &= \mathbb{C}_{M_2}(d_1\mathbb{Q} - b_1\mathbb{P})\mathbb{C}_{M_2}^{-1} = d_1\mathbb{C}_{M_2}\mathbb{Q}\mathbb{C}_{M_2}^{-1} - b_1\mathbb{C}_{M_2}\mathbb{P}\mathbb{C}_{M_2}^{-1} \\ &= (c_2b_1 + d_2d_1)\mathbb{Q} - (a_2b_1 + b_2d_1)\mathbb{P} =: \mathbb{C}_{M_{12}}\mathbb{Q}\mathbb{C}_{M_{12}}^{-1}, \end{aligned} \tag{9.13a}$$

$$\begin{aligned}\mathbb{P}'' &= \mathbb{C}_{M_2}\mathbb{P}'\mathbb{C}_{M_2}^{-1} = \mathbb{C}_{M_2}\mathbb{C}_{M_1}\mathbb{P}(\mathbb{C}_{M_2}\mathbb{C}_{M_1})^{-1} \\ &= \mathbb{C}_{M_2}(-c_1\mathbb{Q} + a_1\mathbb{P})\mathbb{C}_{M_2}^{-1} = -c_1\mathbb{C}_{M_2}\mathbb{Q}\mathbb{C}_{M_2}^{-1} + a_1\mathbb{C}_{M_2}\mathbb{P}\mathbb{C}_{M_2}^{-1} \\ &= -(c_2a_1 + d_2c_1)\mathbb{Q} + (a_2a_1 + b_2b_1)\mathbb{P} =: \mathbb{C}_{M_{12}}\mathbb{P}\mathbb{C}_{M_{12}}^{-1}, \end{aligned} \tag{9.13b}$$

where

$$\mathbb{C}_{M_{21}} := \mathbb{C}_{M_2}\mathbb{C}_{M_1} = \varphi\mathbb{C}_{M_2M_1}, \qquad \varphi \in \mathscr{C}, \tag{9.14a}$$

corresponding to

$$\begin{aligned}\mathbf{M}_2\mathbf{M}_1 &= \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix}\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = \begin{pmatrix} a_2a_1 + b_2c_1 & a_2b_1 + b_2d_1 \\ c_2a_1 + d_2c_1 & c_2b_1 + d_2d_1 \end{pmatrix} \\ &=: \begin{pmatrix} a_{21} & b_{21} \\ c_{21} & d_{21} \end{pmatrix} = \mathbf{M}_{21}. \end{aligned} \tag{9.14b}$$

By thus acting on the operators $\mathbb{Q}$ and $\mathbb{P}$, *the composition of* $\mathbb{C}_{M_2}$ *and* $\mathbb{C}_{M_1}$ (so that $\mathbb{C}_{M_1}$ acts first and $\mathbb{C}_{M_2}$ second) *is a* $\mathbb{C}_{M_2M_1}$ *transform with the parameters of a matrix which is the product of the parameters of the matrices of the constituent transforms.* We have left a free parameter φ in (9.14a) since the similarity transformation, involving $\mathbb{C}_{M_{21}}$ and $\mathbb{C}_{M_{21}}^{-1}$, allows for $\mathbb{C}_{M_{21}}$ and

$\mathbb{C}_{M_2M_1}$ to differ by a constant factor. Whether or not this factor can be chosen to be unity will be seen as we explore now the composition of $\mathbb{C}_M$ transforms on function spaces.

Allowing for exchange of integration order, as the intermediate transformed functions are assumed to exist, we must prove the last equality in

$$\begin{aligned}(\mathbb{C}_{M_2}\mathbb{C}_{M_1}\mathbf{f})(q'') &= \int_{\mathscr{R}} dq' \left[\int_{\mathscr{R}} dq f(q) C_{M_1}(q', q)\right] C_{M_2}(q'', q') \\ &= \int_{\mathscr{R}} dq f(q) \int_{\mathscr{R}} dq' C_{M_2}(q'', q') C_{M_1}(q', q) \\ &\stackrel{?}{=} \varphi \int_{\mathscr{R}} dq f(q) C_{M_2M_1}(q'', q). \end{aligned} \tag{9.15}$$

In performing the integration over q' we must deal with an integrand of the form $\exp[i(r^2q'^2 + sq')]$, which we now proceed to calculate for *complex* r and s. The added generality will serve us later. Completing squares, we obtain

$$\begin{aligned} I(r, s) &:= \int_{\mathscr{R}} dq' \exp[i(r^2q'^2 + sq')] \\ &= \exp(-is^2/4r^2) \int_{\mathscr{R}} dq' \exp[i(rq' + s/2r)^2]. \end{aligned} \tag{9.16a}$$

In reducing the last integral to Euler's, which involves $\exp(-x^2)$, change variables to

$$x := \exp(-i\pi/4)(rq' + s/2r); \tag{9.16b}$$

the integration path will be a line in the complex plane inclined at an angle $-\pi/4 + \arg r$ and passing through the point $x = \exp(-i\pi/4)s/2r$. As the integrand is entire analytic in the whole complex plane, we are allowed to shift the integration contour to pass through the origin of the complex x-plane. If r is in the first or third quadrant [Fig. 9.1(a)], the integration

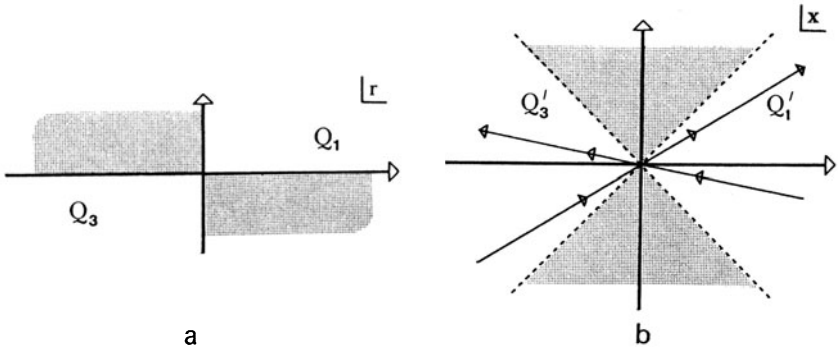


Fig. 9.1. (a) Allowed (unshaded) quadrants for the parameter r and (b) integration contours for the integral (9.16).

contour advances in the $\pi/2$ sector centered on the $+\mathrm{Re}\, x$ or the $-\mathrm{Re}\, x$ axes, respectively [Fig. 9.1(b)]. In these cases the integrand is a decreasing Gaussian function which is integrable by a standard Cauchy–Jordan argument which rotates the contour back to the real axis. If $\arg r$ is in the first quadrant, the integral reduces to Euler's $\pi^{1/2}$, while if $\arg r$ is in the third quadrant, there will be a reversal of the integral bounds, yielding $-\pi^{1/2}$. When r lies *on* the real or imaginary axes, the integral in (9.16a) exists only in the sense $\lim_{L\to\infty}\int_{-L}^{L}$, which can be evaluated to be the limit of the integral as r approaches these axes from the allowed regions. Hence,

$$I(r, s) = \varphi(r)\pi^{1/2}r^{-1}\exp(i\pi/4)\exp(-is^2/4r^2), \qquad |\arg r - \pi/4| \leqslant \pi/2, \tag{9.16c}$$

$$\varphi(r) := \begin{cases} 1 & \text{if } \arg r \in [0, \pi/2](\mathrm{mod}\ 2\pi), \\ -1 & \text{if } \arg r \in [-\pi, -\pi/2](\mathrm{mod}\ 2\pi). \end{cases} \tag{9.16d}$$

Convergence will be absolute when the strict inequality on $\arg r$ holds.

We can now establish the result we claimed in (9.15), as

$$\begin{aligned} \int_{\mathscr{R}} dq' C_{M_2}(q'', q')C_{M_1}(q', q) &= \theta_{M_2}\theta_{M_1}\exp[i(a_1q^2/2b_1 + d_2q''^2/2b_2)] \\ &\quad \times I\big((a_2/2b_2 + d_1/2b_1)^{1/2}, -(q''/b_2 + q/b_1)\big) \\ &= \theta_{M_{21}}\varphi(b_{21}/b_2b_1)\exp[i(a_{21}q^2 - 2q''q + d_{21}q''^2)/2b_{21}] \\ &= \varphi(b_{21}/b_2b_1)C_{M_{21}}(q'', q), \end{aligned} \tag{9.17}$$

where we have collected the terms in the exponents and used the algebraic equalities in (9.14b) (in particular, note that $a_2/b_2 + d_1/b_1 = b_{21}/b_2b_1$). We see that the arbitrary constant φ has been made unity by the proper choice of modulus of θ_M in (9.8b), while the phase of (9.8b) assures us that, for $b_1, b_2, b_{21} > 0$ at least, the constant is unity. It turns out to be impossible to redefine the phases θ_M so as to get rid of φ in the composition formula (9.17). [In group theory, the kernels C_M are said to constitute a *ray* representation of the group $SL(2, \mathscr{R})$ of 2×2 unimodular real matrices.] Note carefully that we have proven the validity of the composition formula for *complex* values of the parameters. The only restriction has been that the integrand in (9.16a) be a bounded function.

Exercise 9.2. Show that the composition relation (9.17) is *associative*, namely, that $(\mathbb{C}_{M_3}\mathbb{C}_{M_2})\mathbb{C}_{M_1} = \mathbb{C}_{M_3}(\mathbb{C}_{M_2}\mathbb{C}_{M_1})$. This is slightly tedious, but the fact that no extra phase enters into this relation is important.

Having shown that the unitary linear real canonical transforms $\mathbb{C}_M$ multiply as the parameter matrices do—modulo a sign—we would like to see

that the other two axioms of group composition (Section 1.4) also hold. These are the existence of an identity element and the inverse for every element in the set.

9.1.5. The Identity Transform Limit

The identity $\mathbb{C}_M$ transform, we should expect, corresponds to the unit matrix $\mathbf{M} = \mathbf{1}$. The integral kernel (9.8) looks peculiar in this case, as it does for the whole class of lower triangular matrices $\mathbf{M}$ which have the 1-2 element $b = 0$. We shall prove that for $b \to 0$ the integral kernel provides a sequence of oscillating Gaussians whose limit (in the *weak* sense of Section 7.3) is a Dirac δ. To this end we use (9.3a) to replace d in (9.8) and write

$$\begin{aligned} C_M(q', q) &= \theta_M \exp\{i[aq^2 - 2q'q + a^{-1}(1 + bc)q'^2]/2b\} \\ &= \theta_M \exp(icq'^2/2a) \exp[i(a^{1/2}q - a^{-1/2}q')^2/2b] \\ &= \beta \exp(icq'^2/2a) G_{|b|}\big(\beta(a^{1/2}q - a^{-1/2}q')\big), \end{aligned} \tag{9.18a}$$

where we have used the Gaussian function (7.20) and defined the phase

$$\beta := \exp[-i(\pi/2 + \arg b)/2]. \tag{9.18b}$$

Again, it will behoove us to work with complex parameters so as to understand the multivaluation features of the set of transforms. Note first that the integral transform (9.5) exists in $\mathscr{L}^2(\mathscr{R})$ only when (9.8a) is bounded. This means

$$\mathrm{Re}(ia/b) \leqslant 0 \quad \text{or} \quad \mathrm{Im}(a/b) \geqslant 0, \qquad \text{i.e.,} \quad \arg(a/b) \in [0, \pi] \ (\mathrm{mod}\ 2\pi), \tag{9.19a}$$

and

$$\text{if } a = 0, \quad \text{then Im } b = 0. \tag{9.19b}$$

The phase of the Gaussian's argument q is $\alpha := \arg(\beta a^{1/2}) = \frac{1}{2}\arg(a/b) - \pi/4$. Hence, if $\arg(a/b) \in [0, \pi]$, $\alpha \in [-\pi/4, \pi/4]$, while if $\arg(a/b) \in [-2\pi, -\pi]$ or $[2\pi, 3\pi]$, $\alpha \in [-5\pi/4, -3\pi/4]$ or $[3\pi/4, 5\pi/4]$. Thus in the first interval, $\beta a^{1/2}$ lies in the "forward" sector of Fig. 9.1(b), while in the last two it lies in the "backward" sector of the same figure. The upper and lower sectors are forbidden. Although the Gaussian in (9.18a) has a complex argument, we can relate its $|b| \to 0$ limit to a Dirac δ showing that (a) for any $q \neq a^{-1}q'$ the function either vanishes (for Im $b \neq 0$) or oscillates with infinite rapidity (for Im $b = 0$); (b) the integral of the function over $\mathscr{R}$ is finite:

$$\begin{aligned} \lim_{|b|\to 0} \int_{\mathscr{R}} dq G_{|b|}\big(\beta(a^{1/2}q - a^{-1/2}q')\big) &= \beta^{-1}a^{-1/2} \lim_{|b|\to 0} \int_{\alpha\mathscr{R}} dx G_{|b|}(x - \beta a^{-1/2}q') \\ &= \beta^{-1}a^{-1/2}\varphi\big((a/b)^{1/2}\big), \end{aligned} \tag{9.20a}$$

where we have made use of the integration contour deformation of Fig. 9.1(b) and introduced the phase function (9.16d). Hence

$$\lim_{|b|\to 0} G_{|b|}(\beta(a^{1/2}q - a^{-1/2}q')) = \beta^{-1}a^{-1/2}\varphi((a/b)^{1/2})\delta(q - a^{-1}q'). \quad (9.20b)$$

Substitution of (9.20b) into (9.18) yields, for $|b| \to 0$ and $(a/b)^{1/2}$ in the first complex quadrant,

$$\lim_{|b|\to 0} C_M(q', q) = a^{-1/2}\exp(icq'^2/2a)\delta(q - a^{-1}q'), \quad (9.21)$$

while if $(a/b)^{1/2}$ is in the third complex quadrant, a minus sign is necessary.

Near to the identity matrix, the parameter a is near to unity, c is near to zero, and if we agree to let b approach zero from the *lower* complex half-plane, including the real axis, then

$$\lim_{\mathbf{M}\to\mathbf{1}} C_M(q', q) = \delta(q - q'). \quad (9.22)$$

The integral kernel thus acts as the simple reproducing kernel for functions under integral transformations. Equation (9.22) thus constitutes the *identity* for the group of real linear canonical transforms. This result determined our choice of phase for θ_M in (9.8b).

Equation (9.21) also specifies the action of the operators for the class of lower-triangular matrices $\mathbf{M}$ ($b = 0$), as

$$(\mathbb{C}_{M(b=0)}\mathbf{f})(q) = a^{-1/2}\exp(icq^2/2a)f(a^{-1}q). \quad (9.23)$$

These will be called *geometric* transformations. They consist of dilatations by a and/or multiplication by an oscillating Gaussian of (imaginary) width a/ic. Note that the three parameters of $\mathbf{M}$ in (9.3b) have dropped to two, a and c, as $d = a^{-1}$.

Exercise 9.3. Compare the case of dilatations in (9.23) with (7.34) and with (7.71). Verify that the multivaluation "paradoxes" disappear in the complex parameter plane.

As to the inverse of the canonical transform $\mathbb{C}_M$, we remark that the inverse of the 2×2 unimodular matrix $\mathbf{M}$ in (9.3b) is

$$\mathbf{M}^{-1} := \begin{pmatrix} d & \exp(-i\pi)b \\ \exp(i\pi)c & a \end{pmatrix}. \quad (9.24)$$

We have used the sign definition since, insofar as matrices are concerned, the 1-2 matrix element is simply $-b$, the sheet in the complex b-plane being irrelevant. Due to the bivaluation property of the canonical transforms, $-b = \exp(in\pi)b$ for $n = \ldots, -1, 3, 7, \ldots$, etc., is needed. In this case, from (9.8) it follows that

$$C_{M^{-1}}(q', q) = C_M(q, q')^*. \quad (9.25)$$

Comparison with (9.9) shows that this is the proper transform kernel for the inverse of the real canonical transformation $\mathbb{C}_M$. Note that b and $\exp(-i\pi)b$ correspond to $(a/b)^{1/2}$ on the same parameter quadrant [Fig. 9.1(a)] for a close to unity in $\mathbb{C}_M$ and $\mathbb{C}_M^{-1}$.

9.1.6. One-Parameter Transform Subgroups

We have shown that the set of real linear canonical transforms $\mathbb{C}_M$ forms a *group* of unitary transformations of $\mathscr{L}^2(\mathscr{R})$ onto itself, in correspondence with (as a two-valued *ray homomorphism* of) the set of real 2×2 unimodular matrices $\mathbf{M}$. This group will be denoted, as is customary in the literature, by $SL(2, \mathscr{R})$, meaning special (unimodular) linear group in two real dimensions. It will prove worthwhile to examine in detail some of the one-parameter *sub*groups of $SL(2, \mathscr{R})$ and establish some connections with previously treated transformations. The fact that each set constitutes a group by itself is evident.

(a) *Dilatations* [recall Eqs. (7.34) and (7.71)], Eq. (9.23):

$$\mathbf{M}^d(a) \coloneqq \begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix}, \qquad (\mathbb{C}_M\mathbf{f})(q') = a^{-1/2} f(a^{-1}q') = (\mathbb{D}_a\mathbf{f})(q'). \tag{9.26}$$

(b) *Imaginary Gauss–Weierstrass transforms* [recall Eqs. (7.74), (7.75), and (8.90), setting the parameter ω or t to pure imaginary values]:

$$\mathbf{M}^I(-b) \coloneqq \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix},$$

$$(\mathbb{C}_M\mathbf{f})(q') = \theta_M \int_{\mathscr{R}} dq f(q) \exp[i(q - q')^2/2b] = (\mathbb{G}_{ib}\mathbf{f})(q'). \tag{9.27}$$

(c) *Multiplication by a Gaussian* of imaginary width, from (9.23):

$$\mathbf{M}^g(c) \coloneqq \begin{pmatrix} 1 & 0 \\ c & 1 \end{pmatrix}, \qquad (\mathbb{C}_M\mathbf{f})(q') = \exp(icq'^2/2) f(q'). \tag{9.28}$$

Exercise 9.4. Because of the composition property (9.17), show that (*almost*) every $\mathbb{C}_M \in SL(2, \mathscr{R})$ can be written as the product of elements of the three subgroups (9.26)–(9.28), following the decomposition

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ c/a & 1 \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix} \begin{pmatrix} 1 & b/a \\ 0 & 1 \end{pmatrix} = \mathbf{M}^g(c/a)\mathbf{M}^d(a)\mathbf{M}^I(-b/a). \tag{9.29}$$

This fails, however, for the special class of $\mathbf{M}$'s with $a = 0$, including the Fourier transform.

There is another triad of one-parameter subgroups of $SL(2, \mathscr{R})$ which avoids the failure in Exercise 9.4 and has by itself some interesting properties. The subgroups are

(α) *Hyperbolic* subgroup, defined as

$$\mathbf{M} = \begin{pmatrix} \cosh(\alpha/2) & -\sinh(\alpha/2) \\ -\sinh(\alpha/2) & \cosh(\alpha/2) \end{pmatrix}, \qquad \alpha \in \mathscr{R}. \tag{9.30}$$

(β) *Parabolic* subgroup, defined as the subgroup of dilatations but for $a = \exp(-\beta/2)$, $\beta \in \mathscr{R}$.

(γ) *Elliptic* subgroup, defined by

$$\mathbf{M} = \begin{pmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{pmatrix}, \qquad \gamma \equiv \gamma \bmod 4\pi. \tag{9.31}$$

The last subgroup is interesting since for $\gamma = -\pi$ the corresponding integral kernel can be seen to be essentially the Fourier transform, but for a phase

$$\mathbb{C}_F = \exp(-i\pi/4)\mathbb{F}, \qquad \mathbf{F} := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{9.32}$$

[The reader familiar with Lie group theory will see immediately that the hyperbolic and elliptic subgroups can be used to decompose $SL(2, \mathscr{R}) \simeq SO(2, 1)$ uniquely and parametrize $\mathbb{C}_M$ by Euler angles on a hyperboloid.]

Exercise 9.5. A decomposition of the general canonical transform $\mathbb{C}_M$ which involves the Fourier transform can be made by

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} b & 0 \\ d & b^{-1} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ a/b & 1 \end{pmatrix}, \tag{9.33}$$

which means that a function is first multiplied by Gaussian (9.28) and then Fourier-transformed; finally it undergoes a "geometric" transformation (9.23).

Exercise 9.6. Using (9.1), show that the following self-adjoint operators are left *invariant* under the corresponding subgroups of canonical transforms:

$$\mathbb{J}_2 := \tfrac{1}{4}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}) =: \tfrac{1}{2}\mathbb{H}^d \quad \text{[under (a) or } (\beta)\text{]}, \tag{9.34a}$$

$$\tfrac{1}{2}\mathbb{P}^2 =: \mathbb{H}^f \quad \text{[under (b)]}, \tag{9.34b}$$

$$\tfrac{1}{2}\mathbb{Q}^2 =: \mathbb{H}^g \quad \text{[under (c)]}, \tag{9.34c}$$

$$\mathbb{J}_1 := \tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2) =: \tfrac{1}{2}\mathbb{H}^r \quad \text{[under } (\alpha)\text{]}, \tag{9.34d}$$

$$\mathbb{J}_0 := \tfrac{1}{4}(\mathbb{P}^2 + \mathbb{Q}^2) =: \tfrac{1}{2}\mathbb{H}^h \quad \text{[under } (\gamma)\text{]}. \tag{9.34e}$$

[Operators $\mathbb{J}_i$ have appeared before, in Eqs. (7.174).] Note that this implies that, under all $\mathbb{C}_M$ transforms of each subgroup, the eigenfunctions of the corresponding operator will transform into multiples of themselves, that is, they will be *self-reciprocal* under $\mathbb{C}_M$. Thus, the eigenfunctions of $\mathbb{J}_0$ are the harmonic oscillator wave functions of Section 7.5 which were built as self-reciprocal under the Fourier transform. They are also, therefore, self-reciprocal under any elliptic

$\mathbb{C}_M$ transform (9.31). The eigenfunctions of the repulsive oscillator are the $\chi_\lambda{}^\pm$ functions (7.203), self-reciprocal under hyperbolic $\mathbb{C}_M$ transforms (9.30). The free-particle Schrödinger eigenfunctions of $\mathbb{H}^f$, basis for the Fourier partial-wave decomposition, are self-reciprocal under imaginary—and real—Gauss–Weierstrass transforms. Eigenfunctions of $\mathbb{J}_2$ are the basis functions for the Mellin transform and are self-reciprocal under dilatations. Finally, the eigenfunctions of $\mathbb{H}^g$ are in general displaced Dirac δ's. Multiplication by a Gaussian obviously leaves them as multiples of themselves. A description of self-reciprocating functions can be found in Wolf (1977a, and the references therein).

Exercise 9.7. Note that $\mathbb{J}_1$ in (9.34d) can be transformed into $\mathbb{J}_2$ in (9.34a) by a linear, real canonical transform:

$$\mathbb{C}_A[\tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2)]\mathbb{C}_A^{-1} = \tfrac{1}{4}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}), \qquad \mathbf{A} := 2^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \tag{9.35}$$

and thus the eigenfunctions $\chi_\lambda{}^\pm(q)$ of the repulsive oscillator Hamiltonian $\mathbb{H}^r$ are the $\mathbb{C}_A^{-1}$ transforms of the Mellin-basis functions $(2\pi)^{-1/2}q_\pm^{-i\lambda-1/2}$, eigenfunctions of $\mathbb{J}_2$. Show that this is precisely the way they were found in Eq. (7.203a), although the process appeared more circuitous there. Note also that [Eqs. (9.32) and (9.35)] $\mathbf{A}^2 = \mathbf{F}$. The transform $\mathbb{C}_A$ thus qualifies as the *square root* of the Fourier transform, i.e., $\chi_\lambda{}^\pm = (2\pi)^{-1/2}\,\mathbb{F}^{-1/2}\mathbf{q}_\pm^{-i\lambda-1/2}$, but for a constant phase. [Watch out for a dummy change of scale in p in Eq. (7.203a).]

Exercise 9.8. Show that the *parity* of a function is preserved under linear canonical transforms.

Exercise 9.9. Study the $\mathbb{C}_M$ version of convolution. Let $f^M(q')$ and $g^M(q')$ be the $\mathbb{C}_M$ transforms of $f(q)$ and $g(q)$, respectively. Show that the real $\mathbb{C}_M$ transform of $h(q) := f(q)g(q)$ is

$$h^M(q') = \int_{\mathscr{R}} dq_1 \int_{\mathscr{R}} dq_2 f^M(q_1)g^M(q_2)C^{(M)}(q'; q_1, q_2), \tag{9.36a}$$

where

$$\begin{aligned} C^{(M)}(q'; q_1, q_2) &:= \int_{\mathscr{R}} dq C_M(q, q')C_M(q, q_1)^* C_M(q, q_2)^* \\ &= \exp(-i\pi/4)[2\pi b a^{1/2}]^{-1} \\ &\quad \times \exp\{i[a\,d(q^2 - q_1{}^2 - q_2{}^2) + (q - q_1 - q_2)^2]/ab\} \end{aligned} \tag{9.36b}$$

is the $\mathbb{C}_M$ *coupling* coefficient. [Recall the convolution structure and coupling coefficients for the finite case in Eqs. (3.3)–(3.4).] Verify that for the Fourier transform (9.32) the usual convolution formula (7.43) is regained.

Exercise 9.10. Show that the product of the dispersion Δ_f of a function $f(q)$ [Eq. (7.217)] times the dispersion Δ_{f^M} of its real $\mathbb{C}_M$ transform is given by

$$\Delta_f \Delta_{f^M} \geqslant b^2/4. \tag{9.37}$$

This generalizes Heisenberg's Fourier uncertainty relation (7.218).

The program of unifying several different integral transforms as particular cases of canonical transforms is quite incomplete up to this point. The Fourier transform and its inverse transform have been successfully incorporated into a continuous $SL(2, \mathscr{R})$ group, but other transforms such as those of Laplace and Gauss–Weierstrass are still outside the general case (9.8). If we allow ourselves to tamper with the reality of the parameters we see that for

$$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

we have the bilateral Laplace transform kernel and for

$$\begin{pmatrix} 1 & -ib \\ 0 & 1 \end{pmatrix}, \qquad b \geqslant 0,$$

the Gauss–Weierstrass kernel. In Section 9.2 we shall see that other important transforms appear, notably the *Bargmann* transform. We shall let the parameters go complex but shall be required to amend the inner product of the transform space so as to preserve unitarity. Comments on canonical transforms other than linear ones will be deferred until the end of Section 9.2.

9.2. Complex Linear Transforms and Bargmann Space

The creation and annihilation operators for the quantum harmonic oscillator presented in Section 7.5 have commutation relations [see Eqs. (7.163)] which suggest their representation as $\mathbb{Z} \mapsto d/dz$ and $\mathbb{Z}^\dagger \mapsto z$. This was done quite early by Fok (1928), following the lead of Schrödinger. The ensuing developments made use of the considerable algebraic simplifications which "boson calculus" brought both in second-quantized field theories and in many-body quantum systems which were based, in one form or another, on harmonic oscillator models [see Biedenharn and Louck (1979, Chapter 5)]. The fact remained, however, that the dagger of the $\mathbb{Z}^\dagger$ in the Fok representation did not mean the adjoint of $\mathbb{Z}$, as d/dz is not the adjoint of z under the usual $\mathscr{L}^2(\mathscr{R})$ inner product. Segal (1963) and Bargmann (1961, 1967) put Fok's representation on a proper mathematical frame by the introduction of a Hilbert space of analytic functions.

During a visit to Mexico in 1972, Professor Peter Kramer suggested some problems in nuclear cluster theory which could be solved by the complexification of the linear transformation parameters of Moshinsky and Quesne (1971a, 1971b). This was accomplished in 1973 (Kramer *et al.*, 1975; references to the original canonical transformation program can be found within). The present formulation was completed shortly thereafter (Wolf,

1974a) during the author's stay at the Centre de Recherches Mathématiques in Montréal, Canada. Further works will be cited as they arise.

9.2.1. Introducing an Inner Product

The original setup in Section 9.1 was to describe the $SL(2, \mathscr{R})$ canonical transformation operators $\mathbb{C}_M$ as those which transform linearly the pair of operators $\mathbb{Q}$ and $\mathbb{P}$ as

$$\begin{pmatrix} \mathbb{Q}' \\ \mathbb{P}' \end{pmatrix} = \mathbb{C}_M \begin{pmatrix} \mathbb{Q} \\ \mathbb{P} \end{pmatrix} \mathbb{C}_M^{-1} = \mathbf{M}^{-1} \begin{pmatrix} \mathbb{Q} \\ \mathbb{P} \end{pmatrix}, \qquad \mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{9.38}$$

We are using here a rather obvious vector notation. When the parameters of $\mathbf{M}$ are allowed to go complex, we retain most of the results of Section 9.1 such as the transform kernel (9.8) with the restrictions (9.19) and its composition properties. What falls through is the unitarity of the transform [in mapping $\mathscr{L}^2(\mathscr{R})$ into itself] and consequently the inversion formula (9.9). The primed operators (9.38) are no longer self-adjoint under the $\mathscr{L}^2(\mathscr{R})$ inner product (9.12). Instead,

$$\begin{pmatrix} \mathbb{Q}'^{\dagger} \\ \mathbb{P}'^{\dagger} \end{pmatrix} = \mathbf{M}^{*-1} \begin{pmatrix} \mathbb{Q}^{\dagger} \\ \mathbb{P}^{\dagger} \end{pmatrix} = \mathbf{M}^{*-1} \begin{pmatrix} \mathbb{Q} \\ \mathbb{P} \end{pmatrix} = \mathbf{M}^{*-1} \mathbf{M} \begin{pmatrix} \mathbb{Q}' \\ \mathbb{P}' \end{pmatrix}, \tag{9.39}$$

where $\mathbf{M}^*$ is the matrix whose elements are the complex conjugates of those of $\mathbf{M}$. Of course $\mathbf{M}^{*-1}\mathbf{M} = \mathbf{1}$ if and only if $\mathbf{M}$ is real. In asking for self-adjointness, an inner product and a space of functions, domain of the operator, must be specified. Accordingly, if we are able to define a sesquilinear inner product $(\mathbf{f}^M, \mathbf{g}^M)_M$ such that $\mathbb{Q}'$ and $\mathbb{P}'$ *do* satisfy $(\mathbb{Q}'\mathbf{f}^M, \mathbf{g}^M)_M = (\mathbf{f}^M, \mathbb{Q}'\mathbf{g}^M)_M$ and correspondingly for $\mathbb{P}$, *then* unitarity of $\mathbb{C}_M$ could be upheld in the form

$$(\mathbf{f}, \mathbf{g})_1 = (\mathbb{C}_M\mathbf{f}, \mathbb{C}_M\mathbf{g})_M = (\mathbf{f}^M, \mathbf{g}^M)_M, \tag{9.40}$$

which would then be the new form of the Parseval identity. As we shall show in proceeding to implement this program, the inversion formula follows. We first characterize the function space $\mathscr{B}_M$ to which $(\mathbb{C}_M\mathbf{f})(q')$ belongs as determined from the transform kernel $C_M(q', q)$ in (9.8) with the restrictions (9.19) and $f(q) \in \mathscr{L}^2(\mathscr{R})$. We claim that (for b *not* real) $f^M(q')$ is an *entire analytic function*. This means that the functions have a convergent Taylor series in q' in the whole complex plane. Thus they have no singularities except at the point at infinity, and they are functions of q' only, and *not* of its complex conjugate q'^*. This property can be seen from the fact that the Taylor expansion $(\mathbb{C}_M\mathbf{f})(q')$ converges everywhere in the complex plane since the integrand contains a decreasing Gaussian in the integration variable and is entire analytic in q'. Note that as $|q'| \to \infty$ along a ray in the complex plane, a Gaussian $G_{\omega^{-1}}(q')$ is a *decreasing* function of $|q|$ along the direction where

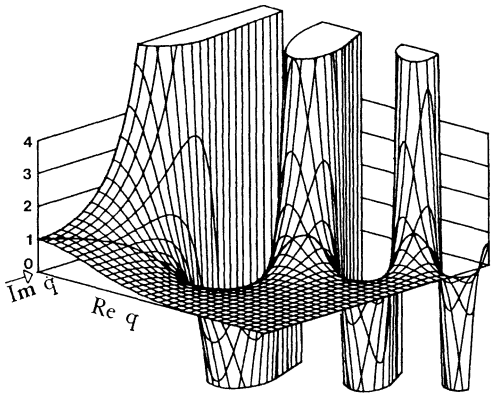


Fig. 9.2. Real part of the Gaussian function in the complex argument plane. The width is $\omega = \frac{1}{2}$, Re q and Im q are plotted in the interval (0, 3), and the vertical scale is in units of $\pi^{-1/2}$. We have marked the bisector line Re q = Im q, where the function oscillates with increasing rapidity. This line separates the "convergent" from the "divergent" directions.

$\arg \omega + 2 \arg q = 0$, *increasing* at right angles to it and oscillating along the bisectors. See Fig. 9.2. It is for entire analytic functions of at most Gaussian growth that the inner product $(\cdot\,,\cdot)_M$ for $\mathscr{B}_M$ can be defined. Specification of this growth will be done below.

9.2.2. The Weight Function

Bargmann (1961) has proposed the following sesquilinear inner product form involving q and its complex conjugate q^*,

$$(\mathbf{f}, \mathbf{g})_M = \int_{\mathscr{C}} d^2\mu_M(q, q^*) f(q)^* g(q), \tag{9.41a}$$

where the integral is taken *over the complex q-plane* $\mathscr{C}$ with

$$d^2\mu_M(q, q^*) = \nu_M(q, q^*)\, d \operatorname{Re} q\, d \operatorname{Im} q =: \nu_M(q, q^*)\, d^2q. \tag{9.41b}$$

The *weight factor* $\nu_M(q, q^*)$ will depend on $\mathbf{M}$ and on the independent variables q and q^*. This weight function will be found for $\mathscr{B}_M$ by requiring that $(\mathbb{Q}'\mathbf{f}, \mathbf{g})_M = (\mathbf{f}, \mathbb{Q}'\mathbf{g})_M$ and $(\mathbb{P}'\mathbf{f}, \mathbf{g})_M = (\mathbf{f}, \mathbb{P}'\mathbf{g})_M$. It will be easier to set up the determining equations from $\mathbb{Q}$ and $\mathbb{P}$ as

$$\begin{aligned}(\mathbb{Q}\mathbf{f}, \mathbf{g})_M &= \big((a\mathbb{Q}' + b\mathbb{P}')\mathbf{f}, \mathbf{g}\big)_M = a^*(\mathbf{f}, \mathbb{Q}'\mathbf{g})_M + b^*(\mathbf{f}, \mathbb{P}'\mathbf{g})_M \\ &= \big(\mathbf{f}, (u\mathbb{Q} + iv\mathbb{P})\mathbf{g}\big)_M, \end{aligned} \tag{9.42a}$$

$$\begin{aligned}(\mathbb{P}\mathbf{f}, \mathbf{g})_M &= \big((c\mathbb{Q}' + d\mathbb{P}')\mathbf{f}, \mathbf{g}\big)_M = c^*(\mathbf{f}, \mathbb{Q}'\mathbf{g})_M + d^*(\mathbf{f}, \mathbb{P}'\mathbf{g})_M \\ &= \big(\mathbf{f}, (iw\mathbb{Q} + u^*\mathbb{P})\mathbf{g}\big)_M, \end{aligned} \tag{9.42b}$$

where

$$u := a^*d - b^*c = \omega \exp(i\phi), \qquad \omega = |u|,\ \phi = \arg u, \tag{9.43a}$$

$$iv := b^*a - a^*b, \qquad \text{i.e.,} \quad v = 2 \operatorname{Im}(b^*a), \tag{9.43b}$$

$$iw := c^*d - d^*c, \qquad \text{i.e.,} \quad w = 2 \operatorname{Im}(c^*d). \tag{9.43c}$$

In (9.43b) we see that the restriction (9.19) implies that $v > 0$. Note that the unimodularity condition $\det \mathbf{M} = 1$, Eq. (9.3a), implies

$$\omega^2 + vw = 1. \tag{9.43d}$$

The extreme members of (9.42) thus read

$$\int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q q^* f^c(q^*) g(q)$$

$$= \int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q f^c(q^*)(uq + v\, d/dq) g(q), \tag{9.44a}$$

$$\int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q\, df^c(q^*)/dq^* g(q)$$

$$= \int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q f^c(q^*)(wq - u^*\, d/dq) g(q), \tag{9.44b}$$

where we have used the fact that $\mathbf{f}, \mathbf{g} \in \mathscr{B}_M$ are *analytic* functions in order to write $f(q)^* = f^c(q^*)$, f^c being a function of q^* only.

Exercise 9.11. Show that for $F = F(q, q^*)$,

$$B_F := \int_{\mathscr{C}} d^2q\, \partial F/\partial q^* = \frac{1}{2}\int_{-\infty}^{\infty} d(\operatorname{Im} q) F\Big|_{\operatorname{Re} q = -\infty}^{\infty} + \frac{i}{2}\int_{-\infty}^{\infty} d(\operatorname{Re} q) F\Big|_{\operatorname{Im} q = -\infty}^{\infty}. \tag{9.45a}$$

This is the boundary term for integration by parts for $F(q, q^*) = G(q, q^*) \cdot H(q, q^*)$:

$$\int_{\mathscr{C}} d^2q\, \partial G/\partial q^* H = B_{GH} - \int_{\mathscr{C}} d^2q G\, \partial H/\partial q^*. \tag{9.45b}$$

Integrating (9.44) by parts by (9.45b), noting that $\partial f^c(q^*)/\partial q = 0 = \partial g(q)/\partial q^*$, and assuming that the boundary term B_{vf^*g} in (9.45a) vanishes, we find as a sufficiency condition a pair of partial differential equations,

$$q^* \nu_M(q, q^*) = (uq - v\partial/\partial q)\nu_M(q, q^*), \tag{9.46a}$$

$$-\partial \nu_M(q, q^*)/\partial q^* = (wq + u^*\partial/\partial q)\nu_M(q, q^*), \tag{9.46b}$$

which will determine the weight function.

This equation pair is of the same form as the pair which determined the transform kernel in (9.7). Its solution, with a proper choice of normalization, is a real function

$$\nu_M(q, q^*) = (\pi v/2)^{-1/2} \exp[(uq^2 - 2qq^* + u^* q^{*2})/2v]$$

$$= (\pi v/2)^{-1/2} \exp\{-\rho^2[1 - \omega \cos(\phi + 2\theta)]/v\}. \tag{9.47}$$

The last expression uses the polar representation of u in (9.43a) and $q =: \rho \exp(i\theta)$. We note that as long as $v > 0$, the weight function is well defined.

The limit $v \to 0^+$, $\mathrm{Im}(a/b) \to 0^+$, which includes real matrices $\mathbf{M}$, will be examined later in this section.

The Parseval identity

$$(\mathbf{f}, \mathbf{g})_1 = \int_{\mathscr{R}} dq f(q)^* g(q) = \int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q f^M(q)^* g^M(q) = (\mathbf{f}^M, \mathbf{g}^M)_M \tag{9.48}$$

will fix the normalization constant for the weight function (see Exercise 9.14).

Having found the explicit form of the weight function, we can verify that the boundary term B_{vf^*g} vanishes for functions with a finite inner product (9.48). Let $f^M(q) =: \exp(uq^2/2v) f_B{}^M(q)$. Upon substituting (9.47) into (9.48), we see that the $\mathscr{C}$-integral of $\exp(-|q|^2/v)|f_B{}^M(q)|^2$ must be finite. The part $f_B{}^M(q)$ must therefore be of *growth* less than $(2, \frac{1}{2}v)$. [Recall the definition of growth in (8.2).] As the integrand is a Gaussian of finite width, in all directions in the complex plane the boundary integral (9.45a) is zero. We can thus characterize $\mathscr{B}_M$ as the space of entire analytic functions on $\mathscr{C}$ which are $\exp(uq^2/2v)$ times a function of growth less than $(2, 1/2v)$. Polynomials times $\exp(uq^2/2v)$, in particular, are seen to be elements of $\mathscr{B}_M$.

Exercise 9.12. To provide an example for $\mathbb{C}_M$ transforms, consider $\Psi_0(q)$, the lowest harmonic oscillator wave function (7.156), namely,

$$\Psi_0(q) \coloneqq \pi^{-1/4} \exp(-q^2/2). \tag{9.49a}$$

Using (9.16) and the associated phase function, show its $\mathbb{C}_M$ transform to be

$$\begin{aligned} \Psi_0{}^M(q) &= \exp(-i\pi/4)\pi^{-3/4}(2b)^{-1/2} \exp(idq^2/2b) I\big([(a + ib)/2b]^{1/2}, -q/b\big) \\ &= [\pi^{1/2}(a + ib)]^{-1/2} \varphi\big([(a + ib)/2b]^{1/2}\big) \exp[-q^2(d - ic)/2(a + ib)]. \end{aligned} \tag{9.49b}$$

Follow this function for the various complex one-parameter subgroups of Section 9.1. Check that for the Fourier transform it yields the correct result.

Exercise 9.13. Evaluate the integral, for real $\beta > 0$,

$$\begin{aligned} J(\alpha, \beta, \gamma, \delta, \varepsilon) &= \int_{\mathscr{C}} d^2q \exp(\alpha q^2 - \beta qq^* + \gamma q^{*2} + \delta q + \varepsilon q^*) \\ &= \pi(\beta^2 - 4\alpha\gamma)^{-1/2} \exp[(\alpha\varepsilon^2 + \gamma\delta^2 + \beta\delta\varepsilon)/(\beta^2 - 4\alpha\gamma)], \end{aligned} \tag{9.50a}$$

absolutely convergent if and only if

$$|\alpha + \gamma| < \beta. \tag{9.50b}$$

This integral will be useful later on. The calculation is tedious but straightforward: integrate over $\mathrm{Re}\, q$ and $\mathrm{Im}\, q$ using (9.16) twice. The condition for absolute convergence for this equation, Eq. (9.16c), leads to $|\arg(\alpha + \beta + \gamma)| < \pi$, which means, β being real and positive, that $|\alpha + \gamma| < \beta$. The two φ-factors are unity.

Exercise 9.14. Find the proper normalization constant for the weight function by requiring $(\Psi_0{}^M, \Psi_0{}^M)_M = 1$. Use (9.49), (9.50), and the identity $u/v - (d - ic)/(a + ib) = (a^* + ib^*)/v(a + ib)$.

9.2.3. Inversion

Having found a Parseval relation, we can suggest an inversion formula for the complex $\mathbb{C}_M$ transform which will then be proven. Although we have insisted on dealing with functions $\mathbf{f} \in \mathscr{B}_1 = \mathscr{L}^2(\mathscr{R})$, it is not difficult to argue that our transforms work—as the Fourier transforms do—for Dirac δ's and other generalized functions. If $\boldsymbol{\delta}_p$ is the Dirac δ sitting at $q = p$, its complex $\mathbb{C}_M$ transform will be, by placing the $\delta(q - p)$ in (9.5),

$$\delta_p{}^M(q') := (\mathbb{C}_M \boldsymbol{\delta}_p)(q') = C_M(q', p). \tag{9.51}$$

If this generalized function appears together with a continuous $\mathbf{f} \in \mathscr{B}_1$ in the Parseval identity (9.48), it tells us that

$$\begin{aligned} f(q) = (\boldsymbol{\delta}_q, \mathbf{f})_1 = (\boldsymbol{\delta}_q{}^M, \mathbf{f}^M)_M &= \int_{\mathscr{C}} \nu_M(q', q'^*)\, d^2q' f^M(q') C_M(q', q)^* \\ &= (\mathbb{C}_M^{-1} \mathbf{f}^M)(q), \end{aligned} \tag{9.52}$$

thereby providing an inversion formula for complex canonical transforms. It will be observed that the inverse transform involves the complex conjugate of the direct transform kernel as for the real case (9.9), but the integral is now that of the $\mathscr{B}_M$ inner product.

Equation (9.52) can be found as a limiting formula if we place a kernel $C_{M'}(q', q)^*$ with $\mathbf{M}'$ close to $\mathbf{M}$, asking only for the convergence of the integrals,

$$\begin{aligned} &\int_{\mathscr{C}} \nu_M(q', q'^*)\, d^2q' f^M(q') C_{M'}(q', q)^* \\ &\quad = \int_{\mathscr{C}} \nu_M(q', q'^*)\, d^2q' \left[\int_{\mathscr{R}} dq'' f(q'') C_M(q', q'') \right] C_{M'}(q', q)^* \\ &\quad = \int_{\mathscr{R}} dq'' f(q'') \left[\int_{\mathscr{C}} \nu_M(q', q'^*)\, d^2q' C_M(q', q'') C_{M'}(q', q)^* \right]. \end{aligned} \tag{9.53}$$

The expression between brackets, we suspect, should be $\delta(q - q'')$ for $\mathbf{M}' = \mathbf{M}$. Saving the reader some algebra, we calculate

$$\begin{aligned} &\int_{\mathscr{C}} \nu_M(q', q'^*)\, d^2q' C_M(q', q'') C_{M'}(q', q)^* \\ &\quad = (2\pi^3 v b b'^*)^{-1/2} \exp[i(aq''^2/2b - a'^* q^2/2b'^*)] \\ &\qquad \times J(b^*/2bv, 1/v, u^*/2v - i\, d'^*/2b'^*, -iq''/b, iq/b'^*) \\ &\quad = C_{M' \cdot -1_M \cdot}(q'', q) \xrightarrow[M' \to M]{} \delta(q - q''), \end{aligned} \tag{9.54}$$

the primed parameters being the parameters of $\mathbf{M}'$, $J(\cdots)$ being the integral (9.50), and the conclusion being due to (9.22). Equation (9.54) substituted into (9.53) reproduces (9.52).

9.2.4. The Bargmann Transform and Space

A particular case of complex linear canonical transforms—which will serve as the Fourier transform did for the real transforms—is *Bargmann's* transform, defined as $\mathbb{C}_B$, where

$$\mathbf{B} = 2^{-1/2}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}, \qquad -i = \exp(-i\pi/2). \tag{9.55a}$$

The transform kernel and weight function in $\mathscr{B}_B$-space are

$$C_B(q', q) = (2^{1/2}\pi)^{-1/2} \exp(-q^2/2 + 2^{1/2}qq' - q'^2/2), \tag{9.55b}$$

$$\nu_B(q', q'^*) = (2/\pi)^{1/2} \exp(-|q'|^2), \qquad u_B = 0, v_B = 1. \tag{9.55c}$$

This essentially defines the transform introduced by Bargmann in his 1961 paper. There, the inversion formula (9.52) is rigorously proven. The space $\mathscr{B}_B$ of entire analytic functions—called Segal–Bargmann or *Bargmann space* thereafter—is shown to be a *Hilbert* space, and $\mathbb{C}_B$ is thereby established as a *unitary* operator. The Bargmann transform, as it appeared originally and is currently used in most of the literature, has normalization coefficients different from ours: The constant factor in the transform kernel (9.55b) is $\pi^{-1/4}$ in place of our $(2^{1/2}\pi)^{-1/2}$, and in the weight function (9.55c) it is π^{-1} instead of our $(2/\pi)^{1/2}$. We uphold our choice of constants by the argument that the normalization for all $\mathbb{C}_M$ transforms provides the correct composition formulas and limits for arbitrary parameter values.

9.2.5. Properties of the Harmonic Oscillator Wave Functions

The important feature of the Bargmann transform is that, from (9.1) and (7.160),

$$\mathbb{C}_B\mathbb{Z}^\dagger = \mathbb{Q}\mathbb{C}_B, \tag{9.56a}$$

$$\mathbb{C}_B\mathbb{Z} = i\mathbb{P}\mathbb{C}_B. \tag{9.56b}$$

Hence

$$(\mathbb{C}_B\mathbb{Z}^\dagger\mathbf{f})(q') \coloneqq 2^{-1/2}\big(\mathbb{C}_B(\mathbb{Q} - i\mathbb{P})\mathbf{f}\big)(q') = (\mathbb{Q}\mathbb{C}_B\mathbf{f})(q') = q'f^B(q'), \tag{9.57a}$$

$$(\mathbb{C}_B\mathbb{Z}\mathbf{f})(q') \coloneqq 2^{-1/2}\big(\mathbb{C}_B(\mathbb{Q} + i\mathbb{P})\mathbf{f}\big)(q') = (i\mathbb{P}\mathbb{C}_B\mathbf{f})(q') = df^B(q')/dq'. \tag{9.57b}$$

In other words, application of the harmonic oscillator raising operator $\mathbb{Z}^\dagger$ on $f(q)$ multiplies its Bargmann transform $f^B(q')$ by q', while the lowering operator $\mathbb{Z}$ on $f(q)$ transforms into d/dq' acting on $f^B(q')$. Furthermore, under the $\mathscr{B}_B$ inner product, z is the adjoint of d/dz and vice versa, as we can easily see:

$$(\mathbb{Q}\mathbf{f}^B, \mathbf{g}^B)_B = (\mathbb{Q}\mathbb{C}_B\mathbf{f}, \mathbb{C}_B\mathbf{g})_B = (\mathbb{C}_B\mathbb{Z}^\dagger\mathbf{f}, \mathbb{C}_B\mathbf{g})_B = (\mathbb{Z}^\dagger\mathbf{f}, \mathbf{g})_1 = (\mathbf{f}, \mathbb{Z}\mathbf{g})_1$$
$$= (\mathbb{C}_B\mathbf{f}, \mathbb{C}_B\mathbb{Z}\mathbf{g})_B = (\mathbb{C}_B\mathbf{f}, i\mathbb{P}\mathbb{C}_B\mathbf{g})_B = (\mathbf{f}^B, \nabla\mathbf{g}^B)_B. \tag{9.58}$$

As a consequence, the harmonic oscillator wave functions (Section 7.5) will have a particularly simple Bargmann transform. The oscillator ground state $\Psi_0(q)$ can be seen to transform into the *constant* $(2\pi)^{-1/4}$ [Eqs. (9.49) for the parameters of $\mathbf{B}$ in (9.55a)]. Since we generated the orthonormal set $\{\Psi_n(q)\}_{n=0}^\infty$ as powers of $\mathbb{Z}^\dagger$ acting on the ground state, we immediately deduce from (9.57a) that

$$\Psi_n{}^B(q') = [(2\pi)^{1/2}n!]^{-1/2}q'^n. \tag{9.59}$$

As we are assured that the Bargmann transform is unitary and we know that $\{\Psi_n(q)\}_{n=0}^\infty$ constitutes a complete and orthonormal basis for $\mathscr{L}^2(\mathscr{R})$, it follows that *the set of power functions* (9.59) *is a complete and orthonormal basis for Bargmann space*. The mathematics of systems described in terms of harmonic oscillator wave functions is particularly streamlined in $\mathscr{B}_B$ as these wave functions involve only power functions. Applying operators generally means applying multiplication and differentiation, plus some combinatorics.

Exercise 9.15. Verify directly that the power functions (9.59) are an orthonormal set in $\mathscr{B}_B$. Calculate $(\mathbf{\Psi}_n{}^B, \mathbf{\Psi}_n{}^B)_B$ using the polar representation of the complex q'-plane: $d^2q' = |q'|\,d|q'|\,d\arg q'$. The angular integral will provide the $\delta_{n,n'}$-factor, and the radial integral is Euler's representation of the Γ-function (Appendix A).

Exercise 9.16. Show that the harmonic oscillator Hamiltonian operator $\mathbb{H}^h = 2\mathbb{J}_0$ in (9.34e) is represented in Bargmann space essentially as $\mathbb{J}_2$ in (9.34a); i.e., $\mathbb{C}_B\mathbb{J}_0\mathbb{C}_B^{-1} = i\mathbb{J}_2$. Accepting the hyperdifferential representation (7.197) as the Fourier transform $\mathbb{F} = \exp(i\pi/4)\exp(-i\pi\mathbb{J}_0)$, show that *Fourier transformation in Bargmann space appears as a dilatation by a factor* $i = \exp(i\pi/2)$ [as in (7.71) and (9.26)], namely, $\mathbb{C}_B\mathbb{F}\mathbb{C}_B^{-1} = \exp(i\pi/4)\mathbb{D}_i$. Using (7.72), verify the self-reciprocity relation (7.167) of the harmonic oscillator wave functions. Note that, as *matrices* [Eqs. (9.26), (9.32), and (9.55a)],

$$\mathbf{BFB}^{-1} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

9.2.6. Transform and Reproducing Kernels as Generating Functions

The transform kernel $C_B(q', q)$ has a rather transparent series expression as a *generating function* relating two orthonormal bases:

$$\sum_{n=0}^{\infty} \Psi_n{}^B(q')\Psi_n(q)^* = (2\pi)^{-1/4} \sum_{n=0}^{\infty} (n!)^{-1/2} q'^n \Psi_n(q) = (2\pi)^{-1/4} G_\psi(2^{1/2}q', q)$$
$$= C_B(q', q) = 2^{-1/4}\pi^{-1/2} \exp[-q^2/2 + 2^{1/2}qq' - q'^2/2], \tag{9.60}$$

where we have used the harmonic oscillator generating function (7.178).

Exercise 9.17. The Bargmann transform maps $\mathscr{L}^2(\mathscr{R})$ functions onto functions with convergent Taylor expansions in $\mathscr{C}$. Relate the harmonic oscillator "partial waves" of a given function (7.180) with the Taylor coefficients of its Bargmann transform. Equation (9.60) provides a very handy relation.

Exercise 9.18. The representation of transform kernels as generating functions relating orthonormal bases can be applied to other cases; for example, the Fourier transform kernel [Eq. (9.32)] under the integral sign can be represented as

$$(2\pi)^{-1/2} \exp(ipq) = \sum_{n=0}^{\infty} i^n \Psi_n(p)\Psi_n(q) = \exp(i\pi/4) C_F(p, q). \tag{9.61}$$

Exercise 9.19. Perform the Bargmann transform of (9.61) and show that

$$(2\pi)^{-1/2}[\mathbb{C}_B \exp(ip\cdot)](q') = \sum_{n=0}^{\infty} \Psi_n(p)\Psi_n{}^B(iq') = C_B(iq', p). \tag{9.62}$$

Notice that this holds in spite of the fact that the oscillating exponential function is "just" outside $\mathscr{L}^2(\mathscr{R})$. Correspondingly, the Bargmann transform kernel behaves as $\exp(q'^2/2)$, i.e., it is "just" outside $\mathscr{B}_B$. The treatment of generalized functions has been developed in Bargmann's second paper (1967).

Generating functions built out of pairs of orthonormal bases have a deep relation with transform kernels. This is suggested by (9.60) and (9.61). In $\mathscr{L}^2(\mathscr{R})$ when a generating function has orthonormal basis functions in two different arguments, a Dirac δ results as in Eq. (7.180d). In Bargmann space the orthonormal basis (9.59), for two different arguments, yields

$$K_B(q_1, q_2) := \sum_{n=0}^{\infty} \Psi_n{}^B(q_1)\Psi_n{}^B(q_2)^* = (2\pi)^{-1/2} \sum_{n=0}^{\infty} (n!)^{-1} q_1{}^n q_2^{*n}$$
$$= (2\pi)^{-1/2} \exp(q_1 q_2^*). \tag{9.63}$$

This well-defined function is the *reproducing* kernel under the Bargmann inner product integral, since for any $\mathbf{f}^B \in \mathscr{B}_B$,

$$\int_{\mathscr{C}} \nu(q, q^*)\, d^2q f^B(q) K_B(q', q) = f^B(q'), \tag{9.64}$$

as its Taylor series converges. The role of the Dirac δ in $\mathscr{L}^2(\mathscr{R})$ is thus taken by K_B in $\mathscr{B}_B$.

Exercise 9.20. Prove that

$$\int_{\mathscr{C}} \nu(q_2, q_2^*)\, d^2q_2 K_B(q_1, q_2) K_B(q_2, q_3) = K_B(q_1, q_3) \tag{9.65}$$

is the analogue of the convolution relation between Dirac δ's in Exercise 7.31.

9.2.7. The Coherent-State Basis

There are two generalized bases of the Dirac kind for $\mathscr{L}^2(\mathscr{R})$ and $\mathscr{B}_B$ on which we would like to comment briefly. First, there is *the* Dirac basis which "expands" a function in terms of a continuum of Dirac δ's sitting on points $q' \in \mathscr{R}$ with continuous linear combination coefficients $f(q')$ as suggested by Eq. (7.86). Correspondingly, Eq. (9.64) expands a function $f^B(q')$ in a continuum of functions $K_B(q, q')$ for $q \in \mathscr{C}$ with linear combination coefficients $f^B(q)$. This set is *overcomplete* in the sense that the functions are linearly independent but not orthogonal [Eq. (9.65)]. Second, we can point out that the inverse and direct Bargmann transforms are

$$f(q) = (2\pi)^{1/4} \int_{\mathscr{C}} \nu_B(q', q'^*)\, d^2q' f^B(q') \Upsilon_{q'}(q), \qquad q \in \mathscr{R}, \tag{9.66a}$$

$$f^B(q') = (2\pi)^{1/4} \int_{\mathscr{R}} dq f(q) \Upsilon_q(q'), \qquad q' \in \mathscr{C}, \tag{9.66b}$$

where we have introduced the *coherent states* (7.188), which are, note, essentially the Bargmann transform kernel. Equation (9.66a) can be interpreted as *the expansion of a function in a complex continuum of coherent states.* This basis is again overcomplete, although a strictly complete subset can be found [see Bargmann *et al.* (1971)]. Conversely, Eq. (9.66b) expands a function $\mathbf{f}^B \in \mathscr{B}_B$ in a real continuum of the same states. Several other generalized bases, complete and orthonormal, can be found for Bargmann space, including, strangely enough, the repulsive oscillator wave-function basis, which happens to be self-reciprocal under $\mathbb{C}_B$ [see Wolf (1977a) and Exercise 9.29].

9.2.8. The Gauss–Weierstrass Transform as a Complex Canonical Transform

The main features of the Bargmann transform can be extended to all other permissible complex canonical transforms. We shall not burden the reader with generalities, however. We *are* interested, nevertheless, in two other important particular cases of $\mathbb{C}_M$ transforms, the Gauss–Weierstrass "diffusive" transform and the bilateral Laplace transform.

The Gauss–Weierstrass transform (for time t) arises for the matrix parameters

$$\mathbf{W}(t) = \begin{pmatrix} 1 & -2it \\ 0 & 1 \end{pmatrix}, \qquad t > 0, \; -i = \exp(-i\pi/2). \tag{9.67}$$

The general $\mathbb{C}_{w(t)}$ kernel (9.8) then becomes the Gauss–Weierstrass kernel (8.90) which is the diffusion equation Green's function for time t. The applications of canonical transforms to the study of the diffusion equation will occupy Section 10.1. The main points we want to emphasize here are the following: (a) The $\mathbb{C}_{w(t)}$ transform provides us with the known results on analyticity of the heat equation's solution [see Widder (1975)]. (b) Diffusive time evolution has, as the energy in the wave equation, a *sesquilinear* invariant associated with a conserved inner product $(\cdot, \cdot)_{w(t)}$ in $\mathscr{B}_{w(t)}$. Previously, only *total heat*, a linear invariant, was counted. (c) The problem of the *backward* time evolution takes a new aspect as a $\mathbb{C}^{-1}_{w(t)}$ operator acting on $\mathscr{B}_{w(t)}$. [In this connection, recall the discussion of the Gauss–Weierstrass transform in Section 8.5 and its inversion. The problem has been tackled by Doetsch (1928, 1936) and Tricomi (1936). More modern treatments can be found in the work of Bilodeau (1961) and Rooney (1957, 1958, 1963). Its relevance in physics is connected with the quantum mechanics of unstable particles; see the articles by Horwitz *et al.* (1971) and Sinha (1972).]

9.2.9. The Collapse of Bargmann to $\mathscr{L}^2(\mathscr{R})$-Spaces, the Laplace Transform

The bilateral Laplace transform kernel will now be seen to arise as the particular case of (9.8) for the parameter values

$$\mathbf{L} \coloneqq \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \qquad i = \exp(i\pi/2). \tag{9.68}$$

The problem with (9.68), however, is that when setting up a $\mathscr{B}_L$-space we are faced with an apparently singular weight function in (9.47), since for $a = 0$ the values of the parameters (9.43) are $u = -1$, $v = 0 = w$. We shall examine in general the behavior of the real weight function $\nu_M(q, q^*)$ as $v \to 0$. Basically, we shall see that the integral over the complex plane in the inner product and the inversion formula becomes a $\int_{\mathscr{R}_\phi} dq \cdots$ in the complex plane along a ray depending in the phase of u. In the case when $\mathbf{M}$ becomes real, the integration contour becomes the real axis. To follow the expression for $\nu_M(q, q^*)$ as $v \to 0^+$ we use the polar form given by the last member of Eq. (9.47). From (9.43d) as $v \to 0^+$, $\omega = (1 - vw)^{1/2} \simeq 1 - vw/2$, so that $\nu_M(q, q^*)$ has its maximum along the line in the complex q-plane where $\cos(\phi + 2\theta) = 1$, i.e., for $\arg q = \theta = -\phi/2 = -\frac{1}{2} \arg u$ and for $\theta = -\phi/2 + \pi$. This approximation and a trigonometric identity allow us to write, for $v \to 0^+$,

$$\nu_M(q, q^*) \simeq (\pi v/2)^{-1/2} \exp(-w\rho^2/2) \exp[-2\rho^2 \sin^2(\theta + \phi/2)/v]. \tag{9.69}$$

In the limit $v \to 0^+$ we can use a sequence of Gaussians of decreasing width which define the Dirac δ in (7.83), writing, as a *weak* limit,

$$\nu_M(q, q^*) \xrightarrow[v\to 0^+]{} 2^{-1/2} \exp(-w\rho^2/2)\delta\big(2^{1/2}\rho \sin(\theta + \phi/2)\big). \tag{9.70}$$

Since this appears under the double integral $\int_0^\infty \rho\, d\rho \int_{-\pi}^{\pi} d\theta$, the point $\rho = 0$ is immaterial insofar as the δ is concerned and only the integration over θ is reduced to the integrand's value at the roots of the sine function: $\theta = -\phi/2$ and $\theta = \pi - \phi/2$, the former with a plus and the latter with a minus sign. If we define $x := \rho \exp(-i\phi/2)$ and $-x := \rho \exp[i(\pi - \phi/2)]$, the limit of the inner product will be a *line* integral,

$$\lim_{v\to 0^+} \int_{\mathscr{C}} \nu_M(q, q^*)\, d^2q f^M(q)^* g^M(q) = \int_{\mathscr{R}_\phi} \exp(-w|x|^2/2)\, dx f^M(x)^* g^M(x), \tag{9.71}$$

along $\mathscr{R}_\phi := \mathscr{R} \exp(-i\phi/2)$, tilted by $-\frac{1}{2}\arg u$ with respect to the real axis. When the matrix $\mathbf{M}$ is real, $u = 1$, $\phi = 0$, and $w = 0$; hence $(\mathbf{f}^M, \mathbf{g}^M)_M = (\mathbf{f}^M, \mathbf{g}^M)_1$, and the defining inner product for $\mathscr{B}_M$ is that of $\mathscr{B}_1 = \mathscr{L}^2(\mathscr{R})$.

We return now to the canonical transform $\mathbb{C}_L$ determined by (9.68). The transform kernel (9.8) is $-(2\pi)^{-1/2} i \exp(-qq')$, which is the bilateral Laplace kernel (although unfortunately off by a factor and phase). The corresponding $\mathscr{B}_L$-space has an inner product (9.71) for $w = 0$, and, since $u = -1$, $\phi = \pm\pi$. The inner product therefore involves *integration up along the imaginary axis.* (See Exercise 9.21.) This agrees with (8.1). The inverse Laplace transform integrates, along this contour, the function in company with the complex conjugate kernel: $(2\pi)^{-1/2} i \exp(xq)$. As x is the value of q' for pure imaginary values, complex conjugation produces the correct inverse transform kernel.

It should be noted that the Laplace transform has been correctly described in spite of the fact that $\mathbf{L}$ in (9.68) does *not* satisfy the integrability conditions (9.19)—in fact, we know that the bilateral Laplace transform is not defined on all of $\mathscr{L}^2(\mathscr{R})$ but only on a *dense* subset: causal functions. We shall comment briefly on this below.

Exercise 9.21. The Laplace transform matrix (9.68) has $u = -1$ [Eq. (9.43a)]. This could mean $u = \exp(in\pi)$ for any odd integer n. Concentrate on $n = \pm 1$. Show that the two cases give rise to the same integral: $x = \rho \exp(\mp i\pi/2)$ along the ray at $\mp i\pi/2$ minus $x = \rho \exp(\pm i\pi/2)$ along the ray at $\pm i\pi/2$.

9.2.10. Further Extensions and References

To sum up, we have shown that the class of complex linear transforms $\mathbb{C}_M$ is a set of unitary transformations between $\mathscr{L}^2(\mathscr{R})$ and Bargmann-like spaces $\mathscr{B}_M$, which properly include the Bargmann, Gauss–Weierstrass, Moshinsky–Quesne (real linear), and—somewhat improperly—bilateral Laplace transforms.

Certain further developments will be left for the interested reader to look up in the literature. The first one concerns the composition of complex linear canonical transforms, generalizing the real case discussed in Section 9.1 and proceeding essentially from the composition property (9.54). Second, we can repeat our program in N dimensions, dealing with $2N$-dimensional *symplectic* matrices $\mathbf{M}$ and defining integral transforms in N-space (Wolf, 1974a). Third, there is the question of existence of transforms *violating*—as the Laplace transform—the integrability conditions (9.19). It turns out that the *unitary* canonical transforms constitute a *subsemigroup* of the group of $2N \times 2N$ symplectic matrices. [See Kramer and Schenzle (1973) and Brunet and Kramer (1976).] It *also* turns out *apropos* that many of the nuclear cluster model calculations need transforms which lie outside this subsemigroup. [See Zahn (1975), Seligman (1976), and Seligman and Zahn (1976a).] Fourth, N-dimensional transforms invite the consideration of *complex radial transforms* (Moshinsky *et al.*, 1972; Wolf, 1974b), which include the Hankel transform and—corresponding to the Bargmann case—the *Barut–Girardello* transform [see Barut and Girardello (1971)]. [See also Kramer *et al.* (1975, Section VI), where Girardello's name has been unjustly left out, and Seligman and Zahn (1976b).] The role of canonical transformations in quantum mechanics has suggested several generalizations (Moshinsky, 1973; Mello and Moshinsky, 1975). Finally, studies in group representations have been done with the aid of canonical transforms. [See Boyer and Wolf (1975, 1976) and Wolf (1977b).]

9.3. Canonical Transforms by Hyperdifferential Operators

We have a parametrized continuum of integral transforms, one for each complex 2×2 unimodular matrix. Since these matrices form a *group*, and integral transforms compose following matrix multiplication—up to a sign—we have at our disposal the powerful results of Lie theory to define and solve many questions. Our aim here does not require the full use of group theory language; rather, we shall phrase the subject of integral transforms in the following terms.

9.3.1. Operators Generating Transforms

Given a one-parameter integral transform family

$$(\mathbb{C}_{M(\tau)}\mathbf{f})(q') = \int_{\mathscr{R}} dq f(q) C_{M(\tau)}(q', q) =: f(q', \tau), \tag{9.72}$$

which includes the identity for $\tau = 0$ [i.e., $\mathbf{M}(0) = \mathbf{1}$ and $f(q, 0) = f(q)$], we

want to find a differential operator $\mathbb{H}$ which we can write as a function of q and d/dq such that

$$(\mathbb{C}_{M(\tau)}\mathbf{f})(q) = \exp(i\tau\mathbb{H})f(q) =: \sum_{n=0}^{\infty} (n!)^{-1}(i\tau\mathbb{H})^n f(q). \tag{9.73}$$

Operators of this kind have appeared before mainly in connection with the time evolution of the wave and diffusion equations, translations, and dilatations. They involve arbitrarily high derivatives so their domain must be a subset of the $\mathscr{C}^\infty$ functions (although we have seen that *weakly* their action can be defined on larger function spaces).

The operator $\mathbb{H}$ can be formally obtained from (9.73) by differentiating with respect to τ and setting $\tau = 0$:

$$\mathbb{H}f(q') = -i\frac{\partial}{\partial\tau}\int_{\mathscr{R}} dq f(q) C_{M(\tau)}(q', q)|_{\tau=0}. \tag{9.74}$$

The operator $\mathbb{H}$ will be said to *generate* the integral transform family (9.72). The theory of Lie groups assures us that once we have found the operator $\mathbb{H}$ by (9.74) its exponentiated (and properly defined) action is that of (9.72)–(9.73).

The following one-parameter subgroups of the group $SL(2, \mathscr{R})$ are of particular interest:

$$\mathbf{M}^d(e^{-\tau}) := \begin{pmatrix} e^{-\tau} & 0 \\ 0 & e^{\tau} \end{pmatrix},$$

$$\begin{aligned} \frac{\partial}{\partial\tau} C_M(q', q)\bigg|_{\tau=0} &= \frac{1}{2} C_M(q', q) - \exp\left(\frac{\tau}{4}\right) q'\delta'\left(q - \exp\left(\frac{\tau}{2}\right) q'\right)\bigg|_{\tau=0} \\ &= \frac{1}{2}\delta(q - q') - q'\frac{\partial}{\partial q}\delta(q - q') \\ &= \left(\frac{1}{2} - q\frac{\partial}{\partial q}\right) C_M(q', q)\bigg|_{\tau=0}, \end{aligned} \tag{9.75a}$$

$$\mathbf{M}^I(\tau) := \begin{pmatrix} 1 & -\tau \\ 0 & 1 \end{pmatrix},$$

$$\begin{aligned} \frac{\partial}{\partial\tau} C_M(q', q)\bigg|_{\tau=0} &= -(2\tau)^{-1} C_M(q', q) + i\frac{1}{2}\tau^{-2}(q - q')^2 C_M(q', q)|_{\tau=0} \\ &= -i\frac{1}{2}\frac{\partial^2}{\partial q^2} C_M(q', q)\bigg|_{\tau=0}, \end{aligned} \tag{9.75b}$$

$$\mathbf{M}^g(\tau) := \begin{pmatrix} 1 & 0 \\ \tau & 1 \end{pmatrix},$$

$$\frac{\partial}{\partial\tau} C_M(q', q)\Big|_{\tau=0} = i\frac{1}{2} q'^2 C_M(q', q)\Big|_{\tau=0} = i\frac{1}{2} q^2 \delta(q - q')$$

$$= i\frac{1}{2} q^2 C_M(q', q)\Big|_{\tau=0}, \tag{9.75c}$$

$$\mathbf{M}^r(\tau) := \begin{pmatrix} \cosh\tau & -\sinh\tau \\ -\sinh\tau & \cosh\tau \end{pmatrix},$$

$$\frac{\partial}{\partial\tau} C_M(q', q)\Big|_{\tau=0} = \left[\frac{1}{2}\coth\tau + i\frac{1}{2}(q^2 - 2qq'\cosh\tau + q'^2)/\sinh^2\tau\right]$$

$$\times C_M(q', q)|_{\tau=0}$$

$$= i\frac{1}{2}\left(-\frac{\partial^2}{\partial q^2} - q^2\right) C_M(q', q)\Big|_{\tau=0}, \tag{9.75d}$$

$$\mathbf{M}^h(\tau) := \begin{pmatrix} \cos\tau & -\sin\tau \\ \sin\tau & \cos\tau \end{pmatrix},$$

$$\frac{\partial}{\partial\tau} C_M(q', q)\Big|_{\tau=0} = \left[\frac{1}{2}\cot\tau - i\frac{1}{2}(q^2 - 2qq'\cos\tau + q'^2)/\sin^2\tau\right]$$

$$\times C_M(q', q)|_{\tau=0}$$

$$= i\frac{1}{2}\left(-\frac{\partial^2}{\partial q^2} + q^2\right) C_M(q', q)\Big|_{\tau=0}. \tag{9.75e}$$

We have used the labeling (9.26)–(9.28), (9.30), and (9.31) for the matrices and formulas (9.8) and (9.21) for the transform kernels. The final expression for each case is put in a form where integration by parts can be readily implemented so as to have the differential operators acting—with a minus sign—on the integrand function $f(q)$ in (9.74). The generating operators are thus found to be, respectively,

$$\mathbb{H}^d := \tfrac{1}{2}(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}) = 2\mathbb{J}_2, \tag{9.76a}$$

$$\mathbb{H}^f := \tfrac{1}{2}\mathbb{P}^2 = \mathbb{J}_0 + \mathbb{J}_1, \tag{9.76b}$$

$$\mathbb{H}^g := \tfrac{1}{2}\mathbb{Q}^2 = \mathbb{J}_0 - \mathbb{J}_1, \tag{9.76c}$$

$$\mathbb{H}^r := \tfrac{1}{2}(\mathbb{P}^2 - \mathbb{Q}^2) = 2\mathbb{J}_1, \tag{9.76d}$$

$$\mathbb{H}^h := \tfrac{1}{2}(\mathbb{P}^2 + \mathbb{Q}^2) = 2\mathbb{J}_0, \tag{9.76e}$$

where we have introduced the three $\mathbb{J}_i$ operators from Eqs. (7.174) and (9.34).

Lie theory customarily works with the exponentiation of first-order differential operators such as $\mathbb{P}$ [generating translations: Eq. (7.69)], $\mathbb{J}_2$ [generating dilatations: Eq. (7.71)], $\mathbb{Q}$, or $\mathbb{Q}^2$ (multiplying the function by an exponential or Gaussian). Here we are exponentiating *second*-order differential operators of which only $\mathbb{P}^2$ has been seen before [in Eqs. (7.74)–(7.75)]. When substituted into (9.73), Eqs. (9.76) lead to

$$\exp(i\beta\mathbb{J}_2) = \mathbb{C}\begin{pmatrix} \exp(-\beta/2) & 0 \\ 0 & \exp(\beta/2) \end{pmatrix}, \tag{9.77a}$$

$$\exp(ib\mathbb{P}^2/2) = \mathbb{C}\begin{pmatrix} 1 & -b \\ 0 & 1 \end{pmatrix}, \tag{9.77b}$$

$$\exp(ic\mathbb{Q}^2/2) = \mathbb{C}\begin{pmatrix} 1 & 0 \\ c & 1 \end{pmatrix}, \tag{9.77c}$$

$$\exp(i\alpha\mathbb{J}_1) = \mathbb{C}\begin{pmatrix} \cosh(\alpha/2) & -\sinh(\alpha/2) \\ -\sinh(\alpha/2) & \cosh(\alpha/2) \end{pmatrix}, \tag{9.77d}$$

$$\exp(i\gamma\mathbb{J}_0) = \mathbb{C}\begin{pmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{pmatrix}. \tag{9.77e}$$

The matrix subindex of $\mathbb{C}_M$ has been written, for clarity, as $\mathbb{C}(\mathbf{M})$. If we allow complex parameters in the $SL(2,\mathscr{R})$ matrices, we can denote the resulting group by $SL(2,\mathscr{C})$: complex two-dimensional special (unimodular) linear transformations. We can now state that *linear canonical transforms are generated by all operators constructed out of quadratic expressions in* $\mathbb{Q}$ *and* $\mathbb{P}$. It is easy to see that (9.76) constitute bases for *all* second-order operators in $\mathbb{Q}$ and $\mathbb{P}$ and, only slightly less easy, that the one-parameter subgroups generated by (9.76) exhaust, by multiplication, all of $SL(2,\mathscr{R})$. [See (9.29), (9.33), or the "Euler angle" decomposition involving (9.77d) and (9.77e).] It does, however, require a good amount of mathematical finesse to fully condition and justify that the correspondence between hyperdifferential operators and integral transforms does hold over a continuous parameter range as suggested by our deceptively simple approach. Some of the aspects related to the domains of the hyperdifferential and integral forms of operators have been indicated at the end of Section 7.2. In dealing interchangeably with the two forms, we shall not encounter any major pitfalls and shall be able to simplify rather messy calculations to simple 2×2 matrix algebra. The results can always be verified by the more traditional methods.

We now have *three* sets of mathematical objects at our disposal: (a) integral transforms $\mathbb{C}(\mathbf{M})$, (b) hyperdifferential operators $\exp(i\tau\mathbb{H})$, and (c) 2×2 matrices $\mathbf{M}$. For every element in one there are corresponding elements in the other two, and this correspondence is preserved under composition, sum, and multiplication save for a possible sign in the com-

position of integral transforms. As we shall see, the key element for many applications is that all $b = 0$ "integral" transforms do not involve integration at all but are purely *geometric* transformations such as (9.23).

Exercise 9.22. Verify that the Fourier transform hyperdifferential form suggested in (7.197) holds as it belongs to the family (9.77e) for $\gamma = -\pi$. Show that $\mathbb{F}^2$ is the inversion operator (9.77a) times $\exp(i\pi/2)$ and $\mathbb{F}^4 = \mathbb{1}$.

Exercise 9.23. Verify that the square of the Bargmann transform is the inverse of the bilateral Laplace transform.

Exercise 9.24. Let $\mathbb{A}$ and $\mathbb{H}$ be operators. Prove the following relation:

$$\exp(\theta\mathbb{H})\mathbb{A}\exp(-\theta\mathbb{H}) = \sum_{n=0}^{\infty}\frac{\theta^n}{n!}[\mathbb{H},[\mathbb{H},\cdots[\mathbb{H},\underbrace{\mathbb{A}]\cdots]}_{n}]. \tag{9.78}$$

This can be seen for the first few powers of θ and then by induction on n.

Exercise 9.25. Use Eq. (9.78) in order to verify that the exponentiated second-order operators (9.77) indeed transform $\mathbb{Q}$ and $\mathbb{P}$ as in (9.38). The subgroups (9.77b) and (9.77c) lead to a terminating series. The series obtained from (9.77a) can be summed. The subgroups (9.77d) and (9.77e) require a recursion argument.

9.3.2. Baker–Campbell–Hausdorff Formulas

Consider the following matrix identity:

$$\begin{pmatrix}\cosh\theta & -\sinh\theta\\ -\sinh\theta & \cosh\theta\end{pmatrix} = \begin{pmatrix}1 & -\tanh\theta\\ 0 & 1\end{pmatrix}\begin{pmatrix}\operatorname{sech}\theta & 0\\ 0 & \cosh\theta\end{pmatrix}\begin{pmatrix}1 & 0\\ -\tanh\theta & 1\end{pmatrix}, \tag{9.79a}$$

i.e., a decomposition along the lines of (9.29). Using the correspondence (9.77) with hyperdifferential operators, we are led to

$$\begin{aligned}\exp[-i\theta\tfrac{1}{2}(d^2/dx^2 + x^2)] &= \exp(-i\tfrac{1}{2}\tanh\theta\, d^2/dx^2)\\ &\quad\times\exp[\tfrac{1}{2}\ln\cosh\theta\,(x\,d/dx + d/dx\cdot x)]\\ &\quad\times\exp(-i\tfrac{1}{2}\tanh\theta x^2).\end{aligned} \tag{9.79b}$$

This is a *Baker–Campbell–Hausdorff* relation between hyperdifferential operators. [See, for instance, Wilcox (1967) and Eriksen (1968).] By substituting the value $\theta = i\pi/4$ into (9.79), this becomes the Bargmann transform matrix [Eqs. (9.55)], as $\cosh(i\pi/4) = 2^{-1/2} = -i\sinh(i\pi/4)$. This implies that, acting on a function,

$$\begin{aligned}(\mathbb{C}_B\mathbf{f})(q) &= \exp[(\pi/8)(d^2/dq^2 + q^2)]f(q)\\ &= 2^{-1/4}\exp(\tfrac{1}{2}\,d^2/dq^2)[\exp(q^2/4)f(2^{-1/2}q)],\end{aligned} \tag{9.80}$$

i.e., reading from right to left, $f(q)$ is multiplied by $\exp(q^2/2)$, unitarily rescaled by a factor $2^{-1/2}$, and finally subjected to a unit Gauss–Weierstrass transform. This produces the Bargmann transform of the function.

Exercise 9.26. Verify that the three operations in (9.80) transform the harmonic oscillator wave functions $\Psi_n(q)$ in (7.166) into power functions. In particular, you will use the inverse of (7.193) in the last step. Conversely, this equation can be proven by (9.80).

Exercise 9.27. Use the decomposition (9.33)—the leftmost factor separated in two—to write another Baker–Campbell–Hausdorff formula for the first member of (9.79).

Exercise 9.28. Use the result of Exercise 9.27 to express the Bargmann transform as (a) multiplication by a decreasing Gaussian of unit width, (b) Fourier transformation, (c) multiplication by another Gaussian, and (d) change of scale.

Exercise 9.29. Find the Bargmann transform of the *repulsive* oscillator functions (7.203). You can either resort to a table of integrals or make use of the eigenfunction equation (7.198) together with the hyperdifferential expression for $\mathbb{C}_B$ in (9.80). You have thus found a new generalized basis for Bargmann space. [See Wolf (1977a).]

9.3.3. Time-Evolution Operators as Generating Canonical Transforms

The hyperdifferential operator realization for canonical transforms will serve us now to bring out the relation between the transform kernels and the Green's functions for a set of quantum-mechanical systems.

Consider partial differential equations of the form

$$\mathbb{H}\psi(q, t) = -i\frac{\partial}{\partial t}\psi(q, t), \tag{9.81}$$

where $\mathbb{H}$ is a differential operator in q only. This is the *diffusion* equation when $\mathbb{H}$ is $-2i\mathbb{H}^f$ as defined in (9.76b). It is Schrödinger's equation for the quantum free particle or the repulsive or the harmonic oscillator when $\mathbb{H}$ is $\mathbb{H}^f$, $\mathbb{H}^r$, or $\mathbb{H}^h$, respectively [Eqs. (9.76b), (9.76d), or (9.76e)—thence the superscript labeling]. The solution to (9.81) at time t can be expressed in terms of the initial or boundary data at time $t = 0$:

$$\psi(q, t) = \exp(it\mathbb{H})\psi(q, 0). \tag{9.82a}$$

This corresponds to a family of canonical transforms parametrized by t,

$$\psi(q, t) = \big(\mathbb{C}_{M(t)}\Psi(\cdot, 0)\big)(q) = \int_{\mathscr{R}} dq'\psi(q', 0)C_{M(t)}(q, q'), \tag{9.82b}$$

where $\mathbf{M}(t)$ is the one-parameter matrix subgroup associated to the generator

$\mathbb{H}$. The canonical transform $\mathbb{C}_{M(t)}$ is the *time-evolution or Green's operator* for the system governed by (9.81). If the initial $\psi(q, 0)$ is a Dirac δ sitting at q' [i.e., $\delta_{q'}(q) \coloneqq \delta(q - q')$], then clearly the solution to (9.82) is

$$G_{q'}(q, t) \coloneqq (\mathbb{C}_{M(t)}\delta_{q'})(q) = C_{M(t)}(q, q'), \tag{9.83}$$

which is the Green's function for the system.

Exercise 9.30. Verify independently that (9.83) is the Green's function of (9.81) for the five one-parameter subgroups $\mathbf{M}(t)$ which we have been handling, since (a) Eqs. (9.75) show that it is a solution to the differential equation, and (b) it is such that $G_{q'}(q, 0) = \delta(q - q')$.

The economy of using matrices to represent canonical transforms is readily apparent when the initial conditions are themselves given as integral transforms. Consider the time development of a real Gaussian wave function, of width ω centered at q' and normalized to unity, under a quantum harmonic oscillator potential, i.e.,

$$\begin{aligned}\psi(q, 0) = G_\omega(q - q') &= \left[\mathbb{C}\begin{pmatrix}1 & \exp(-i\pi/2)\omega \\ 0 & 1\end{pmatrix}\delta_{q'}\right](q) \\ &= (2\pi\omega)^{-1/2}\exp[-(q - q')^2/2\omega].\end{aligned} \tag{9.84}$$

The time evolution is given by the $\mathbf{M}^h(t)$ subgroup of transforms (9.75e)–(9.76e)–(9.77e):

$$\begin{aligned}\psi(q, t) &= \left[\mathbb{C}\begin{pmatrix}\cos t & -\sin t \\ \sin t & \cos t\end{pmatrix}\psi(\cdot, 0)\right](q) \\ &= \left[\mathbb{C}\begin{pmatrix}\cos t & -\sin t \\ \sin t & \cos t\end{pmatrix}\mathbb{C}\begin{pmatrix}1 & -i\omega \\ 0 & 1\end{pmatrix}\delta_{q'}\right](q) \\ &= \left[\mathbb{C}\begin{pmatrix}\cos t & -\sin t - i\omega\cos t \\ \sin t & \cos t - i\omega\sin t\end{pmatrix}\delta_{q'}\right](q).\end{aligned} \tag{9.85}$$

The result is thus a C_M function which can be written by substituting the entries of the last matrix into (9.8). No integration is needed. In Figs. 9.3, 9.4, and 9.5 is the time development of a Gaussian wave function under free, repulsive, and harmonic oscillator potentials. The diffusion equation Green's function is obtained from that of the free-particle Schrödinger case by the simple replacement $t \to 2it$.

Exercise 9.31. Note that the solution (9.85) is periodic with period 2π. This is to be expected, as, classically, the oscillation period of a harmonic oscillator is independent of its energy, and thus the wave function returns to its original shape after that time. At half that period, show that the wave function is inverted. At one-quarter the period, you have the inverse Fourier transform of the initial wave function. See Fig. 9.5.

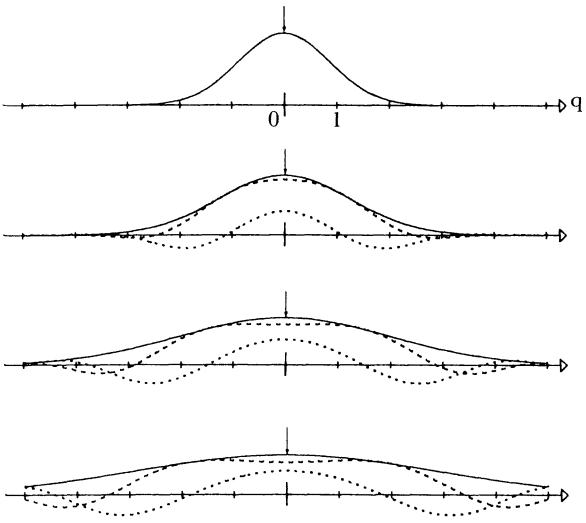


Fig. 9.3. Time development of a Gaussian wave function (of width 0.75, centered at the origin) under the free-particle Schrödinger equation. Real, imaginary, and absolute values are plotted in heavy dotted, light dotted, and continuous lines. The time intervals between two graphs are $\pi/4$. The small arrows indicate the (fixed) peak of the broadening, complex Gaussian.

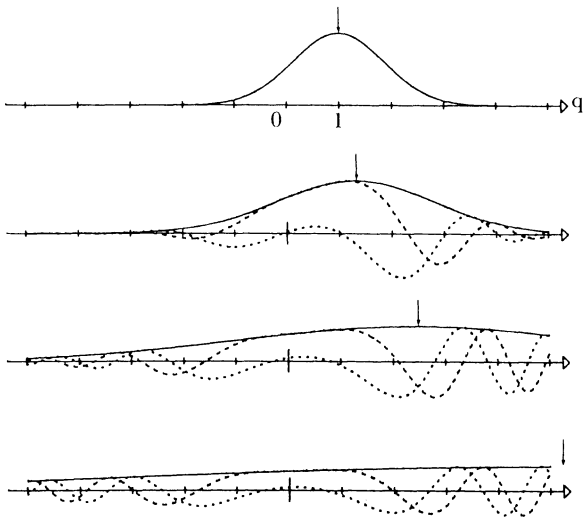


Fig. 9.4. Time development of a Gaussian wave function (of width 0.75, centered at $q = 1$) under the repulsive oscillator Schrödinger equation. Plot marks and parameters are as in Figure 9.3. The peak of the spreading Gaussian moves as a classical particle would under the same potential.

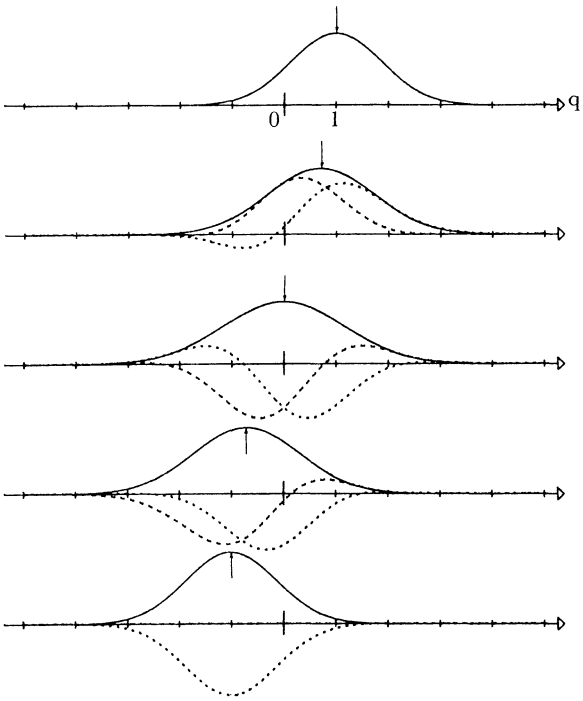


Fig. 9.5. Time development of a Gaussian wave function under the harmonic oscillator Schrödinger equation (9.85). Figure characteristics are as in Fig. 9.4. Here, the Gaussian peak performs the harmonic motion characteristic of coherent states.

9.3.4. Quantum Normal Modes

Wave functions generally lose their original shape under the influence of a quantum potential. One set of functions which *do* preserve their form, remindful of the normal modes of the elastic media, is the *eigenfunctions* of $\mathbb{H}$. If $\Psi_\lambda(q)$ is an eigenfunction of $\mathbb{H}$ with eigenvalue λ, then for $\mathbf{M}(t)$ generated by $\mathbb{H}$,

$$\Psi_\lambda(q, t) \coloneqq \int_{\mathscr{R}} dq' \Psi_\lambda(q') C_{M(t)}(q, q') = \exp(it\mathbb{H})\Psi_\lambda(q) = \exp(it\lambda)\Psi_\lambda(q), \tag{9.86}$$

i.e., it is *self-reproducing* under all $\mathbb{C}_{M(t)}$ and a *separated* function of q and t. Detailing: as the operators which we are interested in are $\mathbb{H}^l$, $\mathbb{H}^r$, and $\mathbb{H}^h$, for the purposes of notational uniformity we shall denote their eigenfunctions by

$\Psi^{\omega}_{\lambda,\sigma}(q)$, $\omega = f, r, h$, with an extra label σ to resolve degeneracy when necessary. These are

$$\mathbb{H}^f: \quad \Psi^f_{\lambda,\sigma}(q) = (2\pi)^{-1/2} \exp[i\sigma(2\lambda)^{1/2}q], \quad \lambda \in \mathscr{R}^+, \sigma = \pm, \tag{9.87a}$$

$$\mathbb{H}^r: \quad \Psi^r_{\lambda,\sigma}(q) = \chi_\lambda{}^\sigma(q), \quad \lambda \in \mathscr{R}, \sigma = \pm \text{ [Eqs. (7.203)]}, \tag{9.87b}$$

$$\mathbb{H}^h: \quad \Psi^h_\lambda(q) = \Psi_n(q), \quad \lambda = n + 1/2, n = 0, 1, 2, \ldots \text{ [Eq. (7.166)]}. \tag{9.87c}$$

Ordinary or Dirac orthonormality and completeness hold for these functions. Hence, multiplying (9.86) by $\Psi_\lambda(q'')^*$ and summing or integrating, as the case may be, over the label set (λ, σ), from the second and last members we obtain

$$C_{M^{\omega}(t)}(q, q'') = \mathop{\S}_{\lambda,\sigma} \exp(it\lambda)\Psi^{\omega}_{\lambda,\sigma}(q)\Psi^{\omega}_{\lambda,\sigma}(q'')^*, \tag{9.88}$$

where the symbol $\S$ is meant to stand appropriately for integration or sum in each case. It becomes

$$\sum_{\sigma=\pm} \int_0^\infty (2\lambda)^{-1/2}\, d\lambda \quad (f \text{ case}), \qquad \sum_{\sigma=\pm} \int_{-\infty}^{\infty} d\lambda \quad (r \text{ case}),$$

$$\sum_{\substack{n=0 \\ \lambda = n+1/2}}^{\infty} \quad (h \text{ case}).$$

Equation (9.88) reduces, in the harmonic oscillator case, to (7.180d) for $t = 0$ and (9.61) for $t = \pi/2$. For the free-particle case, $t = 0$ reproduces the known integral representation of the Dirac δ [Eq. (7.93) for $n = 0$], and similarly for the repulsive oscillator case. The transform kernel is shown by (9.88) to generalize the above completeness relations.

Exercise 9.32. Show that the general $\mathbb{C}_M$ transforms of the harmonic oscillator wave functions are

$$(\mathbb{C}_M\Psi_n)(q) = \left[\left(2\frac{a+ib}{a-ib}\right)^n n!\pi^{1/2}(a+ib)\right]^{-1/2} \exp\left(-\frac{d-icq^2}{a+ib}\frac{2}{2}\right) \times H_n((a^2+b^2)^{-1/2}q). \tag{9.89}$$

Verify the result for Fourier and Bargmann transforms. In the latter case, as $a^2 + b^2 = 0$, it turns out that only the polynomial leading term (of coefficient 2^n) survives. Show that (9.89) is defined for almost all complex M. Equation (9.89) can be proven (a) by straightforward integration, (b) by (9.49) and the appropriate raising operators, or, best, (c) by decomposing $\mathbf{M}$ as $\mathbf{M}^g\mathbf{M}^d\mathbf{M}^h$ [Eqs. (9.75c), (9.75a), and (9.75e)] and noting that under the rightmost factor $\Psi_n(q)$ is only multiplied by a phase.

9.3.5. Coherent States and Their Time Evolution

Another set of states which preserve their shape while under the action of a quantum potential is termed *coherent states* and is particularly important for the harmonic oscillator case. Coherent states $\Upsilon_c(q)$ were defined in (7.188) either as the result of acting with the exponentiated oscillator raising operator on the ground state $\Psi_0{}^h(q)$ or as eigenfunctions of the oscillator lowering operator. They are essentially displaced Gaussian of unit width and centered at $2^{1/2}c$, which reappeared briefly in (9.66), where we noted that they happen to be basically Bargmann's transform kernel (9.55b). They are

$$\begin{aligned}\Upsilon_c(q) &= \pi^{-1/4}\exp(c^2/2)\exp[-(q-2^{1/2}c)^2/2] = (2\pi)^{-1/4}C_B(q,c)\\ &= (2\pi)^{-1/4}\left[\mathbb{C}\begin{pmatrix}2^{-1/2} & -i2^{-1/2}\\ -i2^{-1/2} & 2^{-1/2}\end{pmatrix}\boldsymbol{\delta}_c\right](q).\end{aligned} \tag{9.90}$$

The time evolution of the coherent states (9.90) under the harmonic oscillator potential is thus

$$\begin{aligned}\Upsilon_c(q,t) &= (2\pi)^{-1/4}\left[\mathbb{C}\begin{pmatrix}\cos t & -\sin t\\ \sin t & \cos t\end{pmatrix}\mathbb{C}\begin{pmatrix}2^{-1/2} & -i2^{-1/2}\\ -i2^{-1/2} & 2^{-1/2}\end{pmatrix}\boldsymbol{\delta}_c\right](q)\\ &= (2\pi)^{-1/4}\left[\mathbb{C}\begin{pmatrix}2^{-1/2}e^{it} & -2^{-1/2}ie^{-it}\\ -2^{-1/2}ie^{it} & 2^{-1/2}e^{-it}\end{pmatrix}\boldsymbol{\delta}_c\right](q)\\ &= (2\pi)^{-1/4}\left[\mathbb{C}\begin{pmatrix}2^{-1/2} & -i2^{-1/2}\\ -i2^{-1/2} & 2^{-1/2}\end{pmatrix}\mathbb{C}\begin{pmatrix}e^{it} & 0\\ 0 & e^{-it}\end{pmatrix}\boldsymbol{\delta}_c\right](q)\\ &= \exp(it/2)\Upsilon_{c'(t)}(q), \qquad c'(t) := c\exp(it).\end{aligned} \tag{9.91}$$

The key step has been to write the matrix product $\mathbf{M}^h(t)\mathbf{B}$ as $\mathbf{B}\mathbf{M}^d(-it)$. The last matrix denotes a *dilatation* canonical transform (9.26) which changes $\delta(q-c)$ into $\exp(it/2)\delta(q-e^{it}c)$. The subsequent $\mathbb{C}_B$ transform completes the result. The absolute value of $\Upsilon_{c'(t)}(q)$ is thus a Gaussian of unit width with an oscillating center at $2^{1/2}c\cos t$ representing the motion of a classical point particle moving with harmonic motion under an oscillator potential. As we saw in Section 7.6, coherent states exhibit the minimum dispersion product compatible with Heisenberg's uncertainty relation. Coherent states thus qualify as the *closest* quantum analogue of classical point particles under a harmonic oscillator potential.

Coherent states for Hamiltonians $\mathbb{H}$ other than the harmonic oscillator are of some interest. Our procedure in Eq. (9.91) suggests their definition and calculation. Let $\mathbb{H}$ generate the time-evolution operator $\mathbb{C}_{M(t)}$, and let $\mathbf{A}$ *diagonalize* the matrix subgroup $\mathbf{M}(t)$; then, as $\mathbf{M}(t)\mathbf{A} = \mathbf{A}\mathbf{M}^d(f(t))$, $f(t)$ being some function of t, $\Upsilon_c(q) := (\mathbb{C}_A\boldsymbol{\delta}_c)(q)$ qualifies as a generalized coherent state for $\mathbb{H}$. Its time evolution will be given, following (9.91), by $\varphi\Upsilon_{c'(t)}(q)$, where $c'(t) = cf(t)$ is the "classical" motion of the wave packet and $\varphi = [f(t)]^{1/2}$.

Exercise 9.33. Implement this definition and calculation for the repulsive oscillator (9.76d)–(9.77d). Show that the diagonalizing matrix **A** is given by (9.35) and that $f(t) = \exp t$, which is the classical motion of a particle pushed away by a repulsive oscillator. Unfortunately these repulsive coherent states are oscillating Gaussians, and their absolute values do not peak. The free-particle Hamiltonian generates a triangular-matrix time-evolution operator. This is not diagonalizable, and hence this potential does not possess coherent states.

The coherent-state construction can be carried further for potentials involving "centrifugal" barriers ($\sim q^{-2}$). Thus Barut and Girardello (1971) built eigenfunctions of the second-order lowering operator $\mathbb{J}_-$, the analogue of (7.174c) in more than one dimension. This can also be obtained by a hyperdifferential operator calculus involving $\mathbb{Q}^{-2}$ (Wolf, 1974b). Not surprisingly, the Barut–Girardello coherent states are the precise analogues of (9.90).

10

Applications to the Study of Differential Equations

Canonical transforms, besides generalizing the Fourier and Bargmann integral transforms, provide a fine tool for the analysis of a class of differential equations. The class consists of up-to-second-order differential operators of *parabolic* type. These include the diffusion, the Schrödinger free-particle, the linear potential (free-fall), and the attractive and repulsive oscillator equations. It also includes a few others such as the Fokker–Planck equation. Although this class is far from universal, the ease with which solutions and properties are found makes canonical transforms an attractive tool for problems such as these. In Section 10.1 we start with the introduction of *inhomogeneous* linear canonical transformations and apply the machinery to a deeper study of the diffusion equation: how to find families of solutions out of a known solution (the action of the *similarity group* of the equation) and the question of *separating coordinates*, which brings us to generalized normal modes. In Section 10.2 the analysis is applied to a general member of the differential equation class. We show that all computations reduce to, essentially, 2×2 matrix algebra. This is in the true spirit of group theory.

10.1. The Diffusion Equation: Similarity Group and Separating Coordinates

We shall consider here the set of all up-to-second-order operators in $\mathbb{Q}$ and $\mathbb{P}$,

$$\mathbb{H} = A\mathbb{P}^2 + B(\mathbb{Q}\mathbb{P} + \mathbb{P}\mathbb{Q}) + C\mathbb{Q}^2 + D\mathbb{Q} + E\mathbb{P} + F\mathbb{1}, \qquad A, B, \ldots, F \in \mathscr{C}, \quad (10.1)$$

and shall introduce *inhomogeneous* canonical transforms, i.e., the group of canonical transforms of Chapter 9 plus translations and multiplications by $c \exp(\alpha q)$. Operators (10.1) appear in a class of *parabolic* differential equations

$$\mathbb{H}f(q, t) = -i \frac{\partial}{\partial t} f(q, t), \tag{10.2}$$

for which we can find "normal modes" and separating variables. We shall show that the mathematical techniques we have developed reduce all the needed computations to essentially 2×2 matrix algebra. In this section we shall apply all developments to the *diffusion equation*, where $\mathbb{H}$ in (10.1) is simply $-i\,\partial^2/\partial q^2 = i\mathbb{P}^2$. The slight complication of having complex parameters will be more than offset by the readily interpretable results. Section 10.2 will show how the general case is to be handled.

10.1.1. Heisenberg–Weyl Transformations

The added generality of (10.1)–(10.2) over the corresponding equations we considered in Chapter 9 [Eqs. (9.76) and (9.81)] consists of allowing for terms linear in $\mathbb{Q}$, $\mathbb{P}$, and $\mathbb{1}$. To implement the ideas of Chapter 9 for this enlarged set, we must examine their exponentiated action on functions and operators. Most of this has been done in Chapter 7, where we saw that $\mathbb{P}$ generates *translations* of the space [Eqs. (7.27) and (7.69)], $\mathbb{Q}$ generates multiplication of the function by an exponential [Eq. (7.70)], and $F\mathbb{1}$, quite simply, multiplies the function by a constant. From these we can define the $\mathbb{W}$ *transform* operators

$$\begin{aligned} \mathbb{W}(x, y, z) &\coloneqq \exp[i(x\mathbb{Q} + y\mathbb{P} + z\mathbb{1})] \\ &= \exp[i(z + xy/2)] \exp(ix\mathbb{Q}) \exp(iy\mathbb{P}) \\ &= \exp[i(z - xy/2)] \exp(iy\mathbb{P}) \exp(ix\mathbb{Q}), \qquad x, y, z \in \mathscr{R}. \end{aligned} \tag{10.3a}$$

The equality between the last two expressions can be proven by applying the operators to any analytic function $f(q)$, obtaining in both cases

$$(\mathbb{W}(x, y, z)\mathbf{f})(q) = \exp[i(xq + xy/2 + z)]f(q + y) \tag{10.3b}$$

[recall the Weyl commutation relation (7.33)]. The equality with the first form of $\mathbb{W}$ takes slightly longer to verify (see Exercise 10.1). Moreover, the set of all operators (10.3) for $x, y, z \in \mathscr{R}$ gives rise to a *group* of transformations, which we shall denote by W. (a) The *composition* of two elements of the set (10.3) is a new operator which is again a member of the set. Indeed,

$$\begin{aligned} &\mathbb{W}(x_2, y_2, z_2)\mathbb{W}(x_1, y_1, z_1) \\ &\quad = \mathbb{W}(x_2 + x_1, y_2 + y_1, z_2 + z_1 + (y_2x_1 - x_2y_1)/2), \end{aligned} \tag{10.4}$$

as can easily be verified by acting with both members on any $f(q)$ and using (10.3b). Equation (10.4) shows that the product of two $\mathbb{W}$ transforms is a $\mathbb{W}$ transform. (b) *Associativity* obviously holds. (c) The identity of the group is $\mathbb{W}(0, 0, 0) = \mathbb{1}$. (d) $[\mathbb{W}(x, y, z)]^{-1} = \mathbb{W}(-x, -y, -z)$, as can be verified from (10.4).

Exercise 10.1. Show that the first equality in (10.3a) holds. This can be seen if we develop both members in series and compare coefficients of like powers of x, y, and z inductively.

A simpler proof is obtained if you use (9.38) in order to write the identity

$$\mathbb{C}_M \exp(i\mathbb{P})\mathbb{C}_M^{-1} = \exp[i(x\mathbb{Q} + y\mathbb{P})] \qquad \text{for } \mathbf{M} = \begin{pmatrix} y & 0 \\ -x & y^{-1} \end{pmatrix} \tag{10.5}$$

and then use (9.23), (7.27), and (7.69). The action of (10.5) on any $f(q)$ is given by (10.3b) for $z = 0$. [The parameter z is rather trivial to extract from the Baker–Campbell–Hausdorff relation in (10.3a) as $\mathbb{1}$ commutes with $\mathbb{Q}$ and $\mathbb{P}$.]

Exercise 10.2. Show that for x, y, and z *real* the set of $\mathbb{W}$ transforms is a group of *unitary* mappings of $\mathscr{L}^2(\mathscr{R})$ onto itself. Further description of the *Heisenberg–Weyl* group (10.3b) can be found in Wolf and García (1972) [see also Wolf (1975)].

10.1.2. Inhomogeneous Linear Transformations

The action of the elements of the Heisenberg–Weyl group W on *operators* can be ascertained to be

$$\begin{aligned} \mathbb{W}(D\mathbb{Q} + E\mathbb{P})\mathbb{W}^{-1} &= D\mathbb{W}\mathbb{Q}\mathbb{W}^{-1} + E\mathbb{W}\mathbb{P}\mathbb{W}^{-1} \\ &= D(\mathbb{Q} + y\mathbb{1}) + E(\mathbb{P} - x\mathbb{1}) \\ &= D\mathbb{Q} + E\mathbb{P} + (Dy - Ex)\mathbb{1}. \end{aligned} \tag{10.6}$$

The proof can rely on letting the members act on $\mathscr{C}^\infty$ functions $f(q)$ as with (10.3b) or can use only the linear operators $\mathbb{Q}$ and $\mathbb{P}$ and their properties: (a) linearity; (b) the commutator of $\mathbb{Q}$ and $\mathbb{P}$ is $i\mathbb{1}$ [Eq. (7.59b)]; (c) the set of operators $\mathscr{S}_1 := \{D\mathbb{Q} + E\mathbb{P} + F\mathbb{1};\ D, E, F \in \mathscr{C}\}$ closes on itself under commutation (hence forms a *Lie algebra*) and when exponentiated, generates the group W; (d) the formula (9.78). The group of transformations (10.3) thus acts on the set $\mathscr{S}_1$ as if it were a three-dimensional space with Cartesian coordinates D, E, F, although, note, the parameter z in (10.3) does not appear in (10.6). This three-dimensional space of operators $\mathscr{S}_1$ is thus acted upon by W in addition to being acted upon by the group $SL(2, \mathscr{R})$ of linear canonical transforms which occupied Chapter 9 [Eqs. (9.1)]. The two

groups can then be composed [as a *semidirect product* of $SL(2, \mathscr{R})$ and W] and the elements of the product denoted by

$$\mathbb{I}\{\mathbf{M}, \xi, z\} = \mathbb{I}\left\{\begin{pmatrix} a & b \\ c & d \end{pmatrix}, (x, y, z)\right\} \coloneqq \mathbb{C}\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot \mathbb{W}(x, y, z), \quad (10.7a)$$

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad ad - bc = 1, \qquad \xi \coloneqq (x, y). \quad (10.7b)$$

The set I of transformations (10.7) also forms a group. (a) The product of two of its elements is again an element of the set:

$$\begin{aligned} \mathbb{I}\{\mathbf{M}_2, \xi_2, z_2\} \cdot \mathbb{I}\{\mathbf{M}_1, \xi_1, z_1\} &= \mathbb{C}(\mathbf{M}_2)\mathbb{W}(\xi_2, z_2)\mathbb{C}(\mathbf{M}_1)\mathbb{W}(\xi_1, z_1) \\ &= \mathbb{C}(\mathbf{M}_2)\mathbb{C}(\mathbf{M}_1)\mathbb{C}(\mathbf{M}_1^{-1})\mathbb{W}(\xi_2, z_2)\mathbb{C}(\mathbf{M}_1^{-1})^{-1}\mathbb{W}(\xi_1, z_1) \\ &= \mathbb{C}(\mathbf{M}_2\mathbf{M}_1)\mathbb{W}(\xi_2\mathbf{M}_1, z_2)\mathbb{W}(\xi_1, z_1) \\ &= \mathbb{I}\{\mathbf{M}_2\mathbf{M}_1, \xi_2\mathbf{M}_1 + \xi_1, z_2 + z_1 + \tfrac{1}{2}\xi_2\mathbf{M}_1\Omega\xi_1^T\}, \end{aligned}$$

$$\Omega \coloneqq \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (10.8)$$

The statement is proven in the next to last member. The last equality is again the definition (10.7) written so as to bring out the fact that the product of elements of W in (10.4) can be abbreviated using vector notation: ξ as in (10.7b) and ξ^T as the column vector transpose to ξ. (b) Associativity holds for I as it does for its constituents. (c) The *unit* element for the set is $\mathbb{I}\{\mathbf{1}, \mathbf{0}, 0\}$. (d) The *inverse* of any operator (10.7) is $\mathbb{I}\{\mathbf{M}, \xi, z\}^{-1} = \mathbb{I}\{\mathbf{M}^{-1}, -\xi\mathbf{M}^{-1}, -z\}$, as can easily be verified from (10.8). We shall call I the group of *inhomogeneous linear transformations*.

It can be verified that the subset of I consisting of the $SL(2, \mathscr{R})$ operators $\mathbb{I}\{\mathbf{M}, \mathbf{0}, 0\}$ forms a proper subgroup $SL(2, \mathscr{R}) \subset I$, as does the subset $\mathbb{I}\{\mathbf{1}, x, y, z\}$, which gives $W \subset I$. An important one-parameter subgroup which is not totally contained in $SL(2, \mathscr{R})$ or in W is the following set of operators:

$$\mathbb{I}\left\{\begin{pmatrix} 1 & -\tau \\ 0 & 1 \end{pmatrix}, (\tau, -\tau^2/2, -\tau^3/12)\right\} = \exp[i\tau(\tfrac{1}{2}\mathbb{P}^2 + \mathbb{Q})], \quad (10.9)$$

where the equality still has to be proven.

Exercise 10.3. Show that the elements of I of the form (10.9) do constitute a one-parameter subgroup. If τ_1 and τ_2 are the values of the parameters, their composition will be of the same form with $\tau_1 + \tau_2$. Try disentangling the operator exponential in (10.9) into two such operators following (10.7).

Applying the left-hand side of (10.9) on a function $f(q)$ [as prescribed by (10.7), (10.3b), and the canonical transform (9.5)–(9.8), with $-\tau = \exp(-i\pi)\tau$], we find it is an integral transform with a kernel

$$C_l(q, q') := \exp(3i\pi/4)(2\pi\tau)^{-1/2} \exp\{-i[(q - q')^2/2\tau - (q + q')\tau/2 - \tau^3/24]\}. \tag{10.10}$$

An argument parallel to (9.75) now shows that the one-parameter set (10.9) is indeed generated by the operator $\mathbb{H}^e := \frac{1}{2}\mathbb{P}^2 + \mathbb{Q}$. It is the *linear potential* (free-fall) Schrödinger Hamiltonian, and Eq. (10.10) is the system's Green's function. The eigenfunctions of this operator and its spectrum have been studied in (8.87)–(8.89). Figure 10.1 is a plot of the time evolution of Gaussian initial conditions under the equation (10.2) with $\mathbb{H}^l$ and various values of τ, in analogy to the evolution under $\mathbb{H}^f$, $\mathbb{H}^r$, and $\mathbb{H}^h$ (Figs. 9.3–9.5) with a similar physical interpretation. This *quartet* of operators $\mathbb{H}^\omega$, $\omega = f, r, h, l$, will be quite useful in what follows. In Section 10.2 we shall show that these four are, in fact, *all* the operators we need to consider in connection with the second-order parabolic differential equations (10.1)–(10.2).

10.1.3. Diffusion and Transformation of Initial Conditions

We have assembled most of the mathematical tools we need in order to present the main application in this chapter. The remaining pieces will be

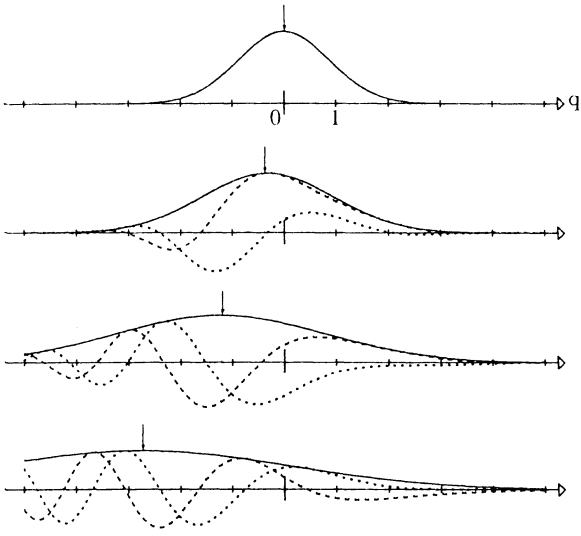


Fig. 10.1. Time development of a Gaussian wave function under the free-fall Schrödinger equation [drawn in the same manner as Figs. 9.3–9.5, following Eq. (9.85) for the evolution operator (10.9)]. The peak of the Gaussian "falls" as a classical particle would.

developed and put in place as we proceed to apply our enlarged set of transforms to answer the following question: Let $f(q)$ be, say, the initial temperature distribution of a thin rod which diffuses in time as $f(q, t)$ subject to

$$\frac{\partial^2}{\partial q^2} f(q, t) = \frac{\partial}{\partial t} f(q, t), \qquad f(q, 0) =: f(q). \tag{10.11}$$

What will be the time development of an *I-transformed* initial condition $(\mathbb{I}\{g\}\mathbf{f})(q)$, where $g = \{\mathbf{M}, \xi, z\} \in I$? The answer turns out to be remarkably simple. As the time development under the diffusion equation is a Gauss–Weierstrass transform (9.67), it follows from (9.81)–(9.82) that

$$f(q, t) = \left[\mathbb{I}\left\{\begin{pmatrix} 1 & -2it \\ 0 & 1 \end{pmatrix}, (0, 0, 0)\right\}\mathbf{f}\right](q) =: (\mathbb{I}_{H(t)}\mathbf{f})(q). \tag{10.12}$$

The $\mathbb{I}\{g\}$-transformed initial conditions thus give rise to the following temperature distribution:

$$\begin{aligned} f_g(q, t) &:= [\mathbb{I}_{H(t)}\mathbb{I}\{g\}\mathbf{f}](q) \\ &= \left[\mathbb{I}\left\{\begin{pmatrix} 1 & -2it \\ 0 & 1 \end{pmatrix}, (0, 0, 0)\right\}\mathbb{I}\left\{\begin{pmatrix} a & b \\ c & d \end{pmatrix}, (x, y, z)\right\}\mathbf{f}\right](q) \\ &= \left[\mathbb{I}\left\{\begin{pmatrix} a - 2ict & b - 2idt \\ c & d \end{pmatrix}, (x, y, z)\right\}\mathbf{f}\right](q) \\ &= \left[\mathbb{I}\left\{\begin{pmatrix} a - 2ict & 0 \\ c & (a - 2ict)^{-1} \end{pmatrix}, (x, y + 2it_g x, z)\right\}\right. \\ &\quad \left. \times\, \mathbb{I}\left\{\begin{pmatrix} 1 & -2it_g \\ 0 & 1 \end{pmatrix}, (0, 0, 0)\right\}\mathbf{f}\right](q). \end{aligned} \tag{10.13}$$

We have used the fact that both the time-development operator $\mathbb{I}_{H(t)}$ and the applied transformation $\mathbb{I}\{g\}$ are elements of the same transformation group I. This allowed us to compose the two by (10.8) and *decompose* the product in such a way that the time-development operator $\mathbb{I}_{H(t_g)}$ acts first but with a *transformed time variable*:

$$t_g = (dt + ib/2)/(a - 2ict). \tag{10.14}$$

This expression follows from ordinary matrix algebra on the two group elements in the last member according to (10.8). Now $\mathbb{I}_{H(t_g)}$ acting on $f(q)$ will produce a function $f(q, t_g)$ that is identical to (10.11) except for having t_g in place of t. The left-most factor in the last member of (10.13) is a special kind of I transform: as the 1-2 element is zero, it is not an integral transform at all but, from (10.3b) and (9.23), only a *geometric transform*:

$$\left[\mathbb{I}\left\{\begin{pmatrix} a & 0 \\ c & a^{-1} \end{pmatrix}, (x, y, z)\right\}\mathbf{f}\right](q) = a^{-1/2} \exp[i(cq^2/2a + xq/a + xy/2 + z)] \times f(q/a + y). \tag{10.15}$$

The geometric transform of a function, we see, involves displacement and change of scale of the argument and multiplication of the function by a Gaussian, an exponential, and a constant factor. Due to the fact that $\mathbb{I}_{H(t)}$ in (10.12) involves an imaginary entry, complex numbers have appeared in (10.13) and (10.14). As the temperature is supposed to be a *real* function of *real* space q and time t, we can redefine for convenience the following group parameters:

$$\beta := ib/2, \qquad \gamma := -2ic, \qquad \xi := -2ix, \qquad \zeta = -iz. \tag{10.16}$$

Writing the entries in (10.13) and (10.14) in terms of these and using the result (10.15), we find that $(\mathbb{I}\{g\}\mathbf{f})(q)$ has developed under diffusion as

$$f_g(q, t) = \mu_g(q, t) f(q_g, t_g), \tag{10.17a}$$

where space q and time t have been transformed to

$$q_g = [q - \xi(\beta + dt)]/(a + \gamma t) + y = q/(a + \gamma t) - \xi t_g + y, \tag{10.17b}$$

$$t_g = (\beta + dt)/(a + \gamma t), \tag{10.17c}$$

and the function f has been factored by a *multiplier* function μ_g with the structure

$$\mu_g(q, t) = C_g(a + \gamma t)^{-1/2} \exp[S(q, t)], \tag{10.17d}$$

$$C_g := \exp[-(\xi y/4 + \zeta)], \tag{10.17e}$$

$$S(q, t) = [-\gamma q^2 - 2\xi q + \xi^2(\beta + dt)]/4(a + \gamma t). \tag{10.17f}$$

Exercise 10.4. Verify these results in all detail.

10.1.4. Manifest and "Hidden" Symmetries of the Diffusion Equation

Our construction guarantees that if $f(q, t)$ is a solution to the heat equation, then $f_g(q, t)$ will also be for all values of the six free parameters a, β, γ, ξ, y, and ζ. The physical meaning of each of these parameters will be brought out now by considering the one-parameter groups.

(a) $g = \{\mathbf{1}, \mathbf{0}, i\zeta\}$: *multiplication by a constant factor.*

$$f_g(q, t) = \exp(-\zeta) f(q, t). \tag{10.18}$$

As the heat equation is *linear*, if $f(q, t)$ is a solution, any multiple of this function will be a solution as well.

(b) $g = \{\mathbf{1}, (0, y), 0\}$: *space translation* [Fig. 10.2(A)].

$$f_g(q, t) = f(q + y, t). \tag{10.19}$$

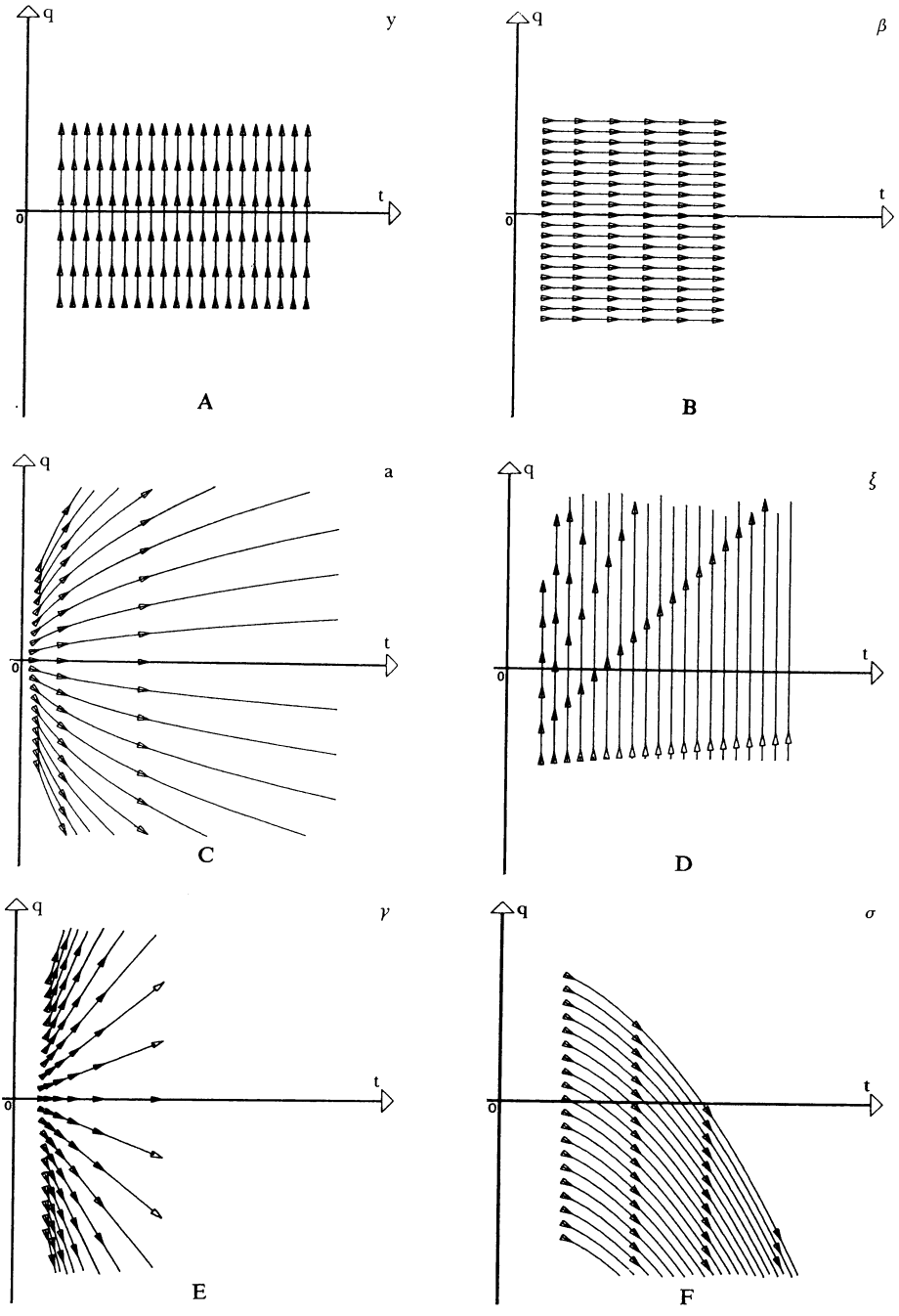


Fig. 10.2 (*see next page for legend*).

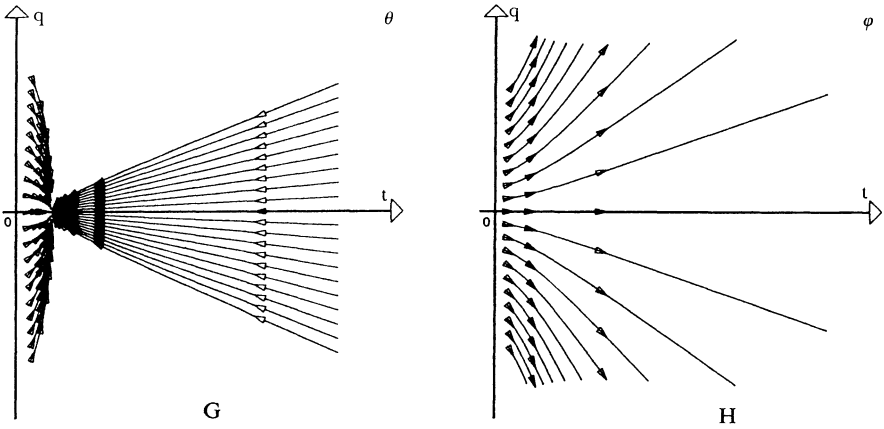


Fig. 10.2. Space and time transformation under various one-parameter subgroups of I, the similarity group of the diffusion equation. On opposite page: (A) space translation, (B) time translation, (C) scale change, (D) Galilean transformation, (E) projective transformation, (F) "linear" transformation. Above: (G) elliptic subgroup, (H) hyperbolic subgroup. Arrowheads are placed at equal intervals of the relevant parameters $\gamma, \beta, a, \ldots$.

The heat equation (10.11) involves only derivatives with respect to q, thus describing a *homogeneous* medium: one where the medium properties are invariant under translation.

(c) $g = \left\{ \begin{pmatrix} 1 & -2i\beta \\ 0 & 1 \end{pmatrix}, \mathbf{0}, 0 \right\}$: *time translation* [Fig. 10.2(B)],

$$f_g(q, t) = f(q, t + \beta) \tag{10.20}$$

is due to the invariance of (10.11) under time translations. [Actually, we must restrict $\beta \geqslant 0$, as we shall see below.]

(d) $g = \left\{ \begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix}, \mathbf{0}, 0 \right\}$: *scale change* [Fig. 10.2(C)],

$$f_g(q, t) = a^{-1/2} f(q/a, t/a^2), \tag{10.21}$$

which states basically that a change of space scale by a must be accompanied by a corresponding change of time scale by a^2.

The four transformations (10.18)–(10.21) have their origin in corresponding symmetries of the heat equation (10.11) which are "inspectionally"

obvious. Our general development, however, points out *two more* transformation symmetries of the diffusion equation.

(e) $g = \{\mathbf{1}, (i\xi/2, 0), 0\}$: *Galilean transformations* [Fig. 10.2(D)].

$$f_g(q, t) = \exp[-\xi(q - \xi t)/2 - \xi^2 t/4] f(q - \xi t, t). \tag{10.22}$$

This transformation is called "Galilean" as it relates the temperature distribution in a fixed rod $f(q, t)$ to that of a rod *moving* with velocity ξ. For f_g to be a solution, f needs to be corrected by a multiplier function (10.17a)–(10.17d)–(10.17f). Figure 10.2(D) only shows the space–time transformation.

(f) $g = \left\{\begin{pmatrix} 1 & 0 \\ i\gamma/2 & 1 \end{pmatrix}, \mathbf{0}, 0\right\}$: *projective transformations* [Fig. 10.2(E)].

$$f_g(q, t) = (1 + \gamma t)^{-1/2} \exp[-\gamma q^2/4(1 + \gamma t)] f\big(q/(1 + \gamma t), t/(1 + \gamma t)\big). \tag{10.23}$$

These transformations deform the (q, t)-space in such a way that the q/t-constant lines are mapped onto themselves [see Fig. 10.2(E)].

The set of all transformations (10.17)–(10.23) constitutes the *similarity group* of the heat equation (10.11). This group, we have seen, is the inhomogeneous, real linear transform group I. Four one-parameter groups are "inspectional" and two are "hidden." Equations (10.17) include all of the transformations at once, so other one-parameter groups can be analyzed.

(g) $g = \left\{\begin{pmatrix} 1 & -2i\sigma \\ 0 & 1 \end{pmatrix}, (2i\sigma, 2\sigma^2, 2i\sigma^3/3)\right\}$ from Eq. (10.9), *linear subgroup* [Fig. 10.2(F)].

$$f_g(q, t) = \exp(-2q\sigma + 4t\sigma^2 + 4\sigma^3/3) f(q - 4t\sigma - 2\sigma^2, t + \sigma). \tag{10.24}$$

(h) $g = \{\mathbf{M}(2i\theta), \mathbf{0}, 0\}$, $\mathbf{M}(2i\theta)$ from Eq. (9.31), *elliptic subgroup* [Fig. 10.2(G)]. The transformations of space–time are

$$\begin{aligned} q_g &= q/(\cosh\theta + 2t \sinh\theta), \\ t_g &= (t \cosh\theta + \tfrac{1}{2} \sinh\theta)/(\cosh\theta + 2t \sinh\theta). \end{aligned} \tag{10.25}$$

(i) $g = \{\mathbf{M}(2i\phi), \mathbf{0}, 0\}$, $\mathbf{M}(2i\phi)$ from Eq. (9.30), *hyperbolic subgroup* [Fig. 10.2(H)]. The space–time transformations are

$$\begin{aligned} q_g &= q/(\cos\phi - 2t \sin\phi), \\ t_g &= (t \cos\phi + \tfrac{1}{2} \sin\phi)/(\cos\phi - 2t \sin\phi). \end{aligned} \tag{10.26}$$

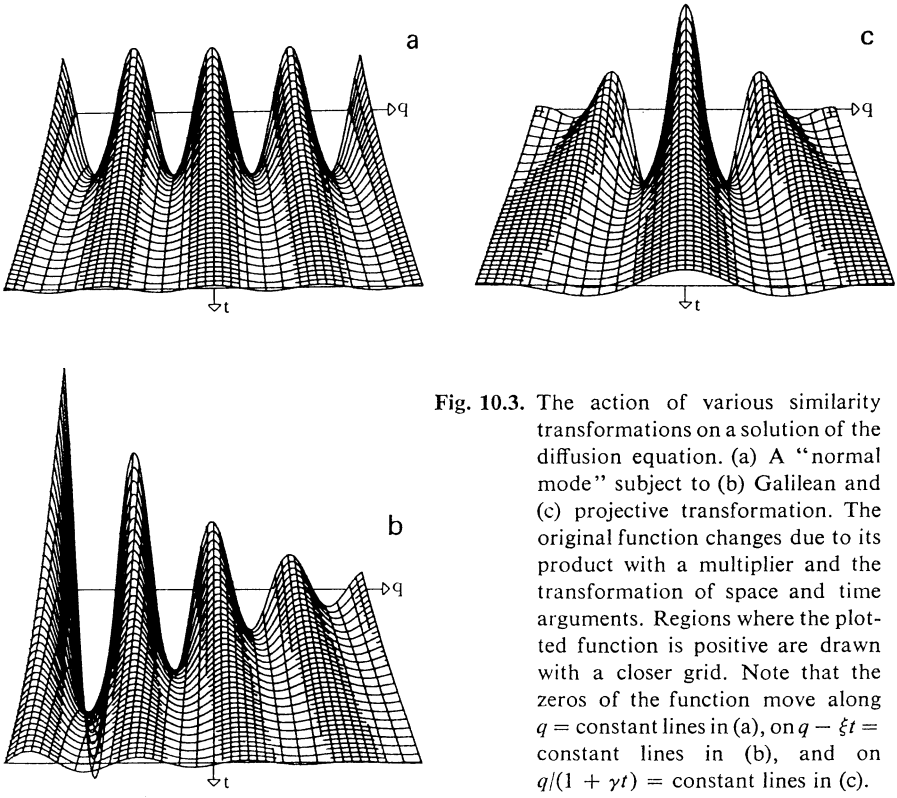


Fig. 10.3. The action of various similarity transformations on a solution of the diffusion equation. (a) A "normal mode" subject to (b) Galilean and (c) projective transformation. The original function changes due to its product with a multiplier and the transformation of space and time arguments. Regions where the plotted function is positive are drawn with a closer grid. Note that the zeros of the function move along $q =$ constant lines in (a), on $q - \xi t =$ constant lines in (b), and on $q/(1 + \gamma t) =$ constant lines in (c).

In the last two cases the appropriate multiplier function can be found from Eqs. (10.17).

The multiplier action of I is a deformation both of space–time and of the solution function. We show this in Fig. 10.3. We present one particular (*separable*) solution in Fig. 10.3(a). After acting on this $f(q, t)$ with a *Galilean* transformation, we obtain Fig. 10.3(b). A projective transformation gives the solution shown in Fig. 10.3(c).

Exercise 10.5. Verify that the set of geometric transforms (10.15) is a five-parameter subgroup of I. What is its effect on the $t = 0$ line?

Exercise 10.6. Verify that (a)–(i) are indeed subgroups of I, in particular, check in the cases of Galilean, projective, and "linear" transformations that under the product of two transformations the coordinates and multipliers compose properly. Note that for a two-variable-function $f(q, t)$ solution of (10.11), all of

I is what we could call a *geometric* transformation group in analogy with (10.15). Find its generators as two-variable first-order differential operators. [See Miller (1977, Section 2.2).]

Exercise 10.7. Verify, especially for Galilean, projective, and linear transformations, that $f_g(q, t)$ is a solution to the diffusion equation (10.11) if $f(q, t)$ is.

Exercise 10.8. Show that, as suggested by Fig. 10.2, the following, considered as sets, are the *invariant contours* under each subgroup: (a) points (q, t); (b) lines t = constant; (c) lines q = constant; (d) convertical parabolas; (e) lines t = constant; (f) concurrent lines; (g) parallel parabolas; (h) concurrent, concentric ellipses and hyperbolas; (i) concentric, nested hyperbolas. Note that all intercepts with the $t = 0$ axis have zero slope in cases (g)–(i).

Exercise 10.9. Not all solutions of the diffusion equation can be meaningfully regressed in time. (Recall Exercise 5.3 and the discussion of the inversion of the Gauss–Weierstrass transform in Section 9.2.) We should thus demand that all time translations (10.20) be nonnegative ($\beta \geqslant 0$), so that the $t = 0$ line remains uncrossed when space–time transformations are applied. Show that consistency then requires that scale and conformal transformations also be nonnegative ($a > 0$ and $\gamma \geqslant 0$) in (10.21) and (10.23). This defines a *subsemigroup* of I. The projective and elliptic transformations, in any case, are not globally continuous. As long as we remain in the vicinity of the $t = 0$ line and use small transformation parameters, however, these features will not bother us.

The solution of differential equations with boundary conditions was the motivation for Sophus Lie to develop his work on continuous groups at the end of the last century. More recently Ovsjannikov (1962) and Bluman and Cole (1974) have updated Lie's work and spurred renewed interest in *similarity* methods. The fact that our I is the similarity group of the diffusion equation was rediscovered by Bluman and Cole (1969) and applied to a variety of boundary conditions [see, for instance, Bluman (1974)]. Another approach to the problem has been to determine all coordinate systems where the diffusion equation (10.11) *separates* into two ordinary differential equations. This has been the theme for a series of papers by Miller, Kalnins, and Boyer. The diffusion equation is specifically analyzed in the article by Kalnins and Miller (1974). A very thorough account of the method and a complete reference list can be found in the recent book by Miller (1977). Canonical transforms, as presented here (Wolf, 1976), allow us to analyze some of these problems for the parabolic differential equations (10.1)–(10.2), reducing them, as we have seen in the sample development (10.13)–(10.17), to 2×2 matrix algebra.

10.1.5. Similarity Solutions, Separation of Variables, and R-Separability

We shall now tackle the problem of separation of variables for the diffusion equation. The completeness of the solution and its extension to

other parabolic equations will be shown in Section 10.2. Here we shall suggest the connection between separation of variables and the *similarity solutions* of the diffusion equation, that is, those solutions which at time $t = 0$ are the eigenfunctions of differential operators (10.1).

Consider the time development of the oscillating eigenfunctions $\Psi^f_{\lambda,\sigma}(q)$ of $\mathbb{H}^f$ [Eqs. (9.76b) and (9.87a)] under diffusion:

$$\Psi^{f;H}_{\lambda,\sigma}(q,t) \coloneqq (\mathbb{I}_{H(t)}\Psi^f_{\lambda,\sigma})(q) = \left[\mathbb{C}\begin{pmatrix}1 & -2it\\ 0 & 1\end{pmatrix}\Psi^f_{\lambda,\sigma}\right](q)$$
$$= \exp[i(2it)\mathbb{H}^f]\Psi^f_{\lambda,\sigma}(q) = \exp(-2\lambda t)\Psi^f_{\lambda,\sigma}(q). \quad (10.27)$$

The key has been the self-reproducing property (9.86) of the eigenfunctions $\Psi^f_{\lambda,\sigma}(q)$ under canonical transforms generated by its operator $\mathbb{H}^f$. See Fig. 10.3(a). Simple as it seems, (10.27) contains the interesting information that $\Psi^{f;H}_{\lambda,\sigma}(q,t)$ is a *separable* function of t and q. In these coordinates the diffusion equation manifestly *separates*, i.e., if we assume the solution has the structure $T(t)Q(q)$ and place this form in (10.11), we obtain two ordinary differential equations for the factors linked by a separation constant which we relate to λ. The solutions for $Q_\lambda(q)$ and $T_\lambda(t)$ yield precisely (10.27). Somewhat redundantly, note that under time translations (10.20), Fig. 10.2(B) draws out the q = constant lines which serve as part of the grid of this coordinate system; vertical t = constant lines are not drawn but can easily be added.

Exercise 10.10. Show that the diffusion equation (10.11) has separable solutions in the coordinates $q' = q - \xi t$, $t' = t$. Verify that the solutions thus obtained by the usual separation of variables method agree. What about (10.23), (10.24), (10.25), and (10.26)? The answer, *R-separation*, is analyzed below.

Now consider the nontrivial problem of exploring the diffusive time development of an initial temperature distribution of the shape of an Airy function (Fig. B.3). More precisely, consider $\Psi_\lambda{}^l(q)$ as given by Eq. (8.88), an eigenfunction of $\mathbb{H}^l$ which is the generator of the *linear* subgroup (10.9). Retracing our steps in (10.27), using the composition formula (10.8)–(10.9) for $\tau = 2it$ and the geometric action (10.15), we proceed as follows:

$$\Psi^{l;H}_\lambda(q,t) \coloneqq (\mathbb{I}_{H(t)}\Psi_\lambda{}^l)(q)$$
$$= \left[\mathbb{C}\begin{pmatrix}1 & -2it\\ 0 & 1\end{pmatrix}\Psi_\lambda{}^l\right](q)$$
$$= \Bigg[\mathbb{I}\{\mathbf{1}, (-2it, 2t^2, -2it^3/3)\}$$
$$\times \mathbb{I}\left\{\begin{pmatrix}1 & -2it\\ 0 & 1\end{pmatrix}, (2it, 2t^2, -2it^3/3)\right\}\Psi_\lambda{}^l\Bigg](q)$$
$$= \exp(-2\lambda t)[\mathbb{I}\{\mathbf{1}, (-2it, 2t^2, -2it^3/3)\}\Psi_\lambda{}^l](q)$$
$$= \exp(2tq + 8t^3/3 - 2\lambda t)\Psi_\lambda{}^l(q + 2t^2)$$
$$= \exp(2tv)\exp(-2\lambda t - 4t^3/3)\Psi_\lambda{}^l(v), \qquad v \coloneqq q + 2t^2. \quad (10.28)$$

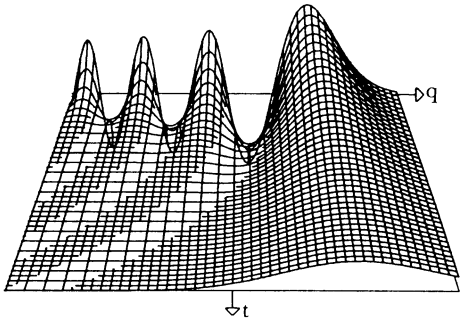


Fig. 10.4. Time development of a linear potential (Airy) $\Psi_\lambda{}^I(q)$ wave function under the diffusion equation. Regions where the function is positive are drawn with a closer grid. Notice that the zeros lie on parallel parabolas.

This function is shown in Fig. 10.4. The same remarks we made about (10.27) are valid here—with some qualification: $\Psi_\lambda^{I,H}(q, t)$ is an *R-separable* function of $v := q + 2t^2$ and t. By R-separability (or *separability with a modulation factor*) we mean a family of functions depending on a parameter λ such that

$$\Phi_\lambda(q, t) = R(u, v)U_\lambda(u)V_\lambda(v), \qquad u = u(q, t), v = v(q, t). \quad (10.29)$$

[See Morse and Feshbach (1953, p. 518) and Kalnins and Miller (1974, and the references therein).] This enlarged separability definition can be seen to work for the problem at hand. We substitute $u := t$ and $v := q + 2t^2$ into the diffusion equation (10.11), using $\partial/\partial q = \partial/\partial v$, $\partial/\partial t = \partial/\partial u + 4u\,\partial/\partial v$ and the assumed solution form (10.29). We divide by Φ_λ, suppressing arguments for brevity and indicating partial derivatives by subindices and total ones by primes. Rearranging terms slightly, we find

$$\frac{V''}{V} + \frac{V'}{V}\left(2\frac{R_v}{R} - 4u\right) - \frac{R_u}{R} = -\frac{R_{vv}}{R} + \frac{U'}{U} + 4u\frac{R_v}{R}. \quad (10.30)$$

If this equation is to separate, one member being only a function of v and the other of u, we expect all terms in R to cancel out and the expression in parentheses to be only a function of v, say, $\varphi(v)$. The solution to $R_v = [2u + \varphi(v)]R$ is $R = \chi(v)\exp(2uv)$ or, since any function of v alone will be absorbed into $V(v)$, $R = c\exp(2uv)$ with c constant. Substituting this result into (10.30), we find

$$\frac{V''}{V} - 2v = \frac{U'}{U} + 4u^2 = k, \quad (10.31)$$

where, by the usual separation argument, k must be a constant. From (10.31) we find that $U = c'\exp(ku - 4u^3/3)$ and V must be the solution of (8.87) for $k = -2\lambda$. Multiplying these results and replacing q and t, we find precisely (10.28) up to a multiplicative constant. Of course, had we not chosen the correct $u(q, t)$ and $v(q, t)$, the terms in $R(u, v)$ would not have canceled cross-variable dependencies. This method can be used in order to *find* R-separating

variables [see Kalnins and Miller (1974)]. In any case, the solution of a partial differential equation is reduced to the solution of three ordinary differential equations. It is the place to point out here that time and again we have simplified partial differential equations into ordinary ones by the device of "uncoupling," i.e., of finding a convenient basis where the Laplacian operator acts by multiplication on the expansion basis functions. This is in essence the transform method. Here, we are simply expanding a function into a similar basis set, eigenfunctions of an operator which is *not* necessarily the one appearing in the differential equation. What we are using are operators which generate various transformation families within a *group* of integral transforms. The useful feature is that a group is binding together the two different operators and their eigenbases.

The separating variables obtained here can be seen in Fig. 10.2(F), where the q-t transformations generated by the *separating* operator $\mathbb{H}^l$ [i.e., Eq. (10.9)] leave the parallel parabolas $q + 2t^2 = v =$ constant invariant. The $u =$ constant lines are vertical. As we did with the q-t-separable functions before, we can subject the initial condition of (10.28) to various kinds of canonical transforms whose effect will be to produce a continuum of other separating variable pairs which will turn the above parabolas into similar conics. As this continuum can be obtained from the $t, v(q, t)$ pair by canonical transformations on the initial conditions, we shall call them all *equivalent*. Note, however, that $t, v = q + 2t^2$, and t, q are *not* equivalent but quite distinct. In Section 10.2 we shall further clarify this notion of equivalence.

We can now use $\mathbb{H}^r$ and $\mathbb{H}^h$ [Eqs. (9.76d)–(9.76e) and (9.77d)–(9.77e)] as separating operators. To this end, we consider the time development of their eigenfunctions $\Psi^r_{\lambda,\mu}(q)$ and $\Psi_n{}^h(q)$ [Eqs. (9.87b)–(9.87c)]. Repeating the basic scheme of Eq. (10.28), we obtain

$$\begin{aligned}
\Psi^{r,H}_{\lambda,\sigma}(q, t) &\coloneqq (\mathbb{I}_{H(t)}\Psi^r_{\lambda,\sigma})(q) \\
&= \exp(-\lambda \arctan 2t) \\
&\quad \times \left[\mathbb{I}\left\{\begin{pmatrix} (1+4t^2)^{1/2} & 0 \\ 2it(1+4t^2)^{-1/2} & (1+4t^2)^{-1/2} \end{pmatrix}, (0,0,0)\right\}\Psi^r_{\lambda,\sigma}\right](q) \\
&= \exp[-tq^2/(1+4t^2)](1+4t^2)^{-1/4} \\
&\quad \times \exp(-\lambda \arctan 2t)\Psi^r_{\lambda,\sigma}\big(q(1+4t^2)^{-1/2}\big), \qquad (10.32)
\end{aligned}$$

$$\begin{aligned}
\Psi^{h,H}_{n}(q, t) &\coloneqq (\mathbb{I}_{H(t)}\Psi_n{}^h)(q) \\
&= \exp[-(n+1/2)\,\operatorname{arctanh} 2t] \\
&\quad \times \left[\mathbb{I}\left\{\begin{pmatrix} (1-4t^2)^{1/2} & 0 \\ -2it(1-4t^2)^{-1/2} & (1-4t^2)^{-1/2} \end{pmatrix}, (0,0,0)\right\}\Psi_n{}^h\right](q) \\
&= \exp[tq^2/(1-4t^2)](1-4t^2)^{-1/4} \\
&\quad \times \exp[-(n+1/2)\operatorname{arctanh} 2t]\Psi_n{}^h\big(q(1-4t^2)^{-1/2}\big). \qquad (10.33)
\end{aligned}$$

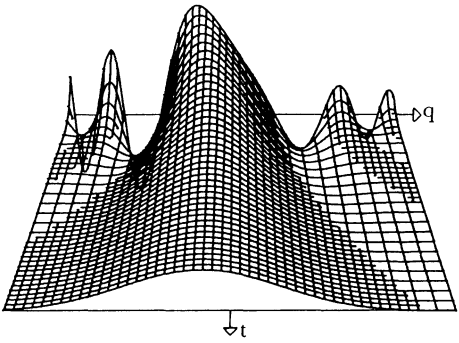


Fig. 10.5. Time development of the repulsive oscillator wave function $\Psi^{r}_{0,+}(q)$ under the diffusion equation. Again, the closer grid marks the regions where the function is positive. The zeros lie on concentric hyperbolas.

These are shown in Figs. 10.5 and 10.6. As in the former case, these function families are R-separable as in (10.29) for $v := q(1 + 4t^2)^{-1/2}$ and $v := q(1 - 4t^2)^{-1/2}$, respectively, and $u := t$. These can be seen in Figs. 10.2(H) and (G). These hyperbolas and ellipses are invariant under transformation generated by $\mathbb{H}^r$ and $\mathbb{H}^h$, respectively. Note that all separating coordinates we have found are such that $v(q, 0) = q$. If we apply the action of the similarity group to the (q, t)-separated normal modes (10.27), we find in general R-separated solutions. Thus, Galilean and projective transformations are R-separated in $(q - \xi t, t)$ and $[q/(1 + \gamma t), t]$, respectively. See Figs. 10.3(d) and (e).

Exercise 10.11. Follow the proof of (10.32) and (10.33) with care. Show that the diffusion equation indeed R-separates as suggested.

Exercise 10.12. In spite of the apparent singularity of (10.33) for $t = 1/2$, show that the solutions extend unscathed beyond this time.

10.1.6. The Heat Polynomials

Exercises 10.13–10.15 introduce certain solutions to the diffusion equation termed *heat polynomials*.

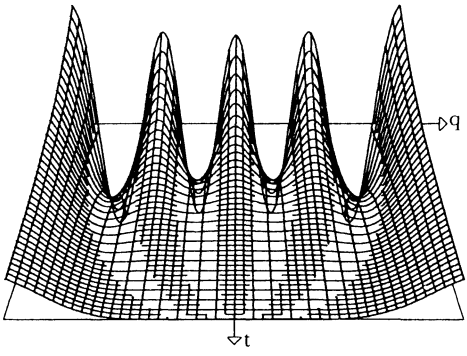


Fig. 10.6. Time development of the harmonic oscillator wave function $\Psi^{h}_{8}(q)$ under the diffusion equation. The zeros lie on concentric, convertical ellipses.

Exercise 10.13. Consider the following one-parameter subgroup of canonical transforms:

$$\exp\left[i\tau\left(-\frac{1}{2}\frac{d^2}{dq^2}+q\frac{d}{dq}+\frac{1}{2}\right)\right]=\mathbb{I}\left\{\begin{pmatrix}\exp(-i\tau) & -\sin\tau\\ 0 & \exp(i\tau)\end{pmatrix},(0,0,0)\right\}. \quad (10.34)$$

Prove the equality along the same lines suggested in (10.9)–(10.10), i.e., find the integral kernel, and then show that its τ derivative equals i times the action of the operator in the exponent [the analogue of (9.75)]. In case this procedure looks tedious, we promise the reader that a streamlined process to relate exponentials of arbitrary second-order operators and the matrices representing their canonical transform subgroups will be given in Section 10.2.

Exercise 10.14. The importance of (10.34) is that the eigenfunctions of the exponent operator are the *Hermite polynomials* $H_n(q)$ with eigenvalue $n + 1/2$. Show this from (7.166) and (7.170). Hermite polynomials can be obtained from $\Psi_n^h(q)$ by a $\mathbb{C}\left(\begin{smallmatrix}-1 & 0\\ 1 & 1\end{smallmatrix}\right)$ transform as it multiplies functions by $\exp(q^2/2)$. Explore this complex canonical transform: in (9.43) $u = 1 = w/2$ but $v = 0$. Refer to (9.71) to show that, indeed, Hermite polynomials are orthogonal with the weight function $\exp(-x^2)$.

Exercise 10.15. Follow the time development of a temperature distribution $H_n(q)$ by the analogue of (10.27), (10.28), (10.32), and (10.33), i.e., expressing $\mathbb{I}_{H(t)}$ as the product of a geometric transform and (10.34) for $\tau = (-i/2)\ln(1 - 4t)$. The result is found to be

$$H_n(q,t) \coloneqq (1-4t)^{n/2}H_n\left(q(1-4t)^{-1/2}\right) =: 2^n v_n(q, t-1/4), \quad (10.35)$$

where $v_n(q, t')$ are the *heat polynomials*. The time evolution of these and their relation to *power* functions for $t = 1/4$ can be seen from Eq. (7.193). There is considerable literature on these [see Hartmann and Wintner (1950), Rosenbloom and Widder (1959), Widder (1962, 1975, Chapter X), and Bilodeau (1974)]. Show that the functions (10.35) have the following properties: (a) They are *polynomials* in q and t. (b) $v_n(q, 0) = q^n$. (c) They are separable functions of t and $v = q(1 - 4t)^{-1/2}$. (d) $v(q, 0) = q$. (e) The multiplier factor R is unity, i.e., we have the case of *ordinary* separation.

We have worked out the simple diffusion equation in some detail, finding new families of solutions which will be shown in Section 10.2 to constitute, up to *equivalence*, *all* separable solutions to the equation. The reasons for being particularly interested in such solutions are the following. We have remarked that all separating coordinates are such that $v(q, 0) = q$. If the initial temperature distribution has a number of zeros at, say, $q_0, q_1, \ldots$, then, for all subsequent times, the separated solution (10.28) will have zeros at these values of v. The zero-temperature points will thus draw out the lines in Fig. 10.2. The solutions appear as in Fig. 10.3, and similar ones produced by different choices of (appropriate) separating operators, as in Figs. 10.4–10.6. Figure 10.3(a) should bring to memory the diffusive medium between *cold*

walls. In a manner reminiscent of the annular membrane of Section 8.3, if we are able to solve the Sturm–Liouville problem between two values, say, q_0 and q_1, of one of the separating operators, we shall be able to describe the solutions of the diffusion equation between *moving* cold walls or similar time-dependent boundary conditions. This is a "distorted image" method adapted to those boundaries which follow conics. In Section 10.2 we shall show how the more general parabolic equation (10.1)–(10.2) is subject to this treatment by nothing more than—properly applied—matrix algebra.

10.2. Inhomogeneous Linear Canonical Transforms and Parabolic Equations

In this section we shall examine the class of second-order parabolic differential equations (10.1)–(10.2) and see that the concepts developed for the diffusion equation in Section 10.1 can be set up in a general framework applicable to the whole class. We first show how all operators of interest can be reduced by *orbit* analysis of I to essentially four subclasses *represented* by $\mathbb{H}^f$, $\mathbb{H}^l$, $\mathbb{H}^r$, and $\mathbb{H}^h$ [respectively, the free-particle, linear potential, repulsive, and harmonic oscillator quantum Hamiltonians, Eqs. (9.76b), (7.61), (9.76d), and (9.76e)]. The similarity group of the whole class is I, the inhomogeneous linear canonical transformation group. This will determine the *similarity* solutions: eigenfunctions of operators in the set, separating variables, and invariant boundaries.

10.2.1. Transformation of Operators

Consider the set of operators $\mathscr{S}_1 := \{D\mathbb{Q} + E\mathbb{P} + F\mathbb{1}; D, E, F \in \mathscr{C}\}$ introduced in Section 10.1 and its transformation under the action of $\mathbb{I}\{g\}$, Eq. (10.7), where $g = \{\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right), (x, y, z)\} \in I$, the group of real inhomogeneous linear transformations. This can be found from (9.1), (10.6), and (10.7) to be

$$\mathbb{I}\{g\}(D\mathbb{Q} + E\mathbb{P} + F\mathbb{1})\mathbb{I}\{g\}^{-1} = (dD - cE)\mathbb{Q} + (aE - bD)\mathbb{P} + (F + yD + xE)\mathbb{1}, \tag{10.36}$$

that is, I transforms $\mathscr{S}_1$ onto itself. *Second-order* operators $\mathscr{S}_2 :=$ {Eq. (10.1); $A, B, \ldots, F \in \mathscr{C}$} can also be transformed by I onto themselves. It will be most convenient to rewrite their general expression as

$$\mathbb{H} = \sum_{k=0}^{5} \theta_k \mathbb{J}_k, \tag{10.37a}$$

$$\theta_0 = 2(A - C), \quad \theta_1 = B, \quad \theta_2 = 2(A + C), \quad \theta_3 = D, \quad \theta_4 = E, \quad \theta_5 = F, \tag{10.37b}$$

where we are using (9.76e), (9.76d), and (9.76a) for $\mathbb{J}_0$, $\mathbb{J}_1$, and $\mathbb{J}_2$ and defining

$$\mathbb{J}_3 := \mathbb{Q}, \qquad \mathbb{J}_4 := \mathbb{P}, \qquad \mathbb{J}_5 := \mathbb{1}. \tag{10.37c}$$

The action of I on $\mathscr{S}_2$ can be determined from (10.36) plus a little algebra. It has the general form

$$\mathbb{H}_g := \mathbb{U}\{g\}\mathbb{H}\mathbb{U}\{g\}^{-1} = \sum_{k=0}^{5} \theta'_k \mathbb{J}_k =: \sum_{j,k=0}^{5} \Gamma_{kj}(g)\theta_j \mathbb{J}_k. \tag{10.38a}$$

The $\{\theta'_k\}_{k=0}^5$ are linear functions of the original $\{\theta_k\}_{k=0}^5$, which transform as the entries of a column vector $\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_5)^T$ under a matrix $\boldsymbol{\Gamma}(g)$ which *represents* the group element $g \in I$. Explicitly,

$$\boldsymbol{\Gamma}(g) = \begin{pmatrix} \frac{1}{2}(a^2+b^2+c^2+d^2) & \frac{1}{2}(a^2-b^2+c^2-d^2) & -cd-ab & 0 & 0 & 0 \\ \frac{1}{2}(a^2+b^2-c^2-d^2) & \frac{1}{2}(a^2-b^2-c^2+d^2) & cd-ab & 0 & 0 & 0 \\ -bd-ac & bd-ac & ad+bc & 0 & 0 & 0 \\ \frac{1}{2}(cx+dy) & \frac{1}{2}(cx-dy) & \frac{1}{2}(-cy-dx) & d & -c & 0 \\ \frac{1}{2}(-ax-by) & \frac{1}{2}(-ax+by) & \frac{1}{2}(ay+bx) & -b & a & 0 \\ \frac{1}{4}(x^2+y^2) & \frac{1}{4}(x^2-y^2) & -\frac{1}{2}xy & y & -x & 1 \end{pmatrix} \tag{10.38b}$$

The reason for being interested in these transformations of $\mathscr{S}_2$ is that a given operator $\mathbb{H}$ may be mapped onto a simpler, known operator $\mathbb{H}_g$. If $\psi_\lambda(q)$ is an eigenfunction of $\mathbb{H}$ with eigenvalue λ, then $\psi_\lambda{}^g(q) := (\mathbb{U}\{g\}\psi_\lambda)(q)$ will be an eigenfunction of $\mathbb{H}_g$ with the same eigenvalue. If the latter eigenfunctions are known and the transformation g is a *geometric* one [Eq. (10.15)], then the eigenfunctions of $\mathbb{H}$ can be found simply as $\psi_\lambda(q) = (\mathbb{U}\{g\}^{-1}\psi_\lambda{}^g)(q)$.

Exercise 10.13. Prove (10.36) by considering $g = \{\mathbf{A}, \boldsymbol{\xi}, z\}$,

$$\mathbb{U}\{g\}\mathbb{U}\{\mathbf{1}, (D, E), F\}\mathbb{U}\{g\}^{-1} = \mathbb{U}\{\mathbf{1}, (D, E)\mathbf{A}^{-1}, F - (D, E)\boldsymbol{\Omega}\boldsymbol{\xi}^T\}, \tag{10.39}$$

where $\boldsymbol{\Omega} := \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ as in (10.8). Elements $\mathbb{H}$ of $\mathscr{S}_1$ may be seen as vectors in three-dimensional space with components $(D, E, F)^T$ which transform as the entries of (10.39) under the lower-right 3×3 submatrix of (10.38b). Note in particular that the column vector $(D, E)^T \to \mathbf{A}^{-1T}(D, E)^T$.

Exercise 10.17. Consider the composition of two transformations (10.39). Show that $\mathbb{U}\{g_1\}\mathbb{U}\{g_2\} = \mathbb{U}\{g_1 g_2\}$ acting on $(D, E, F)^T$. You may come to use $\mathbf{A}\boldsymbol{\Omega}\mathbf{A}^T = \boldsymbol{\Omega}$ [this only says that $\mathbf{A}$, an $SL(2, \mathscr{R})$ matrix, is also a two-dimensional *symplectic* one].

Exercise 10.18. Extend the above considerations to $\mathbb{H}$ seen as six-dimensional column vectors $\boldsymbol{\theta}$. Show that $\boldsymbol{\Gamma}(g_1)\boldsymbol{\Gamma}(g_2) = \boldsymbol{\Gamma}(g_1 g_2)$, $\boldsymbol{\Gamma}(\{\mathbf{1}, \mathbf{0}, 0\}) = \mathbf{1}$, and $\boldsymbol{\Gamma}(g^{-1}) = \boldsymbol{\Gamma}(g)^{-1}$ and that associativity holds. The set of matrices $\{\boldsymbol{\Gamma}(g), g \in I\}$ constitutes a 6×6 *matrix representation* of I.

10.2.2. Orbit Analysis

The concrete form of $\mathbf{\Gamma}(g)$ can be used to obtain all operators $\mathbb{H}_g = \mathbb{I}\{g\}\mathbb{H}\mathbb{I}\{g\}^{-1}$, $g \in I$, which can be "reached" from a given, fixed, operator $\mathbb{H}$. We shall consider first the case of operators with *real* coefficients θ_i. We are here specifically interested in *second*-order parabolic equations (10.1), with a nonzero leading coefficient, which will generate one-parameter subgroups (or *subsemigroups*) of canonical transforms describing the time evolution of initial conditions. If we multiply an operator $\mathbb{H}$ by a real constant κ, we are effectively only changing the time scale without affecting anything essential in the system. Similarly, addition of a term $k\mathbb{1}$ to $\mathbb{H}$ in (10.37) only multiplies the solution of the equation by a factor of $\exp(ikt)$, which we deem unimportant (see, however, Exercise 10.20).

We are led thus to consider equivalence classes of operators,

$$\Omega^{\omega} := \{\kappa\mathbb{I}\{g\}\mathbb{H}^{\omega}\mathbb{I}\{g\}^{-1} + k\mathbb{1}; g \in I; \kappa, k \in \mathscr{R}\}, \tag{10.40}$$

which we shall call *the orbit of* $\mathbb{H}^{\omega}$. Transformation by I, multiplication by κ, and addition of a constant define an equivalence relation (see Exercise 10.19) which will *divide* $\mathscr{S}_2$ *into disjoint orbits.*

Exercise 10.19. Show that (10.40) are indeed *equivalence* classes; that is, the defining equivalence relation ($\equiv$) is (a) reflexive, $\mathbb{H} \equiv \mathbb{H}$; (b) symmetric, $\mathbb{H} \equiv \mathbb{H}' \Leftrightarrow \mathbb{H}' \equiv \mathbb{H}$; and (c) transitive, $\mathbb{H} \equiv \mathbb{H}'$, $\mathbb{H}' \equiv \mathbb{H}'' \Rightarrow \mathbb{H} \equiv \mathbb{H}''$. The relation ($\equiv$) thus divides $\mathscr{S}_2$ into disjoint sets.

We shall now show that there are exactly *six* orbits (10.40) in $\mathscr{S}_2$ of which two are trivial (one is in $\mathscr{S}_1$ and the other is the orbit of the zero operator). For the four remaining orbits we shall choose $\mathbb{H}^f$, $\mathbb{H}^l$, $\mathbb{H}^r$, and $\mathbb{H}^h$ as representatives.

The orbit analysis of $\mathscr{S}_2$ is aided by constructing

$$\Theta := \theta_0^2 - \theta_1^2 - \theta_2^2, \tag{10.41}$$

associated to the vector $\boldsymbol{\theta}$ which characterizes a given $\mathbb{H} \in \mathscr{S}_2$. It is straightforward to verify that this number is *invariant* under all transformations (10.38). [In group language, the subspace of $\mathscr{S}_2$ with $\theta_3 = \theta_4 = \theta_5 = 0$ is isomorphic to a three-dimensional Minkowski space–time under $SL(2, \mathscr{R}) \simeq SO(2, 1)$ transformations.] By multiplying $\mathbb{H}$ by the constant κ, Θ is multiplied by κ^2; this cannot change its *sign*, and hence we know that there are at least three orbits in $\mathscr{S}_2$ corresponding to $\Theta > 0$, $\Theta < 0$, and $\Theta = 0$. Examples of operators in these orbits are $\mathbb{H}^h$ (with $\theta_0 = 2$) for which $\Theta = 4$; $\mathbb{H}^r$ ($\theta_1 = 2$), $\Theta = -4$; and $\mathbb{H}^l$ and $\mathbb{H}^f$ ($\theta_0 = 1 = \theta_1$), $\Theta = 0$. We shall now examine these three cases and see whether we can find transformations g which map arbitrary operators with these values of Θ onto the four chosen operators,

which will then serve as orbit representatives. We need consider only *geometric* transformations (10.15).

(a) $\theta^2 := \Theta > 0$. For $\mathbb{H}$ given by (10.37), $\mathbb{H}^h = 2\theta^{-1}\mathbb{I}\{g\}\mathbb{H}\mathbb{I}\{g\}^{-1} + k\mathbb{1}$, with

$$a = [|\theta|/(\theta_0 + \theta_1)]^{1/2}, \qquad c = \theta_2[|\theta|(\theta_0 + \theta_1)]^{-1/2},$$
$$x = 2[\theta_4(\theta_0 - \theta_1) - \theta_3\theta_2]/\Theta, \tag{10.42}$$
$$y = 2[\theta_4\theta_2 - \theta_3(\theta_0 + \theta_1)]/\Theta.$$

We can assume that $\theta_0 + \theta_1 \neq 0$, as otherwise the operator $\mathbb{H}$ would contain no second derivative. These operators are not physically interesting and yield to simpler methods.

(b) $-\theta^2 := \Theta < 0$, $\mathbb{H}^r = 2\theta^{-1}\mathbb{I}\{g\}\mathbb{H}\mathbb{I}\{g\}^{-1} + k\mathbb{1}$, with g given again by (10.42).

(c) $\Theta = 0$. Assume first that θ_0, θ_1, and θ_2 are not all identically zero. Then $\mathbb{I}\{g\}\mathbb{H}\mathbb{I}\{g\}^{-1}$, by a free parameter μ and

$$a = [2\mu/(\theta_0 + \theta_1)]^{1/2}, \qquad c = [(\theta_0 - \theta_1)/2\mu]^{1/2}, \tag{10.43a}$$

can be brought to a form where $\theta_0' = \mu = \theta_1'$, $\theta_2' = 0$, i.e., an operator $\mu\mathbb{P}^2/2$ plus terms *linear* in $\mathbb{Q}$ and $\mathbb{P}$. A further choice of x and y such that

$$\theta_4' = -\tfrac{1}{2}a[x(\theta_0 + \theta_1) - y\theta_2 - 2\theta_4] = 0 \tag{10.43b}$$

will eliminate all first derivatives from $\mathbb{H}$. The value of the coefficient θ_3' of $\mathbb{Q}$ is then fixed, determined only by the free parameter μ as

$$\theta_3' = (2\mu)^{-1/2}[\theta_3(\theta_0 + \theta_1)^{1/2} - \theta_4(\theta_0 - \theta_1)^{1/2}]. \tag{10.43c}$$

The operator we have is thus $\mathbb{H}' = \mu\mathbb{P}^2/2 + \theta_3'\mathbb{Q} + k\mathbb{1}$. We *cannot* make θ_3' vanish, however, *unless* the expression in brackets in (10.43c) is zero to start with. The case $\Theta = 0$ therefore contains at least two subcases:

(c1) When θ_3' in (10.43c) is nonzero, we can fix μ so that $\theta_3'/\mu = 1$, thereby bringing the operator to $\mu\mathbb{H}^l$.

(c2) When $\theta_2\theta_3 - (\theta_0 - \theta_1)\theta_4 = 0$, θ_3' in Eq. (10.43c) is zero, and a choice of $\mu = 1$ transforms the operator $\mathbb{H}$ to $\mathbb{H}^f$.

There are two more orbits in the $\theta = 0$ case:

(c3) When $\theta_0 = \theta_1 = \theta_2 = 0$ but the operator is nonzero, it belongs to $\mathscr{S}_1$. It can be always "rotated" to become $\kappa\mathbb{P}$ + constant $\mathbb{1}$.

(c4) All θ's are zero. A representative of this equivalence class is $\mathbb{1}$. We shall not consider the last two subcases in what follows.

We asked for the operators $\mathbb{H}$ in (10.37) to have real coefficients. When this condition is relaxed, Θ can be a complex number which under real I

transformations is still invariant. We now have in infinity of orbits (10.40), one for each phase of Θ, and for $\Theta = 0$ a similar unfolding. Our interest here, however, centers on real Θ's: Schrödinger-type equations where the coefficients are real and diffusive-type equations where the $\mathbb{P}^2$ term is pure imaginary. An example of the latter is, of course, the diffusion equation of Section 10.1. Another example, a *Fokker–Planck* equation, will be given in Exercises 10.20 and 10.22. For diffusive equations it seems best to place the i on the time variable and use real I transformations, as before, to relate the $\mathbb{H}$ operator to a simpler operator in the same orbit.

Now, if we allow the parameters in $g \in I$ to become complex, all $\Theta \neq 0$ orbits coalesce. A change of phase $q \to q \exp(-i\pi/4)$ will turn $\mathbb{J}_0$ into $i\mathbb{J}_1$, for example. For quantum-mechanical Schrödinger equations, complex transformations are generally meaningless as the $\mathscr{L}^2(\mathscr{R})$ norm is changed, although this may be just what one needs in order to describe *decay*. For diffusion equations, the requirement that the coordinates and function remain real usually restricts the useful transformations to a real parameter subset.

To illustrate the possibilities at hand we propose the following example.

Exercise 10.20. Consider the *Fokker–Planck*-type of differential equation,

$$\frac{\partial^2}{\partial q^2} f(q, t) + \frac{\partial}{\partial q}[qf(q, t)] = \frac{\partial}{\partial t} f(q, t), \tag{10.44a}$$

which can be written as

$$\mathbb{H}^{\mathrm{FP}} f(q, t) \coloneqq (2\mathbb{J}_0 + 2\mathbb{J}_1 - 2i\mathbb{J}_2 - \tfrac{1}{2}\mathbb{1}) f(q, t) = -i\partial f(q, t)/\partial(it), \tag{10.44b}$$

with $\Theta = 4$. It is thus in the same orbit as the harmonic oscillator. Verify that, for

$$g_0 \coloneqq \left\{ 2^{-1/2} \begin{pmatrix} 1 & 0 \\ -i & 2 \end{pmatrix}, \mathbf{0}, 0 \right\}, \qquad \mathbb{I}\{g_0\}\mathbb{H}^{\mathrm{FP}}\mathbb{I}\{g_0\}^{-1} = \mathbb{H}^h - \tfrac{1}{2}\mathbb{1}. \tag{10.45a}$$

The "normal mode" solutions for (10.44) will thus be

$$\begin{aligned} \Psi_n^{\mathrm{FP},h}(q, t) &\coloneqq \exp(t/2) \exp[i(n + 1/2)(it)](\mathbb{I}\{g_0\}^{-1}\Psi_n^h)(q) \\ &= 2^{1/4} \exp(-nt) \exp(-q^2/4)\Psi_n^h(2^{-1/2}q) \\ &= k \exp(-nt) \exp(-q^2/2) H_n(2^{-1/2}q), \end{aligned} \tag{10.45b}$$

where k is a constant. Check that (10.45b) solves (10.44a). Note that this solution is separable in q and t. Its time evolution will propagate the zeros along $q =$ constant lines, in analogy with the normal mode solutions (10.27) of the heat equation.

Exercise 10.21. Note that, in asking for a *geometric* transformation to do the job of bringing an arbitrary $\mathbb{H}$ to one of the four chosen representatives, we are leaving out three rather important operators: (a) $\mathbb{J}_2$, which generates changes of scale [Eqs. (9.77a) and (10.21)], in the same orbit as $\mathbb{H}^r = 2\mathbb{J}_1$ by (9.35); (b) $\frac{1}{2}\mathbb{Q}^2$, which generates projective transformations for the diffusion equation

[Eqs. (9.77c) and (10.23)], in the same orbit as $\frac{1}{2}\mathbb{P}^2$ by a Fourier $\left(\begin{smallmatrix} 0 & \frac{1}{2} \\ -1 & 0 \end{smallmatrix}\right)$ transform; and (c) $\mathbb{Q}$, generator of Galilean transformations (10.22) which belong to the nonzero orbit in $\mathscr{S}_1$. Show that the cases $\theta_0 = \theta_1$, specifically excluded in our treatment, can easily be incorporated by Fourier transformation.

10.2.3. Transforming Initial Conditions: The Similarity Group

To find the relation of a given operator $\mathbb{H}$ to its chosen, known, orbit representative, we can construct solutions of the former in terms of those of the latter. It is thus sufficient to treat only the orbit representative in what follows, leaving for exercises a sample calculation for the Fokker–Planck equation (10.44). Each of the operators $\mathbb{H}^\omega$ generates a one-parameter subgroup of canonical transformations

$$\mathbb{I}_{\omega(t)} := \exp(it\mathbb{H}^\omega) =: \mathbb{I}\left\{\begin{pmatrix} h_a & h_b \\ h_c & h_d \end{pmatrix}, (h_x, h_y, h_z)\right\}, \qquad h_k = h_k(t), \quad (10.46)$$

which, acting on a function $f(q)$, defines a two-variable function

$$f^\omega(q, t) := (\mathbb{I}_{\omega(t)}\mathbf{f})(q), \qquad f^\omega(q, 0) = f(q), \quad (10.47)$$

which will be a solution to the differential equation

$$\mathbb{H}^\omega f^\omega(q, t) = -i\partial f^\omega(q, t)/\partial t. \quad (10.48)$$

Now, if the initial condition $f(q)$ is subject to an I transformation $\mathbb{I}\{g\}$ and turned into another function $f_g(q)$, the subsequent time evolution of the latter—following (10.13)—will be

$$\begin{aligned} f_g{}^\omega(q, t) &:= (\mathbb{I}_{\omega(t)}\mathbf{f}_g)(q) = (\mathbb{I}_{\omega(t)}\mathbb{I}\{g\}\mathbf{f})(q) \\ &= \left[\mathbb{I}\left\{\begin{pmatrix} a_t & 0 \\ c_t & a_t^{-1} \end{pmatrix}, (x_t, y_t, z_t)\right\}\mathbb{I}_{\omega(t_g)}\mathbf{f}\right](q) = [\mathbb{I}\{G_t\}\mathbf{f}^\omega(\cdot, t_g)](q) \\ &= a_t^{-1/2}\exp[i(c_t q^2/2a_t + x_t q/a_t + x_t y_t/2 + z_t)]f^\omega(q/a_t + y_t, t_g). \end{aligned} \quad (10.49)$$

The parameters $a, c, \ldots, z$ of G_t which depend on t and the function $t_g(t)$ can be calculated from identities between the elements of the matrix representatives of $\mathbb{I}_{\omega(t)}\mathbb{I}\{g\}$ and $\mathbb{I}\{G_t\}\mathbb{I}_{\omega(t_g)}$, where, note, G_t is a *geometric* transformation. In Table 10.1 we summarize the results for the four orbit representative operators. It follows that if $f^\omega(q, t)$ is a solution to (10.48), we generate a six-parameter continuum of solutions. We thus state that the group I is the *similarity group* for the operator $\mathbb{H}^\omega$. The association seen in Section 10.1 between the various parameters and geometrical transformations such as changes of scale and Galilean and projective transformations is seen to be peculiar to the $\mathbb{H}^f$ and $\mathbb{H}^I$ cases. In general, the $v(q, t) =$ constant lines will be rather complicated curves in the (q, t)-plane. In all cases, however, we

stress that I is the *full* similarity group of the differential equation (10.48) including both *manifest* and *hidden* invariances.

Exercise 10.22. Continuing with the Fokker–Planck equation introduced in Exercise 10.20, show $\mathbb{I}_{\mathrm{FP}(t)}$ to be

$$\begin{aligned}\mathbb{I}_{\mathrm{FP}(t)} &= \mathbb{I}\{g_0\}^{-1}\exp[i(it)(\mathbb{H}^h - \tfrac{1}{2}\mathbb{1})]\mathbb{I}\{g_0\} \\ &= \mathbb{I}\left\{\begin{pmatrix}\exp(-t) & -2i\sinh t\\ 0 & \exp(t)\end{pmatrix}, \mathbf{0}, -it/2\right\} \qquad (10.50)\end{aligned}$$

from (10.44), (10.45), and (9.77e). Now, comparing the matrix elements of $\mathbb{I}_{\mathrm{FP}(t)}\mathbb{I}\{g\}$ and $\mathbb{I}\{G_t\}\mathbb{I}_{\mathrm{FP}(t_g)}$, show that

$$\exp(2t_g) - 1 = \{ib + d[\exp(2t) - 1]\}/\{a - ic[\exp(2t) - 1]\}, \qquad (10.51a)$$

$$a_t = \exp(t_g)[a\exp(-t) - 2ic\sinh t], \qquad (10.51b)$$

$$c_t = c\exp(t + t_g), \qquad (10.51c)$$

$$x_t = x\exp(t_g), \qquad (10.51d)$$

$$y_t = y\exp(-t_g) + 2ix\sinh t_g. \qquad (10.51e)$$

In asking for the time variable and the solution to be real, we are led to consider b, c, and x pure imaginary—as in the diffusion equation of Section 10.1.

10.2.4. Similarity Solutions and Separation of Variables

In keeping with the general plan of presentation of Section 10.1, we would now like to examine the time evolution, under $\mathbb{H}^\omega$, of *similarity* solutions, i.e., eigenfunctions $\Psi_\lambda{}^v(q)$ of a second operator $\mathbb{H}^v$. One of the results of this development will be the definition and explicit calculation of four equivalence classes of separating coordinates for our set of differential equations. As before, let $\mathbb{I}_{\omega(t)}$ and $\mathbb{I}_{v(t)}$ be the one-parameter time-evolution subgroups generated by $\mathbb{H}^\omega$ and $\mathbb{H}^v$ [Eq. (10.46)]. Then for a finite neighborhood of $t = 0$ we can always write

$$\mathbb{I}_{\omega(t)} = \mathbb{I}\{G_t^{\omega v}\}\mathbb{I}_{v(t')}, \qquad (10.52)$$

where $G_t^{\omega v}$ is a time-dependent geometric transformation binding the two evolution subgroups for $t' = t'(t)$. The parameters of $G_t^{\omega v}$ and $t'(t)$ have been collected in Table 10.2 for pairs of orbit representative operators.

Now we proceed as we did in (10.27), (10.28), (10.32), and (10.33), using the fact that $\mathbb{I}_{v(t')}$ acting on $\Psi_\lambda{}^v(q)$ multiplies it only by a factor of $\exp(i\lambda t')$:

$$\begin{aligned}\Psi_\lambda{}^{v,\omega}(q,t) &:= (\mathbb{I}_{\omega(t)}\boldsymbol{\Psi}_\lambda{}^v)(q) = (\mathbb{I}\{G_t^{\omega v}\}\mathbb{I}_{v(t')}\boldsymbol{\Psi}_\lambda{}^v)(q) \\ &= \exp(i\lambda t')(\mathbb{I}\{G_t^{\omega v}\}\boldsymbol{\Psi}_\lambda{}^v)(q) \\ &= a_t^{-1/2}\exp[i(c_tq^2/2a_t + x_tq/a_t + x_ty_t/2 + z_t + \lambda t')] \\ &\quad\times \Psi_\lambda{}^v(q/a_t + y_t) \\ &= \exp\{i[c_ta_tv^2/2 + (x_t - c_ta_ty_t)v]a_t^{-1/2} \\ &\quad\times \exp\{i[-y_t(x_t - c_ta_ty_t)/2 + z_t + \lambda t'(t)]\}\Psi_\lambda{}^v(v). \qquad (10.53)\end{aligned}$$

In the last expression, we have rearranged the factors so as to display the *R-separability* of the function $\Psi_\lambda^{v,\omega}(q, t)$ as the function $\Psi_\lambda{}^v(v)$ of $v(q, t) = q/a_t + y_t$ times a function of t times a *multiplier* involving v and t but independent of λ. [Recall Eq. (10.28) and the ensuing discussion.] The pair of coordinates (v, t) are the coordinates *separated by* $\mathbb{H}^v$ of the differential equation (10.48) for $\mathbb{H}^\omega$. In Table 10.3 we have collected these coordinates and the multiplier functions for all pairs of orbit representative operators.

10.2.5. Equivalent and Nonequivalent Separating Coordinates

To bring out the significance of *equivalent* coordinate systems, consider first the case when $\mathbb{H}^\omega$ and $\mathbb{H}^v$ belong to the *same* orbit, i.e., there exists a similarity group element $g \in I$ such that

$$\mathbb{H}^v = \mathbb{I}\{g\}\mathbb{H}^\omega\mathbb{I}\{g\}^{-1}, \qquad \Psi_\lambda{}^v(q) = (\mathbb{I}\{g\}\Psi_\lambda{}^\omega)(q). \tag{10.54}$$

Then

$$\begin{aligned}\Psi_\lambda^{v,\omega}(q, t) &\coloneqq (\mathbb{I}_{\omega(t)}\Psi_\lambda{}^v)(q) = (\mathbb{I}_{\omega(t)}\mathbb{I}\{g\}\Psi_\lambda{}^\omega)(q) = (\mathbb{I}\{G_t\}\mathbb{I}_{\omega(t')}\Psi_\lambda{}^\omega)(q)\\ &= \exp(i\lambda t')(\mathbb{I}\{G_t\}\Psi_\lambda{}^\omega)(q).\end{aligned} \tag{10.55}$$

Indeed, this is just (10.49) when the choice for $f(q)$ is $\Psi_\lambda{}^\omega(q)$, so that $f(q, t)$ is $\exp(i\lambda t')\Psi_\lambda{}^\omega(q)$, a separable function in q and t. The conclusion is that *when* $\mathbb{H}^\omega$ *and the separating operator* $\mathbb{H}^v$ *belong to the same orbit, the separating coordinates* (v, t) *of the former can be obtained from the Cartesian ones by a transformation in the similarity group of the equation.* These will be taken to be *equivalent*. (Compare Fig. 10.3.) Now, if $\mathbb{H}^\omega$ and $\mathbb{H}^v$ belong to *different* orbits, the separating coordinates are inequivalent.

To find all coordinate systems equivalent to a given $[v(q, t), t]$ defined by an orbit representative operator $\mathbb{H}^v$, consider the action of $\mathbb{I}_{\omega(t)}$ on $(\mathbb{I}\{g\}\Psi_\lambda{}^v)(q)$. This will give the coordinates associated to $\mathbb{I}\{g\}\mathbb{H}^v\mathbb{I}\{g\}^{-1}$. Proceeding by (10.49) and (10.53), we obtain

$$\begin{aligned}(\mathbb{I}_{\omega(t)}\mathbb{I}\{g\}\Psi_\lambda{}^v)(q) &= (\mathbb{I}\{G_t\}\mathbb{I}_{\omega(t_g)}\Psi_\lambda{}^v)(q)\\ &= (\mathbb{I}\{G_t\}\mathbb{I}\{G_{t_g}^{\omega v}\}\mathbb{I}_{v(t_g')}\Psi_\lambda{}^v)(q)\\ &= \exp(i\lambda t_g')(\mathbb{I}\{G_tG_{t_g}^{\omega v}\}\Psi_\lambda{}^v)(q).\end{aligned} \tag{10.56}$$

In other words, we have only to apply the transformations of Table 10.1, representing G_t and t_g, to those of Table 10.2, representing $G_t^{\omega v}$ and $t'(t)$. If the former are the identity, we obtain Table 10.3 from (10.53).

Exercise 10.23. Implement (10.56) for the case of the free-particle Schrödinger equation. This case leads both to algebraically manageable results and to conclusions which are relevant for the diffusion equation. Show that the coordinate systems equivalent to (q, t) (*f-f* box in Table 10.3) are given by

$$v = [q + (dx - cy)t + (ay - bx)]/(a - ct) \tag{10.57a}$$

and t. The coordinate systems equivalent to $(q - t^2/2, t)$ (*f-l* box in Table 10.3) are

$$v = [q + (dx - cy)t + (ay - bx)]/(a - ct) - \tfrac{1}{2}[(dt - b)/(a - ct)]^2 \quad (10.57b)$$

and t, and those equivalent to $\left(q(1 \mp t^2)^{-1/2}, t\right)$ (boxes *f-r* and *f-h* of Table 10.3) are

$$v = [q + (dx - cy)t + (ay - bx)][(a - ct)^2 \mp (dt - b)^2]^{-1/2} \quad (10.57c)$$

and t. Note that all the coordinate lines v = constant are conic sections. Can you find their axes and foci?

Exercise 10.24. Find the multiplier exponents $S(v, t)$ which generalize those of Table 10.3 according to (10.57). Recall the transform in Exercise 10.15 which led to the heat polynomials. Show that the multiplier function which corresponds to the coordinate system separated by the generator of (10.34) is unity, as (10.35) clearly shows. This is the free-particle counterpart of the heat polynomials. Can you show that this system and the Cartesian one are essentially (up to translations and dilatations) the *only* completely ($R = 1$) separating coordinate systems?

Table 10.1 Geometric and Time Transformation Parameters for the Action of a General Element in I on the Solutions of the Differential Equation $\mathbb{H}^{\omega}\mathbf{f} = -i\partial_t\mathbf{f}$ [a]

Operator $\mathbb{H}^{\omega}$	Time $t_g(t)$ transformation	Geometrical transformation
$\mathbb{H}^f = \frac{1}{2}\mathbb{P}^2$	$t_g = \dfrac{dt - b}{a - ct}$	$a_t = a - ct,\ c_t = c,\ z_t = z,$ $(x_t, y_t) = (x, y)\begin{pmatrix} 1 & t_g \\ 0 & 1 \end{pmatrix}$
$\mathbb{H}^l = \frac{1}{2}\mathbb{P}^2 + \mathbb{Q}$	$t_g = \dfrac{dt - b}{a - ct}$	$a_t = a - ct,\ c_t = c,\ z_t = z,$ $(x_t, y_t) = \left[(x, y) + (t, -t^2/2)\begin{pmatrix} a & b \\ c & d \end{pmatrix} - (t_g, -t_g^2/2)\right]\begin{pmatrix} 1 & t_g \\ 0 & 1 \end{pmatrix}$
$\mathbb{H}^r = \frac{1}{2}(\mathbb{P}^2 - \mathbb{Q}^2)$	$\tanh t_g = \dfrac{d\tanh t - b}{a - c\tanh t}$	$a_t = (a\cosh t - c\sinh t)/\cosh t_g = (d\sinh t - b\cosh t)/\sinh t_g,$ $c_t = (c\cosh t - a\sinh t + a_t^{-1}\sinh t_g)/\cosh t_g,$ $(x_t, y_t) = (x, y)\begin{pmatrix} \cosh t_g & \sinh t_g \\ \sinh t_g & \cosh t_g \end{pmatrix},$ $z_t = z$
$\mathbb{H}^h = \frac{1}{2}(\mathbb{P}^2 + \mathbb{Q}^2)$	$\tan t_g = \dfrac{d\tan t - b}{a - c\tan t}$	$a_t = (a\cos t - c\sin t)/\cos t_g = (d\sin t - b\cos t)/\sin t_g,$ $c_t = (c\cos t + a\sin t - a_t^{-1}\sin t_g)/\cos t_g,$ $(x_t, y_t) = (x, y)\begin{pmatrix} \cos t_g & \sin t_g \\ -\sin t_g & \cos t_g \end{pmatrix},$ $z_t = z$

[a] The heat equation can be related to case *f* by substituting $t \to 2it,\ b =: -2i\beta,\ c =: i\gamma/2,\ x =: i\xi/2,\ z =: i\zeta$.

Table 10.2 Parameters and Time Transformation for the Evolution, Governed by $\mathbb{H}^{\omega}\psi^{\upsilon}_{\lambda} = -i\partial_t\psi^{\upsilon}_{\lambda}$, of the Eigenfunctions of an Operator $\mathbb{H}^{\upsilon}$ [a]

ω \ υ	f	l	r	h
f	1	$t' = t$ $a_t = 1,$ $x_t = -t$ $y_t = -t^2/2,$ $z_t = -t^3/12$	$\tanh t' = t$ $a_t = (1 - t^2)^{1/2}$ $c_t = t(1 - t^2)^{-1/2}$	$\tan t' = t$ $a_t = (1 + t^2)^{1/2}$ $c_t = -t(1 + t^2)^{-1/2}$
l	$t' = t$ $a_t = 1,$ $x_t = t$ $y_t = t^2/2,$ $z_t = t^3/12$	1	$\tanh t' = t$ $a_t = (1 - t^2)^{1/2}$ $c_t = t(1 - t^2)^{-1/2}$ $x_t = t(1 - t^2/2)(1 - t^2)^{-1/2}$ $y_t = \frac{1}{2}t^2(1 - t^2)^{-1/2}$ $z_t = -t^3/12$	$\tan t' = t$ $a_t = (1 + t^2)^{1/2}$ $c_t = -t(1 + t^2)^{-1/2}$ $x_t = t(1 + t^2/2)(1 + t^2)^{-1/2}$ $y_t = \frac{1}{2}t^2(1 + t^2)^{-1/2}$ $z_t = -t^3/12$
r	$t' = \tanh t$ $a_t = \cosh t$ $c_t = -\sinh t$	$t' = \tanh t$ $a_t = \cosh t$ $c_t = -\sinh t$ $x_t = -t'$ $y_t = -t'^2/2$ $z_t = t'^3/12$	1	$\tan t' = \tanh t$ $a_t = (\cosh 2t)^{1/2}$ $c_t = -\sinh 2t(\cosh 2t)^{-1/2}$
h	$t' = \tan t$ $a_t = \cos t$ $c_t = \sin t$	$t' = \tan t$ $a_t = \cos t$ $c_t = \sin t$ $x_t = -t'$ $y_t = -t'^2/2$ $z_t = t'^3/12$	$\tanh t' = \tan t$ $a_t = (\cos 2t)^{1/2}$ $c_t = \sin 2t(\cos 2t)^{-1/2}$	1

[a] Refer to Eqs. (10.52) – (10.53). The entry 1 means $t' = t$ and $a_t = 1$, $c_t = 0$. Missing entries are zero. (As in Table 10.1, the heat equation is related to case f by $t \to 2it$. The results appear explicitly in Section 10.1.)

If we are faced with a differential equation of the type (10.48) with given initial ($t = 0$) and moving boundary conditions, our procedure would be to see whether we can find separating variables such that the coordinate curves match the boundaries. If they do, there is an associated operator whose Sturm–Liouville problem in the appropriate interval yields the best function set in which to expand the initial $t = 0$ data, so that they naturally follow the constancy conditions at the moving boundary. This is in essence the familiar image method but applied to moving, distorting, mirrors.

Table 10.3 Separating Coordinates $(v(q, t), t)$ and Multiplier Functions $R(v, t) = \exp[iS(v, t)]$ [Eq. (10.56)] for the Differential Equation $\mathbb{H}^{\omega}\mathbf{f} = -i\partial_t\mathbf{f}$, as Separated by the Operator $\mathbb{H}^{v}$ [a]

ω \ v	f	l	r	h
f	$v = q$ $S = 0$	$v = q - t^2/2$ $S = -vt$	$v = q(1 - t^2)^{-1/2}$ $S = v^2t/2$	$v = q(1 + t^2)^{-1/2}$ $S = -v^2t/2$
l	$v = q + t^2/2$ $S = vt$	$v = q$ $S = 0$	$v = (q + \frac{1}{2}t^2)(1 - t^2)^{-1/2}$ $S = v^2t/2 + vt(1 - t^2)^{1/2}$	$v = (q + \frac{1}{2}t^2)(1 + t^2)^{-1/2}$ $S = -v^2t/2 + vt(1 + t^2)^{1/2}$
r	$v = q/\cosh t$ $S = -v^2 \sinh(2t)/4$	$v = q/\cosh t - \frac{1}{2}\tanh^2 t$ $S = -v^2 \sinh(2t)/4$ $- v \tanh t(1 + \frac{1}{2}\sinh^2 t)$	$v = q$ $S = 0$	$v = q(\cosh 2t)^{-1/2}$ $S = -\frac{1}{2}v^2 \sinh 2t$
h	$v = q/\cos t$ $S = v^2 \sin(2t)/4$	$v = q/\cos t - \frac{1}{2}\tan^2 t$ $S = v^2 \sin(2t)/4$ $- v \tan t(1 - \frac{1}{2}\sin^2 t)$	$v = q(\cos 2t)^{-1/2}$ $S = \frac{1}{2}v^2 \sin 2t$	$v = q$ $S = 0$

[a] As before, the heat equation is related to the f case by $t \to 2it$.

Appendix A

The Gamma Function

The *factorial* of a natural number n is defined as

$$n! := n(n-1)(n-2)\cdots 3\cdot 2\cdot 1. \tag{A.1}$$

Recursively, it can be characterized by

$$n! := n(n-1)!, \qquad 0! := 1. \tag{A.2}$$

A function which generalizes the factorial for complex numbers is the *gamma* function, defined by the *Euler integral*

$$\begin{aligned}\Gamma(z) &:= \int_0^\infty dt\, t^{z-1}\exp(-t) \\ &= 2\int_0^\infty du\, u^{2z-1}\exp(-u^2), \qquad \operatorname{Re} z > 0.\end{aligned} \tag{A.3}$$

From this form it follows by integration by parts that

$$\Gamma(z+1) = z\Gamma(z), \qquad \Gamma(1) = 1, \tag{A.4}$$

and hence

$$\Gamma(n) = (n-1)!. \tag{A.5}$$

We can define $\Gamma(z)$ for $\operatorname{Re} z \leqslant 0$ by $\Gamma(z) = \Gamma(z+1)/z$ repeated the number of times necessary for the argument to reach positive values for the real part. A special value is

$$\Gamma(\tfrac{1}{2}) = \pi^{1/2} = 1.7724538509\ldots, \tag{A.6}$$

found from the last expression in (A.3), which is just the integral (7.21). A plot of the gamma function appears in Fig. A.1. It is an analytic function with simple poles at zero and the negative integers, since

$$\begin{aligned}\Gamma(x-n) &= (x-n)^{-1}\Gamma(x-n+1) = \cdots \\ &= (-1)^n[(n-x)(n-1-x)\cdots(1-x)x]^{-1}\Gamma(1+x).\end{aligned} \tag{A.7a}$$

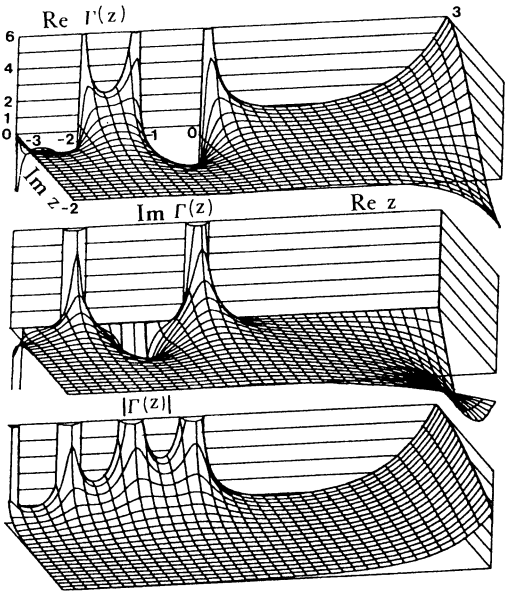


Fig. A.1. Real, imaginary, and absolute values of the gamma function $\Gamma(z)$ in the complex plane of the argument. $\mathrm{Re}\, z \in (-3, 3)$, $\mathrm{Im}\, z \in (-2, 0)$. Simple poles are present at $z = 0, -1, -2, \ldots$.

Thus for $x \to 0$ the residues of the poles are

$$\mathrm{Res}\ \Gamma(z)|_{z=-n} = (-1)^n/n!. \tag{A.7b}$$

Two other expressions for the gamma function, the Euler infinite limit and the Weierstrass infinite product, can be seen, for instance, in Whittaker and Watson (1903, Chapter 12). In the former we can find the proofs of the following useful relations: the Gauss multiplication formula

$$\Gamma(nz) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n=1} \Gamma(z + k/n) \tag{A.8}$$

and the reflection formulas

$$\Gamma(z)\Gamma(1 - z) = \pi \csc(\pi z), \tag{A.9a}$$

$$\Gamma(\tfrac{1}{2} + z)\Gamma(\tfrac{1}{2} - z) = \pi \sec(\pi z). \tag{A.9b}$$

The numerical computation of the gamma function is usually performed by approximating it by the polynomial

$$\begin{aligned}\Gamma(z + 1) = 1 &- 0.577191652z + 0.988205891z^2 - 0.897056936z^3 \\ &+ 0.918206857z^4 - 0.756704078z^5 + 0.482199394z^6 \\ &- 0.193527818z^7 + 0.035868343z^8 + \varepsilon(z),\end{aligned} \tag{A.10}$$

which for $0 \leqslant z \leqslant 1$ is valid with $|\varepsilon(z)| \leqslant 3 \times 10^{-7}$. The argument is moved to the strip $0 \leq \operatorname{Re} z \leq 1$ by repeated use of (A.4) or (A.7a); then, if need be, the absolute value of the imaginary part is contracted to less than $\frac{1}{2}$ with the use of the Gauss formula (A.8). For this and several other computer algorithms and approximations, see Hastings (1955) and the periodically updated communications of the American Computer Society (ACS). The analytic aspects of the gamma function have been elegantly developed by Artin (1964) and Lösch and Schoblik (1951). A summary of properties, tables, and references can be found in Abramowitz and Stegun (1964, Chapter 6).

Appendix B

The Bessel and Related Functions

We define the Bessel function of integer order k as

$$J_k(z) := (2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \cos(z \sin \theta - k\theta). \tag{B.1}$$

This was Bessel's original definition in 1824 [see Watson (1922, Section 2.2 and the references therein)]. It leads to our first use of this function in Eqs. (5.48c)–(5.50) by the following steps involving trigonometric identities, considerations about the parity of the functions, and the invariance of (B.1) under $\theta \to \pm\theta + \alpha$:

$$\begin{aligned} \int_{-\pi}^{\pi} d\theta \cos(z \sin \theta - k\theta) &= \int_{-\pi}^{\pi} d\theta \exp(iz \sin \theta) \exp(-ik\theta) \\ &= \int_{-\pi}^{\pi} d\theta \cos(z \sin \theta) \exp(-ik\theta). \end{aligned} \tag{B.2}$$

With the substitutions $\theta = x/2$, $k = 2(n - m)$, and $z = 2\tau(k/M)^{1/2}$ we obtain (5.48c).

The middle term in (B.2), with the substitution $t = \exp(i\theta)$, gives us (B.1) as a closed contour integral around the origin:

$$J_k(z) = (2\pi i)^{-1} \oint dt t^{-k-1} \exp[z(t - t^{-1})/2]. \tag{B.3}$$

It follows from here that the $J_k(z)$ are the *Laurent* series coefficients of the exponential function in the integrand, i.e.,

$$G_B(z, t) := \exp[z(t - t^{-1})/2] = \sum_{k \in \mathcal{Z}} J_k(z) t^k. \tag{B.4}$$

This is the Bessel *generating function*. For $t = i\exp(i\theta)$ and $z = pq$ we obtain (8.78). From (B.1) we can see that $J_k(z)$ is an analytic function of z in the neighborhood of $z = 0$. Its Taylor expansion can be found from (B.3) by the Taylor expansion of the exponential and the Cauchy integral (8.12) for $g(s) = s^p$:

$$\begin{aligned} J_k(z) &= (2\pi i)^{-1} \oint dt \sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{zt}{2}\right)^m \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-z}{2t}\right)^n t^{-k-1} \\ &= \sum_{m,n=0}^{\infty} \frac{(-1)^n}{m!\,n!} \left(\frac{z}{2}\right)^{m+n} (2\pi i)^{-1} \oint dt t^{m-n-k-1} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,(n+k)!} \left(\frac{z}{2}\right)^{2n+k}. \end{aligned} \tag{B.5}$$

For k an integer it thus follows that

$$J_k(e^{i\pi m} z) = e^{ik\pi m} J_k(z). \tag{B.6}$$

The ratio test shows that this series converges for all finite z. Equation (B.5) can be generalized for complex values of the index by the gamma function:

$$J_k(z) := \sum_{n=0}^{\infty} (-1)^n [n!\,\Gamma(n+k+1)]^{-1} (z/2)^{2n+k}, \qquad k \in \mathbb{C}. \tag{B.7}$$

In particular, for $k = \pm\frac{1}{2}$, we find

$$J_{1/2}(z) = (2/\pi z)^{1/2} \sin z, \tag{B.8a}$$

$$J_{-1/2}(z) = (2/\pi z)^{1/2} \cos z. \tag{B.8b}$$

The Bessel function $J_k(z)$ has a countable infinity of simple real zeros for $z > 0$ and, at $z = 0$, a k-fold zero. The location of $j_{k,n}$, the nth zero of $J_k(z)$, is an increasing function of k. These zeros are transcendental numbers bounded from below by k, and as $n \to \infty$ their spacing increases monotonically, tending toward π. They interlace since $j_{k,n} < j_{k+1,n} < j_{k,n+1} < j_{k+1,n+1} < \cdots$. Table B.1 gives the first zeros of a few low-order Bessel functions.

Table B.1 Zeros of the Bessel Function j_{kn}

n \ k	0	1	2	3	4	5
1	2.40482	3.83171	5.13562	6.38016	7.58834	8.77148
2	5.52007	7.01559	8.41724	9.76102	11.06471	12.33860
3	8.65372	10.17347	11.61984	13.01520	14.37254	15.70017
4	11.79153	13.32369	14.79595	16.22347	17.61597	18.98013
5	14.93091	16.47063	17.95982	19.40942	20.82693	22.21780

A *Christoffel–Darboux* three-term recursion relation for Bessel functions can be obtained by differentiating the generating function (B.4) with respect to t:

$$\sum_{k\in\mathscr{Z}} kJ_k(z)t^{k-1} = \partial G_B(z, t)/\partial t = (z/2 + z/2t^2)G_B(z, t)$$
$$= \sum_{k\in\mathscr{Z}} z[J_k(z) + J_{k+2}(z)]t^k/2, \tag{B.9}$$

where we have shifted the dummy sum index where necessary. Linear independence of the power functions then implies

$$J_{k+1}(z) - 2kz^{-1}J_k(z) + J_{k-1}(z) = 0. \tag{B.10}$$

Similarly, differentiating (B.4) with respect to z and rearranging terms by (B.9), we find the raising and lowering operators,

$$(k/z \mp d/dz)J_k(z) = J_{k\pm1}(z), \tag{B.11}$$

which can also be seen to hold directly by the series expansion (B.7).

Equation (8.65) can be shown to hold for integer N (integer or half-integer μ) by noting that for $N = 2$ ($\mu = 0$) it coincides with (B.1) for $k = 0$. For $N = 3$ ($\mu = 1/2$) the integral is elementary and leads correctly to (B.8a). Last, the Bessel function as given by (8.65) can be seen to satisfy (B.11) by integration by parts.

Applying the raising and lowering operators (B.11) in either order to $J_k(z)$, we find that the Bessel function satisfies the second-order differential equation

$$\left(z^2\frac{d^2}{dz^2} + z\frac{d}{dz} + z^2 - k^2\right)J_k(z) = 0. \tag{B.12}$$

This is Bessel's differential equation. As is true for any (Fuchsian) equation, (B.12) has two independent solutions. They are $J_k(z)$ and $J_{-k}(z)$ for k *not* an integer; when k is an integer, these two functions are not linearly independent, but

$$J_{-k}(z) = (-1)^k J_k(z), \tag{B.13}$$

as can be ascertained from (B.7) by observing that the Γ-function in the denominator of $J_{-k}(z)$ has poles for $n = 0, 1, \ldots, k-1$, so the sum actually starts from $n = k$. In the case of integer k, the *second* solution to (B.12), built for real k as

$$N_k(z) = [J_k(z)\cos(\pi k) - J_{-k}(z)]/\sin \pi k, \tag{B.14}$$

defines the *Neumann* function (also called Bessel of the *second* kind or Y-function). As k approaches integer values, $N_k(z)$ continues to be a well-defined

function which can be found from L'Hospital's rule. Its explicit series expression can be found in the literature [see, for instance, Arfken (1966, Section 11.2), Whittaker and Watson (1903), and, of course, Watson's treatise (1922); the last contains a very complete account of these functions]. Bessel and Neumann functions have been plotted in Figs. B.1 and B.2.

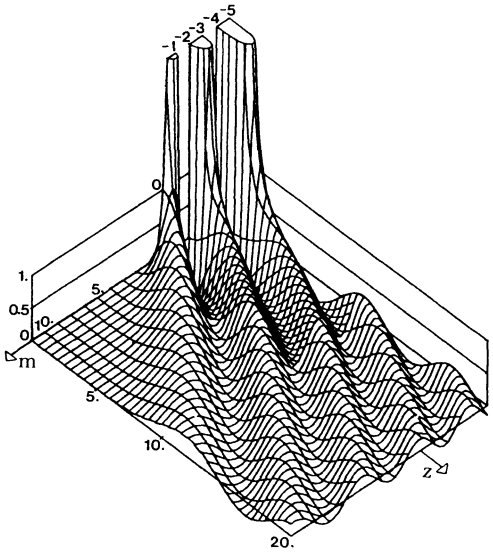


Fig. B.1. The Bessel function $J_m(z)$ for $m \in (-5, 10)$ and $z \in (0, 20)$. The function becomes infinite at $z = 0$ for all noninteger negative m. A closer grid details this region.

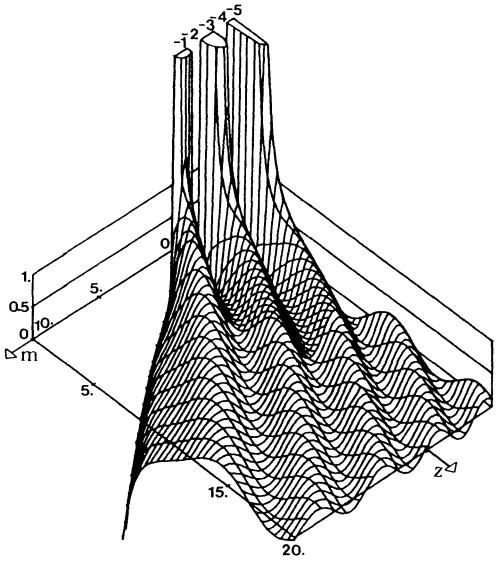


Fig. B.2. The Neumann function $N_m(z)$ for $m \in (-5, 10)$ and $z \in (0, 20)$. The point $z = 0$ is singular. A closer grid details the negative m region.

Some of the main properties of Bessel vs. Neumann functions are their behavior at the origin:

$$J_k(z) \underset{z\to 0}{\simeq} [2^k\Gamma(k+1)]^{-1}z^k, \qquad k \neq -1, -2, -3, \ldots, \tag{B.15a}$$

$$N_k(z) \underset{z\to 0}{\simeq} -2^k\pi^{-1}\Gamma(k)z^{-k}, \qquad k \neq 0, \qquad N_0(z) \underset{z\to 0}{\simeq} 2\pi^{-1}\ln z. \tag{B.15b}$$

Their asymptotic behavior can be shown to be

$$J_k(z) \underset{z\to\infty}{\simeq} (2/\pi z)^{1/2}\cos[z - \pi(k + 1/2)/2], \tag{B.16a}$$

$$N_k(z) \underset{z\to\infty}{\simeq} (2/\pi z)^{1/2}\sin[z - \pi(k + 1/2)/2]. \tag{B.16b}$$

[See Watson (1922, Chapter VII).] Both Bessel and Neumann functions satisfy the three-term and differential recursion equations (B.10) and (B.11). The properties of the zeros (simplicity, reality, spacing, and interlacing) are common to both functions.

The *modified* Bessel differential equation

$$\left(z^2\frac{d^2}{dz^2} + z\frac{d}{dz} - z^2 - k^2\right)f(z) = 0 \tag{B.17}$$

has solutions $J_k(\pm iz)$. It is convenient to introduce the *modified* Bessel functions

$$I_k(z) := \begin{cases} \exp(i\pi k/2)J_k(\exp(i\pi/2)z), & -\pi < \arg z \leqslant \pi/2, \\ \exp(3i\pi k/2)J_k(\exp(-3i\pi/2)z), & \pi/2 < \arg z \leqslant \pi, \end{cases} \tag{B.18}$$

which have the series expansion

$$I_k(z) = \sum_{k=0}^{\infty} [n!\Gamma(n + k + 1)]^{-1}(z/2)^{2n+k}. \tag{B.19}$$

[Compare with (B.7).] For k *not* an integer, independent solutions of (B.17) are provided by $I_k(z)$ and $I_{-k}(z)$. When k is an integer, $I_{-n}(z) = I_n(z)$. Suggesting analogy with Neumann functions, one defines the *Macdonald* function,

$$K_k(z) = (\pi/2)[I_{-k}(z) - I_k(z)]/\sin\pi k, \tag{B.20}$$

which is independent of $I_k(z)$ for all k. The limits and asymptotics of the I- and K-functions are

$$I_k(z) \underset{z\to 0}{\simeq} (z/2)^k/\Gamma(k + 1), \qquad k \neq -1, -2, -3, \ldots, \tag{B.21a}$$

$$K_k(z) \underset{z\to 0}{\simeq} (z/2)^{-k}\Gamma(k)/2, \qquad k \neq 0; \qquad K_0(z) \underset{z\to 0}{\simeq} -\ln z, \tag{B.21b}$$

$$I_k(z) \underset{z\to\infty}{\simeq} (2\pi z)^{-1/2}\exp(z), \tag{B.22a}$$

$$K_k(z) \underset{z\to\infty}{\simeq} (\pi/2z)^{1/2}\exp(-z). \tag{B.22b}$$

For real z and positive k, both functions are free of zeros.

From the Bessel modified equation we shall obtain another important differential equation. Let $y := (3z/2)^{2/3}$ and write (B.17) in terms of it for $g(y) = f(z)$; then define $g(y) =: y^{-1/2}h(y)$. When $k = 1/3$, terms cancel, and we are left with *Airy*'s equation:

$$\left(\frac{d^2}{dy^2} - y\right)h(y) = 0. \tag{B.23}$$

Equation (7.61) is found from here by $y =: 2^{1/3}q$. It thus follows that $y^{1/2}I_{\pm 1/3}(2y^{3/2}/3)$ and $y^{1/2}K_{1/3}(2y^{3/2}/3)$ will be solutions to (B.23). Actually, one defines the *first* and *second Airy* functions:

$$\begin{aligned}\mathrm{Ai}(y) &:= \pi^{-1}(y/3)^{1/2}K_{1/3}(z)\\ &= y^{1/2}[I_{-1/3}(z) - I_{1/3}(z)]/3,\end{aligned} \tag{B.24a}$$

$$\mathrm{Ai}(-y) = y^{1/2}[J_{-1/3}(z) + J_{1/3}(z)], \tag{B.24b}$$

$$\mathrm{Bi}(y) := (y/3)^{1/2}[I_{-1/3}(z) + I_{1/3}(z)], \tag{B.24c}$$

$$\mathrm{Bi}(-y) = (y/3)^{1/2}[J_{-1/3}(z) - J_{1/3}(z)], \qquad z = 2y^{3/2}/3. \tag{B.24d}$$

These are plotted in Figure B.3. The Taylor expansions are of the form

$$\mathrm{Ai}(y) = c_1F_1(y) - c_2F_2(y), \tag{B.25a}$$

$$\mathrm{Bi}(y) = 3^{1/2}[c_1F_1(y) + c_2F_2(y)], \tag{B.25b}$$

where the constants are

$$c_1 = 3^{-2/3}/\Gamma(2/3) = 0.35502805\ldots = \mathrm{Ai}(0) = 3^{-1/2}\mathrm{Bi}(0), \tag{B.26a}$$

$$c_2 = 3^{-1/3}/\Gamma(1/3) = 0.25881940\ldots = -\mathrm{Ai}'(0) = 3^{-1/2}\mathrm{Bi}'(0) \tag{B.26b}$$

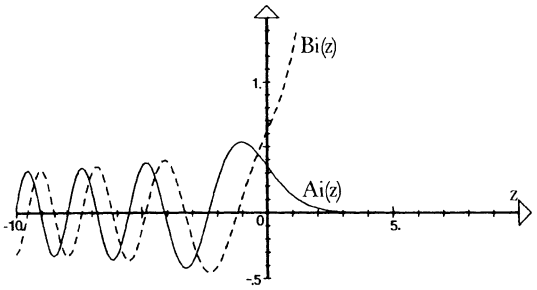


Fig. B.3. The Airy function of first and second kind.

and the functions are

$$F_n(y) = \sum_{m=0}^{\infty} 3^m(n/3)_m[\Gamma(3m + n)]^{-1}y^{3m+n-1}, \qquad n = 1, 2, \quad \text{(B.27a)}$$

where we have used *Pochhammer's symbol*

$$(a)_m := a(a + 1)(a + 2)\cdots(a + m - 1) = \Gamma(a + m)/\Gamma(a). \quad \text{(B.27b)}$$

For $y \to +\infty$, the asymptotics are

$$\mathrm{Ai}(y) \simeq 2^{-1}\pi^{-1/2}y^{-1/4}\exp(-2y^{3/2}/3), \quad \text{(B.28a)}$$

$$\mathrm{Ai}(-y) \simeq \pi^{-1/2}y^{-1/4}\sin(2y^{3/2}/3 + \pi/4), \quad \text{(B.28b)}$$

$$\mathrm{Bi}(y) \simeq \pi^{-1/2}y^{-1/4}\exp(2y^{3/2}/3), \quad \text{(B.29a)}$$

$$\mathrm{Bi}(-y) \simeq \pi^{-1/2}y^{-1/4}\cos(2y^{3/2}/3 + \pi/4). \quad \text{(B.29b)}$$

The integral expression (7.64), which we asserted represents the Airy function, can be put in terms of the usual and modified Bessel functions as in (B.24). The process is rather involved, so we refer the interested reader to the book by Watson (1922, Section 6.4). References to Airy's original "rainbow" equation and the solutions by Stokes and Hardy appear there.

Further properties and tables for the Bessel and related functions can be found in Abramowitz and Stegun (1964, Chapters 9 and 10), while integrals of Bessel functions—as for the Green's functions in Section 5.3—and Struve functions, mentioned in Section 8.5, occupy Chapters 11 and 12 of Abramowitz and Stegun. Further references and tables have been given in Sections 5.2, 5.3, and 6.4.

Appendix C

Some Summation Formulas

Let $A(m, n)$ be a function of two discrete variables $m, n = 0, 1, 2, \ldots$, i.e., on the points of Figure C.1. We assume that the sum S converges, regardless of the order in which it is performed:

$$S := \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A(m, n) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A(m, n). \tag{C.1}$$

This only means that in one case we sum over columns and in the other over rows. We can also perform the summation over diagonals (thin lines in Fig. C.1) as

$$S = [A(0, 0)] + [A(0, 1) + A(1, 0)] + [A(0, 2) + A(1, 1) + A(2, 0)] + \cdots$$
$$+ \left[\sum_{m=0}^{n} A(m, n - m)\right] + \cdots = \sum_{n=0}^{\infty} \sum_{m=0}^{n} A(m, n - m). \tag{C.2}$$

The same sum can be done following 60° directions (broken lines):

$$S = [A(0, 0)] + [A(0, 1)] + [A(0, 2) + A(1, 0)] + [A(0, 3) + A(1, 1)] + \cdots$$
$$+ \left[\sum_{m=0}^{n/2} A(m, n - 2m)\right]_{n \text{ even}} + \left[\sum_{m=0}^{(n-1)/2} A(m, n - 2m)\right]_{n \text{ odd}} + \cdots$$
$$= \sum_{n=0}^{\infty} \sum_{m=0}^{[n/2]} A(m, n - 2m), \tag{C.3}$$

where $[n/2]$ is the largest integer not exceeding $n/2$. For example, $[2] = 2$, $[5/2] = [2.5] = 2$, etc. The same argument can be used to sum the $A(m, n)$ along lines which run one unit to the right and r units down, obtaining

$$S = \sum_{n=0}^{\infty} \sum_{m=0}^{[n/r]} A(m, n - rm). \tag{C.4}$$

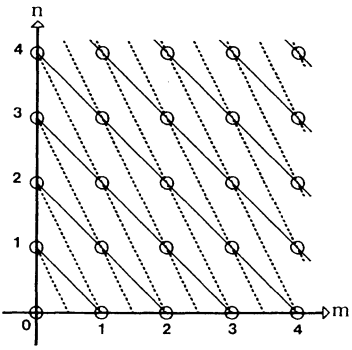


Fig. C.1. Various summation orders on an infinite two-dimensional lattice of non-negative integers.

When triple sums of $A(k, m, n)$ appear, the sum can be performed over diagonals in space; thus

$$\begin{aligned} T &:= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A(k, m, n) \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{min(k,m)} A(k - n, m - n, n) \\ &= \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{min([k/r],[m/s])} A(k - rn, m - sn, n). \end{aligned} \tag{C.5}$$

The middle term has been used in (7.183). Equations (C.1)–(C.4) can now be employed to produce further identities involving the first two indices of the sum.

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Notation

General Conventions

a (lowercase boldface)	vector
A (uppercase boldface)	matrix
$\mathscr{A}$ (script)	set
$\mathbb{A}$ (double)	operator
a^* (asterisk)	complex conjugate
$\mathbf{A}^\dagger$ (dagger)	adjoint

Re	real part
Im	imaginary part
Res	residue
$\mathscr{C}$	set of complex numbers
$\mathscr{R}$	set of real numbers
$\mathscr{Z}$	set of integer numbers
$\mathscr{Z}^+$	set of natural numbers
$\sum$	sum
$\prod$	product
(a, b)	open interval
$[a, b]$	closed interval
$\lvert a \rvert$	absolute value of a
$(\mathbf{a}, \mathbf{b})$	inner product of **a** and **b**
$\lVert \mathbf{a} \rVert$	norm of **a**
(a_n)	vector with components a_n
$\lVert A_{mn} \rVert$	matrix of elements A_{mn}
$\in$	is an element of
$:=$	is defined as
$=:$	defines
$\Rightarrow$	implies, only if
$\Leftarrow$	is implied by, if

Symbol List

$\mathrm{Ai}(z)$	Airy function of the first kind [Eqs. (B.24a), (B.24b)]
$\mathrm{Bi}(z)$	Airy function of the second kind [Eqs. (B.24c), (B.24d)]
$\mathbf{B}$	Bargmann transform matrix [Eqs. (9.55)]
$\mathscr{B}_M$	canonical transform of $\mathscr{L}^2(\mathscr{R})$-space [p. 394]
$C_M(q', q)$	canonical transform integral kernel [Eqs. (9.8)]
$\mathbb{C}_M$	canonical transform operator [p. 382]

$\mathscr{C}_{\downarrow}^{\infty}$	space of infinitely differentiable functions of fast decrease [p. 263]
$\mathbb{D}_a$	dilatation operator [Eq. (7.34)]
$D_k(x)$	Dirichlet kernel [Eq. (4.19)]
$\mathbb{E}_x$	multiplication by exponential operator [Eq. (7.29)]
$\{f_n\}_{n=1}^N$	coordinates of vector $\mathbf{f} \in \mathscr{V}^N$ [Eq. (1.2)]
$\{\tilde{f}_n\}_{n=1}^N$	Fourier transforms of $\{f_n\}_{n=1}^N$ [Eq. (1.51)]
$\{f_n\}_{n\in z}$	Fourier series coefficients of $f(x)$ [Eq. (4.17b)]
$\tilde{f}(p)$	Fourier transform of $f(q)$, $q \in \mathscr{R}$ [Eqs. (7.1)]
$f^B(g')$	Bargmann transform of $f(q)$ [p. 399]
$f^{BL}(s)$	bilateral Laplace transform of $f(q)$ [Eqs. (8.1)]
$f_\sigma^{BM}(\lambda)$	bilateral Mellin transform of $f(q)$ [Eqs. (8.26)]
$f^L(s)$	Laplace transform of $f(q)$ [Eqs. (8.9)]
$f^M(\lambda)$	Mellin transform of $f(q)$ [Eqs. (8.29)]
$f^M(q')$	M-canonical transform of $f(q)$ [Eq. (9.5)]
$\hat{f}_c(p)$	Cauchy representation of $f(q)$ [Eq. (7.136)]
$f_{a\infty}(q)$	function with support on $[a, \infty)$ [Eq. (7.125)]
$\mathbf{f}\,(\boldsymbol{\varepsilon})\,\mathbf{g}$	product relative to $\boldsymbol{\varepsilon}$-basis [p. 102]
$\mathbf{F}$	Fourier canonical transform matrix [Eq. (9.32)]
$\mathbf{F} = \|F_{mn}\|$	Fourier (finite) transform matrix [Eq. (1.48)]
$\mathbb{F}, \mathbb{F}^{-1}$	Fourier integral transform operator and its inverse [Eqs. (7.1)]
$\mathbb{F}_{(N)}, \mathbb{F}_{(N)}^{-1}$	N-dimensional Fourier transform and its inverse [Eqs. (8.38)]
$G_{\cdots}^{\cdots}(q, t)$	Green's function for a system
$G_\omega(q)$	Gaussian bell function of width ω [Eq. (7.20)]
$\mathbb{G}(t)$	time-evolution operator [finite lattice, p. 54; heat equation, p. 199; wave equation, p. 210]
$\mathbb{G}_{\text{II}}(t)$	phase-space evolution operator [Eq. (2.113)]
$\mathbb{G}_\omega$	Gaussian operator [Eq. (7.74)]
$H_n(q)$	hermite polynomials [Eq. (7.192)]
$\mathbb{H}_{\text{II}}$	phase-space evolution generator [Eq. (2.107)]
$\mathbb{H}_\mu, \mathbb{H}_\mu^{-1}$	Hankel transform operator and its inverse [Eqs. (8.83)]
$\mathbb{H}_\mu^B, \mathbb{H}_\mu^{B-1}$	Hankel–Bochner transform operator and its inverse [Eqs. (8. 66)]
$\mathbb{H}^f, \mathbb{H}^l, \mathbb{H}^r, \mathbb{H}^h$	Schrödinger Hamiltonian operators for the free particle, linear potential, repulsive and attractive oscillator [Eqs. (9.34), (9.76)]
I	group of inhomogeneous linear canonical transformations [p. 420]
$I_k(x)$	modified Bessel function [Eq. (B.18)]
$\mathbf{I}_0\ (\mathbb{I}_0)$	inversion matrix (operator) [Eqs. (1.54), (1.82), and (4.41)]
$\mathbb{I}_{\text{FP}(t)}$	time-evolution operator of the Fokker–Planck equation [Eq. (10.50)]

$\mathbb{I}_{H(t)}$ time-evolution operator of the diffusion equation [p. 442]
$\mathbb{I}\{\mathbf{M}, \boldsymbol{\xi}, z\}$ inhomogeneous linear canonical transform operator [Eqs. (10.7)]
$\mathbb{I}_{\omega(t)}$ time-evolution operator generated by $\mathbb{H}^{\omega}$ [Eq. (10.46)]
j_{mn} nth zero of $J_m(x)$ [Table B.1]
$J_m(x)$ Bessel function [Appendix B]
$\mathbb{J}_0, \mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_{\pm}$ set of second-order differential operators [Eqs. (7.174), (9.34), (9.76), (10.37c)]
$K_B(q', q)$ Bargmann reproducing kernel [Eq. (9.63)]
$K_n(x)$ Macdonald function [Eq. (B.20)]
$\mathbb{K}, \mathbb{C}, \mathbb{M}$ lattice interaction, damping, and mass operators [p. 51]
$\mathbf{L}$ Laplace transform matrix [Eq. (9.68)]
$\mathbb{L}, \mathbb{L}^{-1}$ Laplace transform operator and its inverse [Eqs. (8.9)]
$\mathbb{L}_B, \mathbb{L}_B^{-1}$ bilateral Laplace transform operator and its inverse [Eqs. (8.1)]
$\mathscr{L}^2(\mathscr{I})$ space of (Lebesgue) square-integrable functions over the interval $\mathscr{I}$ [p. 142 and 264]
$\mathscr{L}_0^2(R)$ space of (Lebesgue) square-integrable functions which vanish at the boundary of a region R [p. 222]
$\mathscr{L}_{\omega}^2(\mathscr{I})$ space of (Lebesgue) square-integrable functions on $\mathscr{I} \subseteq \mathscr{R}$ with weight function $\omega(x)$ [p. 297]
$\mathbb{M}, \mathbb{M}^{-1}$ Mellin transform operator and its inverse [Eqs. (8.29)]
$\mathbb{M}_B, \mathbb{M}_B^{-1}$ bilateral Mellin transform operator and its inverse [Eqs. (8.26)]
$N_m(x)$ Neumann function [Eq. (B.14)]
$p_{\pm}, q_{\pm}$ "cut" power functions [Eq.(7.202)]
$\mathbf{P}(^{m}_{\pi(m)})$ permutation matrix [Eq. (1.45)]
$\mathbb{P}$ $-i$ times the differentiation operator (the quantum-mechanical momentum operator) [Eq. (7.56)]
$\mathscr{P}\int$ principle value of an integral [Eq. (7.138)]
$\mathbb{Q}$ multiplication by argument operator [Eq. (7.55)]
$R^{(\varepsilon,\eta)}(x)$ rectangle function of width ε and height η [Eqs. (4.24), (7.4)]
$\mathbf{R}$ ($\mathbb{R}$) rotation matrix (operator) [Eq. (1.81)]
$R_{\square}$ (hyper-) rectangular region [p. 223]
$R_{\bigcirc}$ circular region [p. 230]
$R_{\backsim}$ sectorial region [p. 240]
$R_{\odot}$ annular region [p. 243]
S_{N-1} sphere in N dimensions [p. 363]
$S^{(P,\eta)}(x)$ square wave of P pulses and height η [Eqs. (4.39)]
$SL(2, \mathscr{R})$ group of unimodular 2×2 real matrices [p. 390]
$\mathscr{S}_1, \mathscr{S}_2$ set of first- and second-order differential operators [p. 434]
$T^h(x)$ triangle function of height h [Eq. (4.28)]
$\mathbb{T}_a$ translation operator [Eqs. (4.36a), (7.27)]
$\mathscr{U}$ set of unitary matrixes [p. 14]

$\mathscr{V}^N$ N-dimensional complex vector space [Sect. 1.1]
W Heisenberg–Weyl group [p. 418]
W_f equivalent width of $f(q)$ [Eqs. (4.69a), (7.222)]
$\mathbf{W}(t)$ Gauss–Weierstrass transform matrix [Eq. (9.67)]
$\mathbb{W}(x, y, z)$ (Heisenberg–Weyl) $\mathbb{W}$ transform operator [Eqs. (10.3)]
$\mathbb{Z}^\dagger, \mathbb{Z}$ harmonic oscillator raising and lowering operators [Eqs. (7.160)]

$\Gamma(x)$ gamma function [Appendix A]
$\mathbf{\Gamma}(g)$ 6×6 matrix representation of the inhomogeneous canonical transformation g [Eqs. (10.38)]
$\delta(q)$ Dirac δ [Eqs. (4.79), (7.85)]
$\delta^{(n)}(q)$ nth derivative of the Dirac δ [Eqs. (4.94), (7.87)]
$\boldsymbol{\delta}_y,\ y \in \mathscr{I}$ Dirac's generalized basis [pp. 133, 183]
$\delta_{m,n}$ Kronecker δ [Eq. (1.6)]
Δ_f dispersion of $f(q)$ [Eq. (7.217)]
$\mathbf{\Delta}$ matrix representative of $\mathbb{\Delta}$ in the ε-basis [Eq. (1.60)]
$\tilde{\mathbf{\Delta}}$ matrix representative of $\mathbb{\Delta}$ in the $\boldsymbol{\varphi}$-basis [Eq. (1.62)]
$\mathbb{\Delta}$ second-difference operator [p. 21]
$\{\boldsymbol{\varepsilon}_n\}_{n=1}^N$ basis for $\mathscr{V}^N$ [Sect. 1.1]
$\boldsymbol{\varepsilon}^m(t)$ lattice fundamental solutions [Eqs. (2.41), (2.42)]
$\theta(x, t)$ (Jacobi) theta function [Eq. (4.64)]
$\Theta(q)$ Heaviside theta function [Eq. (7.89)]
$\Theta_\varepsilon(q)$ causal exponentially damped function [Eq. (7.123)]
$\nu_M(q, q^*)$ weight function for the $\mathbb{C}_M$ transform space [Eq. (9.47)]
$\Upsilon_c(q)$ coherent states [Eqs. (7.188)]
$\{\boldsymbol{\varphi}_n\}_{n=1}^N$ finite Fourier transform basis [Eqs. (1.52)]
$\boldsymbol{\varphi}^m(t)$ lattice normal modes [Eqs. (2.46)]
$\varphi_n(x)$ imaginary exponential functions [Eq. (4.9)]
$\varphi_n(x, t)$ vibrating string normal modes [Eqs. (5.31)]
$\varphi_n{}^y(t)$ infinite lattice normal modes [Eqs. (5.52)]
$\varphi_{n_1,n_2}(x_1, x_2, t)$ rectangular membrane normal modes [Eq. (6.12)]
$\varphi_{mn}^{\bigcirc}(r, \phi, t)$ circular membrane normal modes [Eq. (6.27)]
$\varphi_{mn}^{\circlearrowright}(r, \phi, t)$ sectorial membrane normal modes [Eq. (6.34)]
$\chi_\lambda{}^{\pm}(q)$ repulsive oscillator wave functions [Eqs. (7.203)]
$\Psi_n(q), \Psi_n{}^h(q)$ harmonic oscillator wave functions [Eq. (7.166)]
$\Psi_\lambda{}^{\cdot, H}(q, t)$ time evolution of $\Psi_\lambda{}^{\cdot}(q)$ under the diffusion equation [Eqs. (10.27), (10.28), (10.32), (10.33)]
$\mathbf{\Omega}$ symplectic 2×2 metric matrix [Eqs. (10.8), (10.39) *et seq.*]
Ω^ω class of operators in the same orbit as $\mathbb{H}^\omega$ [Eq. (10.40)].
$\binom{m}{\pi(m)}$ permutation [p. 14]
$\mathbb{\nabla}$ differentiation operator
$\mathbb{\nabla}^2, \mathbb{\Delta}$ Laplacian operator

Index

The most basic account of a topic is indicated by an italic page number.