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 suggested 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

$$f(q) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dp\tilde{f}(p)\exp(ipq) =: (\mathbb{F}^{-1}\tilde{\mathbf{f}})(q), \tag{7.1a}$$

$$\tilde{f}(p) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dqf(q)\exp(-ipq) =: (\mathbb{F}\mathbf{f})(p). \tag{7.1b}$$

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

$$(\mathbf{f}, \mathbf{g}) := \int_{-\infty}^{\infty} dqf(q)^*g(q) = \int_{-\infty}^{\infty} dp\tilde{f}(p)^*\tilde{g}(p) = (\mathbb{F}\mathbf{f}, \mathbb{F}\mathbf{g}) \tag{7.2}$$

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 $q' \in \mathscr{R}$,

$$\lim_{L\to\infty} (2\pi)^{-1/2}\int_{-L}^{L} dp\left[(2\pi)^{-1/2}\int_{-\infty}^{\infty} dqf(q)\exp(-ipq)\right]\exp(ipq')$$
$$= \lim_{\varepsilon\to 0}\tfrac{1}{2}[f(q'+\varepsilon)+f(q'-\varepsilon)]. \tag{7.3}$$

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

$$\begin{aligned} I(s) &:= \lim_{L\to\infty} \int_0^L dp p^{-1} \sin ps \\ &= \operatorname{sign} s \lim_{v\to\infty} \int_0^b dy y^{-1} \sin vy, \end{aligned} \tag{7.7}$$

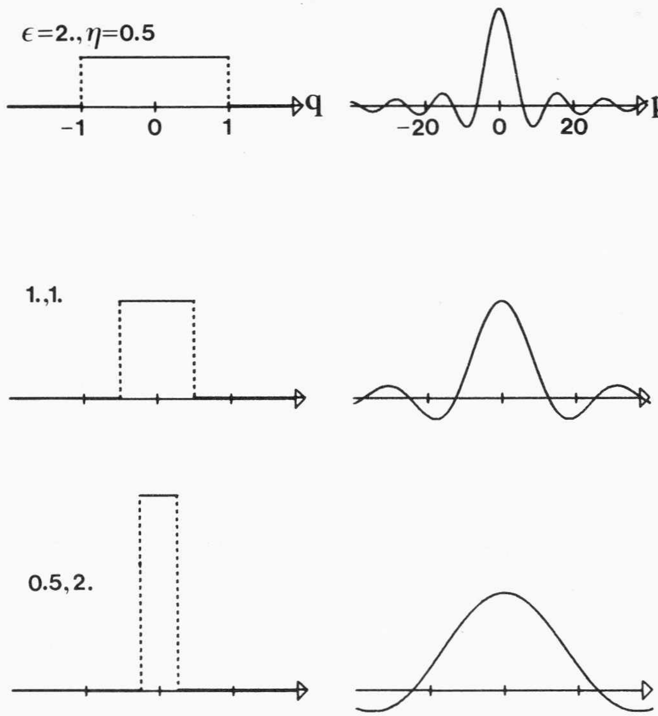

Fig. 7.1. The rectangle function $R^{(\varepsilon,\eta)}(q)$ (right) and its Fourier transform $\tilde{R}^{(\varepsilon,\eta)}(p)$ (left) for various values of ε and η such that $\varepsilon\eta = 1$.

where we have changed variables to $y := bp/L$ and $v := |s|L/b$, $b > 0$, 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

$$[I(s)\,\mathrm{sign}(s) - \pi/2] = \lim_{v\to\infty} \int_0^b dy g(y) \sin vy, \tag{7.9a}$$

$$g(y) := 1/y - \pi[2b \sin(\pi y/2b)]^{-1}. \tag{7.9b}$$

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

$$\lim_{v\to\infty} v^{-1}\left[-g(y)\cos vy\,|_0^b + \int_0^b dy g'(y)\cos vy\right] = 0. \tag{7.9c}$$

We conclude that

$$\lim_{v\to\infty} \int_0^b dy y^{-1}\sin vy = \pi/2, \tag{7.10a}$$

and hence

$$\lim_{L\to\infty} \int_{-L}^{L} dp p^{-1}\sin ps = \pi \operatorname{sign} s. \tag{7.10b}$$

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

$$\tilde{R}(p) = (2\pi)^{-1/2}\eta i p^{-1}[\exp(-ibp) - \exp(-iap)]. \tag{7.12}$$

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

$$(2\pi)^{-1}\int_{-\infty}^{\infty} dq f(q) \int_{-L}^{L} dp \exp[ip(q' - q)]$$
$$= \pi^{-1}\int_{-\infty}^{\infty} dq f(q + q')q^{-1} \sin Lq. \quad (7.13)$$

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

$$\lim_{v\to\infty} \int_a^b dy f(y + c)y^{-1} \sin vy = \begin{cases} \frac{1}{2}\pi[f(c^+) + f(c^-)] & \text{if } a < 0 < b, \\ \frac{1}{2}\pi f(c^+) & \text{if } a = 0 < b \\ \frac{1}{2}\pi f(c^-) & \text{if } a < 0 = b \\ 0 & \text{when } 0 \notin [a, b], \end{cases} \quad (7.14)$$

where $f(c^+) := \lim_{\varepsilon\to 0} f(c + \varepsilon)$, $\varepsilon > 0$. 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

$$s_M(q) := \begin{cases} q, & q \in (-M/2, M/2), \\ 0, & \text{otherwise,} \end{cases} \quad (7.15a)$$

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

$$\lim_{L\to\infty} \int_{-L}^{L} dp \tilde{f}(p)^* \tilde{g}(p) = \int_{-\infty}^{\infty} dq f(q)^* g(q). \tag{7.17}$$

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

$$\left|\int_{-\infty}^{\infty} dq f(q)^* g(q)\right|^2 \leqslant \left[\int_{-\infty}^{\infty} dq\,|f(q)|^2\right]\left[\int_{-\infty}^{\infty} dq\,|g(q)|^2\right], \tag{7.18b}$$

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

$$\begin{aligned} \left|\int_{-\infty}^{\infty} dq f(q)^* g(q)\right| &\leqslant \int_{-\infty}^{\infty} dq\,|f(q)^* g(q)| \\ &\leqslant \left[\int_{-\infty}^{\infty} dq\,|f(q)|^p\right]^{1/p}\left[\int_{-\infty}^{\infty} dq\,|g(q)|^{p'}\right]^{1/p'} \end{aligned} \tag{7.18c}$$

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

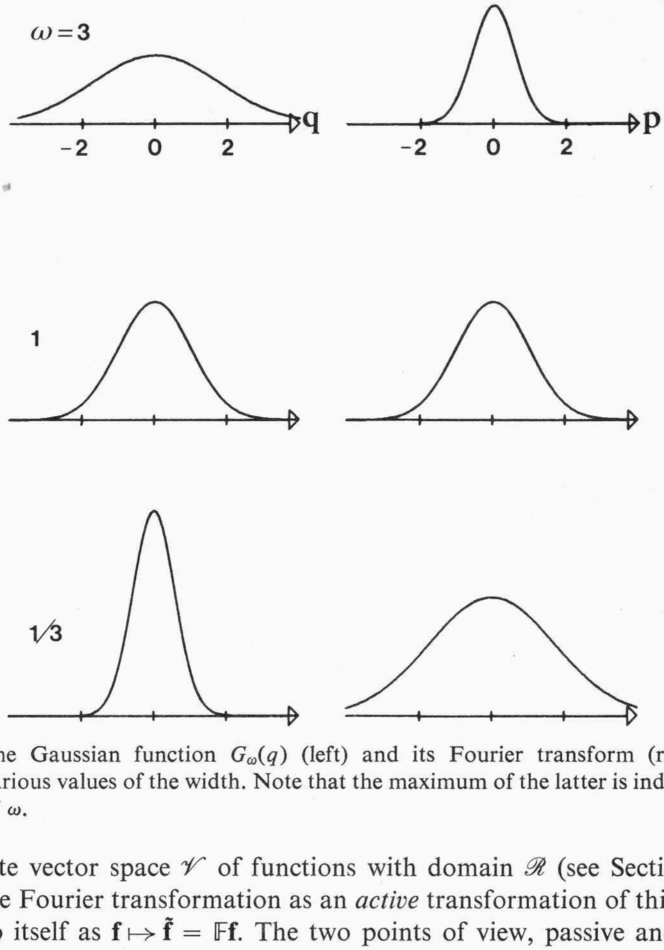

Fig. 7.2. The Gaussian function $G_\omega(q)$ (left) and its Fourier transform (right) for various values of the width. Note that the maximum of the latter is independent of ω.

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 $h(q) := af(q) + bg(q)$, $a, b \in \mathscr{C}$, 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

$$(\mathbb{T}_y\mathbf{f})(q) := f(q + y), \tag{7.27}$$

has the following property under Fourier transformation:

$$\begin{aligned}\widetilde{(\mathbb{T}_y\mathbf{f})}(p) &= (\mathbb{F}(\mathbb{T}_y\mathbf{f}))(p) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq(\mathbb{T}_y\mathbf{f})(q)\exp(-ipq)\\ &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dqf(q+y)\exp(-ipq)\\ &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq'f(q')\exp[-ip(q'-y)]\\ &= \exp(iyp)(\mathbb{F}\mathbf{f})(p) = \exp(iyp)\tilde{f}(p).\end{aligned} \tag{7.28}$$

[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.,

$$(\mathbb{E}_x\mathbf{f})(q) := \exp(ixq)f(q) \tag{7.29}$$

(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

$$(f\cdot g)(q) := f(q)g(q), \qquad q \in \mathscr{R}, \tag{7.41}$$

while we define the *convolution* of $f(q)$ and $g(q)$ as

$$(f * g)(q) := \int_{-\infty}^{\infty} dq' f(q')g(q - q') = \int_{-\infty}^{\infty} dq' f(q - q')g(q'), \qquad q \in \mathscr{R}. \tag{7.42}$$

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

$$(2\pi)^{-1/2}\int_{-\infty}^{\infty} dq(-iq)^m f(q)\exp(-ipq) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dq f(q)\frac{d^m}{dp^m}\exp(-ipq). \tag{7.53}$$

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.,

$$(\mathbb{Q}\mathbf{f})(z) := zf(z), \tag{7.55}$$

where z may be q, p, or any other dummy variable. Similarly, letting

$$(\mathbb{P}\mathbf{f})(z) := -i\frac{d}{dz}f(z) \tag{7.56}$$

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

$$\begin{aligned}(\mathbf{f}, \mathbb{P}\mathbf{g}) &= -i\int_{-\infty}^{\infty} dq f(q)^* \frac{d}{dq} g(q) = -if(q)^* g(q)\Big|_{-\infty}^{\infty} \\ &\quad + i\int_{-\infty}^{\infty} dq \left[\frac{d}{dq}f(q)\right]^* g(q) = (\mathbb{P}\mathbf{f}, \mathbf{g}).\end{aligned} \tag{7.58b}$$

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,

$$[\mathbb{Q}, \mathbb{P}] := \mathbb{Q}\mathbb{P} - \mathbb{P}\mathbb{Q} = i\mathbb{1}. \qquad (7.59b)$$

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

$$\mathbb{H}^{l}\psi(q) := (\tfrac{1}{2}\mathbb{P}^2 + \mathbb{Q})\psi(q) = \left(-\tfrac{1}{2}\frac{d^2}{dq^2} + q\right)\psi(q) = 0. \qquad (7.61)$$

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

$$\psi(q) = c(2\pi)^{-1/2}\int_{-\infty}^{\infty} dp\,\exp(ip^3/6 - ipq) =: c(2\pi)^{1/2}2^{1/3}\,\mathrm{Ai}\,(2^{1/3}q). \quad (7.64)$$

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 $f^{(-1)}(x) := \int_c^x dx' f(x')$, 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)],

$$\mathbb{T}_y = \exp(iy\mathbb{P}) := \sum_{n=0}^{\infty} \frac{(iy)^n}{n!} \mathbb{P}^n. \tag{7.69}$$

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,

$$\exp(ix\mathbb{Q})f(q) := \sum_{n=0}^{\infty} \frac{(ix)^n}{n!} \mathbb{Q}^n f(q) = \exp(ixq)f(q) =: \mathbb{E}_x f(q). \tag{7.70}$$

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	$f(q + y)$	$\exp(iyp)\tilde{f}(p)$
	$\exp(-ixq)f(q)$	$\tilde{f}(p + x)$
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	$d^nf(q)/dq^n$	$(ip)^n\tilde{f}(p)$
	$(-iq)^nf(q)$	$d^n\tilde{f}(p)/dp^n$

Table 7.2 Relation between Some Properties of a Function and Those of Its Fourier Transform

Property	$f(q)$	$\tilde{f}(p)$
Parity	Even	Even
	Odd	Odd
Complex conjugation	Real	$\tilde{f}(-p)^* = \tilde{f}(p)$
	Imaginary	$\tilde{f}(-p)^* = -\tilde{f}(p)$
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)	$f(q) = 0, q < a$	$\lvert\tilde{f}(p)\rvert \leqslant C \exp(-a\lvert\text{Im}\, p\rvert)$; $\tilde{f}(p)$ entire analytic in $\text{Im}\, p < 0$ half-plane
	$f(q) = 0, q > b$	$\lvert\tilde{f}(p)\rvert \leqslant C' \exp(b\, \text{Im}\, p)$; $\tilde{f}(p)$ entire analytic in $\text{Im}\, p > 0$ 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

$$\delta^k(q) := \tilde{R}^{[k,(2\pi)^{-1/2}]}(q) = (\pi q)^{-1}\sin(kq/2), \qquad R^{(1/k,k)}(q), \qquad G_{1/k}(q). \tag{7.83}$$

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

$$f^k(q) := \int_{-\infty}^{\infty} dq' f(q - q')\delta^k(q'). \tag{7.84}$$

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,

$$\begin{aligned}(\Theta' * f)(q) &= \int_{-\infty}^{\infty} dq'\Theta'(q')f(q-q') = -\int_{-\infty}^{\infty} dq'\Theta(q')\, df(q-q')/dq' \\ &= -\int_{0}^{\infty} dq'\, df(q-q')/dq' = f(q) = (\delta * f)(q).\end{aligned} \tag{7.91}$$

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

$$\delta(cq) = |c|^{-1}\delta(q). \tag{7.97}$$

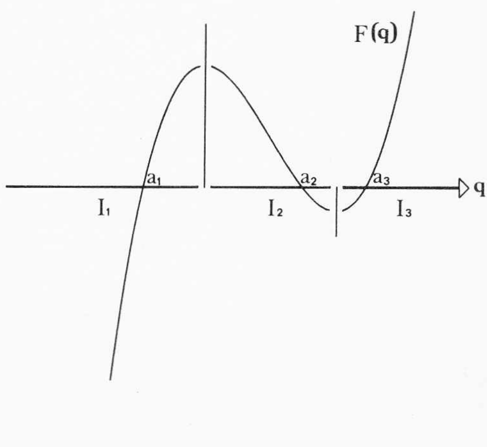

Fig. 7.3. A function broken into its monotonic segments.

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 $U(\mathbb{P})$, $\mathbb{P} := -i d/dq$, 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:

$$\tilde{G}_q(p) = [(2\pi)^{1/2}U(p)]^{-1}\exp(-ipq') = (\mathbb{E}_{-q'}\tilde{\mathbf{V}})(p), \tag{7.104a}$$

$$\tilde{V}(p) := (2\pi)^{-1/2}/U(p). \tag{7.104b}$$

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 $\tilde{f}(p)^{-1} := 1/\tilde{f}(p)$ 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

$$p_\pm := ic/2M \pm [k/M - (c/2M)^2]^{1/2} =: i\Gamma \pm p_e, \tag{7.113a}$$

$$\Gamma := c/2M \geqslant 0, \qquad p_e := (p_0{}^2 - \Gamma^2)^{1/2}, \qquad p_0 := (k/M)^{1/2}. \tag{7.113b}$$

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.

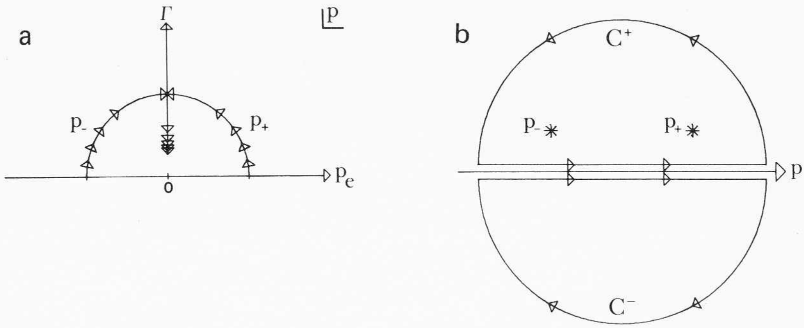

Fig. 7.4. (a) Migration of the complex oscillation frequency poles as a function of the damping constant c. The arrows indicate the points in the complex p-plane where $c = 2(kM)^{1/2}\kappa$ for $\kappa = 0.2, 0.4, \ldots, 1$ (damped oscillating and critical cases) and $\kappa = 1.2, 1.4, \ldots, 2$ (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

$f'_a := df(q)/dq\,|_{q=a}$. 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 $f_b := f(b)$ and $f'_b := df(q)/dq\,|_{q=b}$ 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

$$(\widetilde{f'})_{ab}(p) = (2\pi)^{-1/2}\exp(-ipq)f(q)|_{q=a}^{b} + ip\tilde{f}_{ab}(p), \tag{7.120a}$$

$$(\widetilde{f''})_{ab}(p) = (2\pi)^{-1/2}ip\exp(-ipq)f(q)|_{q=a}^{b} + (2\pi)^{-1/2}\exp(-ipq)f'(q)|_{q=a}^{b} - p^2\tilde{f}_{ab}(p). \tag{7.120b}$$

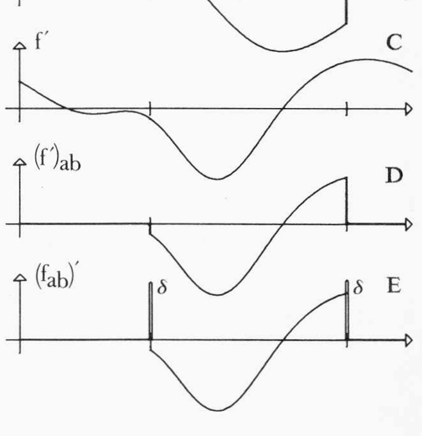

Fig. 7.5. Cuts, derivatives, and cut derivatives. (A) An "arbitrary" uncut function $f(q)$. (B) The cut function $f_{ab}(q)$. (C) The derivative of $f(q)$. (D) The cut derivative. (E) Derivative of the cut function.

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-

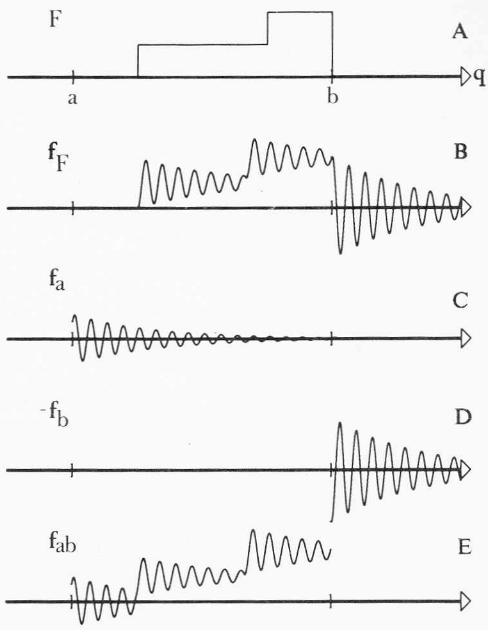

Fig. 7.6. Driving force and causal response. (A) The applied driving force during the time interval $[a, b]$. (B) The pure time-unlimited response of the system to the driving force. (C) "Arbitrary" initial conditions to the measurement process. (D) Boundary conditions at $q = b$ due to the the cut of 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 $[a, \infty)$:

$$\Theta_\varepsilon(q - a) = (\mathbb{T}_{-a}\boldsymbol{\Theta}_\varepsilon)(q) := \begin{cases} \exp[-\varepsilon(q - a)], & q < a, \\ \frac{1}{2}, & q = a, \\ 0, & q < a, \ \mathrm{Re}\,\varepsilon > 0. \end{cases} \tag{7.123}$$

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

$$(\mathbb{F}\mathbb{T}_b \mathbb{I}_0 \boldsymbol{\Theta}_\varepsilon)(p) = i(2\pi)^{-1/2}(p + i\varepsilon)^{-1} \exp(-ibp), \tag{7.132}$$

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 $\tilde{f}(p)$:

$$\tilde{f}_{a\infty}(p) = \lim_{\varepsilon\to 0^+} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p' - i\varepsilon)^{-1} \exp[-ia(p - p')]\tilde{f}(p'), \tag{7.135a}$$

$$\tilde{f}_{-\infty b}(p) = -\lim_{\varepsilon\to 0^+} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p' + i\varepsilon)^{-1} \exp[-ib(p - p')]\tilde{f}(p'), \tag{7.135b}$$

$$\begin{aligned}\tilde{f}_{ab}(p) = {}& (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p')^{-1} \\ & \times \{\exp[-ia(p - p')] - \exp[-ib(p - p')]\}\tilde{f}(p'),\end{aligned} \tag{7.135c}$$

$$\begin{aligned}\tilde{f}(p) = {}& \lim_{\varepsilon\to 0} (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'[(p - p' - i\varepsilon)^{-1} - (p - p' - i\varepsilon)^{-1}] \\ & \times \exp[-ic(p - p')]\tilde{f}(p').\end{aligned} \tag{7.135d}$$

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

$$\hat{f}_c(p) := (2\pi i)^{-1} \int_{-\infty}^{\infty} dp'(p - p')^{-1} \exp[-ic(p - p')]\tilde{f}(p'), \qquad \operatorname{Im} p \neq 0, \tag{7.136}$$

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 $C_\delta^{\mp}$

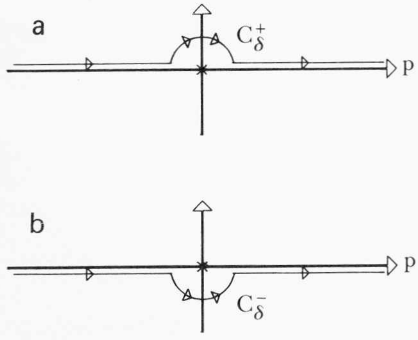

Fig. 7.7. Deformation of the integration contour as the integrand poles slide onto the real axis (a) from below and (b) from above.

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:

$$\mathscr{P}\int_{-\infty}^{\infty} dpp^{-1}F(p) := \lim_{\delta\to 0}\left(\int_{-\infty}^{-\delta} + \int_{\delta}^{\infty}\right) dpp^{-1}F(p). \tag{7.138}$$

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

$$(2\pi i)^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'p'^{-1}\exp[ip'(q - c)]$$

$$= \pi^{-1}\lim_{\substack{\delta\to 0\\ L\to\infty}}\int_{\delta}^{L} dp'p'^{-1}\sin[p'(q - c)] = \tfrac{1}{2}\operatorname{sign}(q - c), \tag{7.142}$$

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

$$\widetilde{s'_{a\infty}}(p) = (2\pi)^{1/2}\tilde{\varphi}_{0\infty}(p)\tilde{s}_{a\infty}(p). \tag{7.149}$$

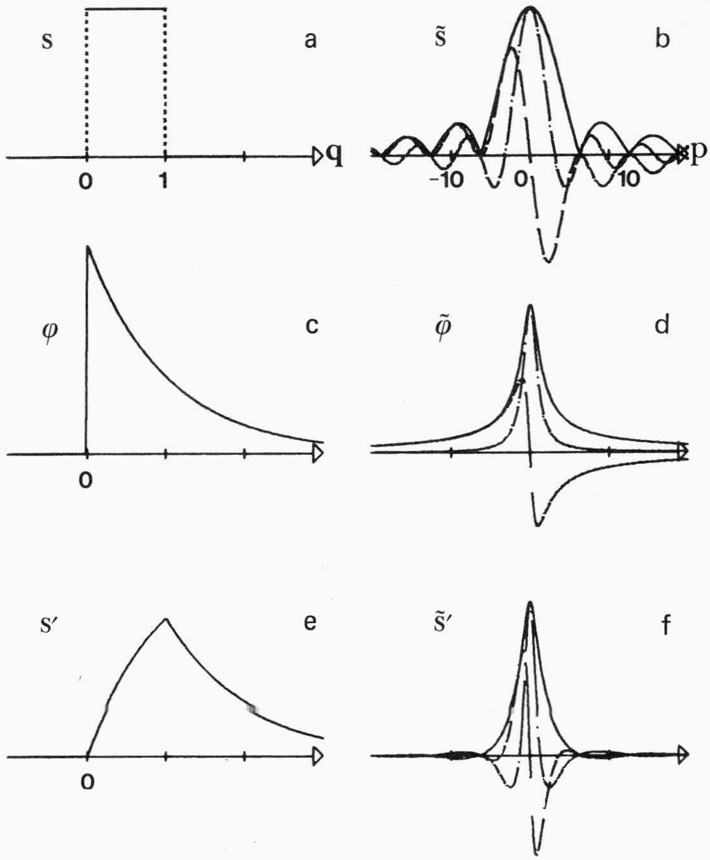

Fig. 7.8. Causal filtering. (a) "Rectangular" signal and (b) its Fourier transform, showing the real and imaginary parts (broken lines) and absolute value (continuous line). (c) Causal filter function $\varphi_{0\infty}$, a decreasing exponential, and (d) its Fourier transform. (e) Causal output signal, 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

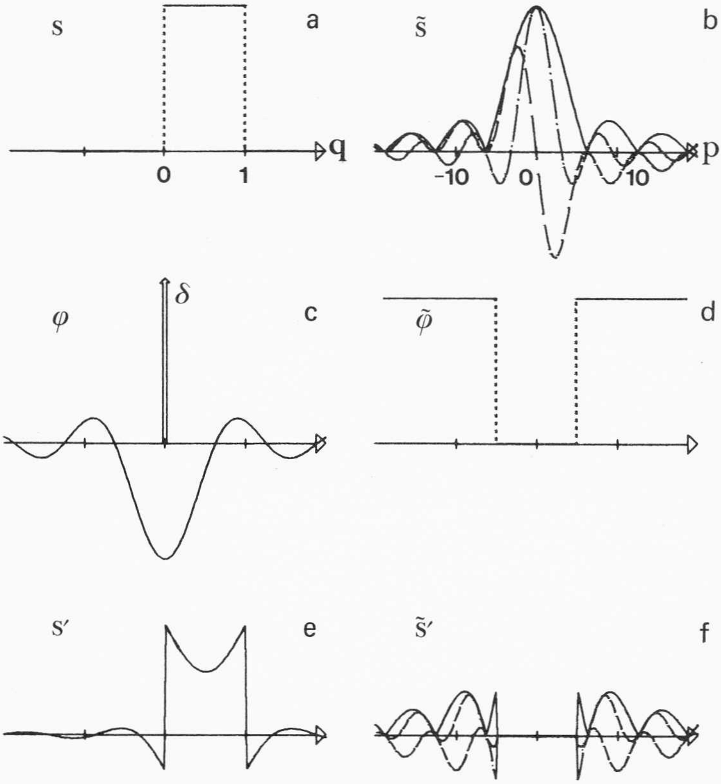

Fig. 7.9. Noncausal filtering. (a) The signal and (b) its Fourier transform—the same as in Figure 7.8. (c) Noncausal filter function built by specifying that its Fourier transform (d) eliminate all partial waves $p \in (-5, 5)$: it is a Dirac δ due to the "background" minus the Fourier transform of the 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

$$\tilde{\varphi}(p) = (2\pi)^{-1/2}[\alpha(p) + i\beta(p)], \qquad \alpha(p), \beta(p) \text{ real for } p \text{ real.} \tag{7.150}$$

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:

$$s(q) = \cos \omega q, \tag{7.151a}$$

$$\tilde{s}(p) = (\pi/2)^{1/2}[\delta(p - \omega) + \delta(p + \omega)]. \tag{7.151b}$$

By taking into account the parity of $\alpha(p)$ and $\beta(p)$ in (7.150), the output signal will be

$$\begin{aligned} \tilde{s}'(p) &= (\pi/2)^{1/2}\{\alpha(p)[\delta(p - \omega) + \delta(p + \omega)] + i\beta(p)[\delta(p - \omega) + \delta(p + \omega)]\} \\ &= (\pi/2)^{1/2}\{\alpha(\omega)[\delta(p - \omega) + \delta(p + \omega)] + i\beta(\omega)[\delta(p - \omega) - \delta(p + \omega)]\} \end{aligned} \tag{7.152a}$$

$$s'(q) = \alpha(\omega) \cos \omega q + \beta(\omega) \sin \omega q. \tag{7.152b}$$

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

$$\alpha(p) = \pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}\beta(p), \tag{7.153a}$$

$$\beta(p) = -\pi^{-1}\mathscr{P}\int_{-\infty}^{\infty} dp'(p - p')^{-1}\alpha(p). \tag{7.153b}$$

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,

$$\Psi_0(q) := 2^{1/2}\pi^{1/4}G_1(q) = \pi^{-1/4}\exp(-q^2/2), \tag{7.156}$$

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

$$\lambda\mathbb{Z} = \mathbb{F}\mathbb{Z}\mathbb{F}^{-1} = a\mathbb{F}\mathbb{Q}\mathbb{F}^{-1} + b\mathbb{F}\mathbb{P}\mathbb{F}^{-1} = -a\mathbb{P} + b\mathbb{Q}, \tag{7.159}$$

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

$$\mathbb{Z} := 2^{-1/2}(\mathbb{Q} + i\mathbb{P}) = 2^{-1/2}\left(q + \frac{d}{dq}\right), \tag{7.160a}$$

$$\mathbb{Z}^\dagger := 2^{-1/2}(\mathbb{Q} - i\mathbb{P}) = 2^{-1/2}\left(q - \frac{d}{dq}\right). \tag{7.160b}$$

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 $\lambda = -i$, $\mathbb{Z}^\dagger\boldsymbol{\Psi}_0$ will be also; $(\mathbb{Z}^\dagger)^2\boldsymbol{\Psi}_0$ will correspond to $\lambda = -1$, $(\mathbb{Z}^\dagger)^3\boldsymbol{\Psi}_0$ to $\lambda = i$, and $(\mathbb{Z}^\dagger)^4\boldsymbol{\Psi}_0$ to $\lambda = 1$. Now, functions corresponding to different eigenvalues of unitary (or hermitian) operators are orthogonal. In fact we shall show that all $\boldsymbol{\Psi}_n := c_n(\mathbb{Z}^\dagger)^n\boldsymbol{\Psi}_0$ 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 $m > n$, $(\boldsymbol{\Psi}_n, \boldsymbol{\Psi}_m)$ is proportional to

$$\begin{aligned}((\mathbb{Z}^\dagger)^n\boldsymbol{\Psi}_0, (\mathbb{Z}^\dagger)^m\boldsymbol{\Psi}_0) &= (\mathbb{Z}^m(\mathbb{Z}^\dagger)^n\boldsymbol{\Psi}_0, \boldsymbol{\Psi}_0) \\ &= ((\mathbb{Z}^\dagger)^n\mathbb{Z}^m\boldsymbol{\Psi}_0, \boldsymbol{\Psi}_0) + ([\mathbb{Z}^m, (\mathbb{Z}^\dagger)^n]\boldsymbol{\Psi}_0, \boldsymbol{\Psi}_0). \end{aligned} \tag{7.164}$$

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 $\boldsymbol{\Psi}_0$ 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:

$$(\Psi_n, \Psi_m) = \delta_{nm}. \tag{7.165b}$$

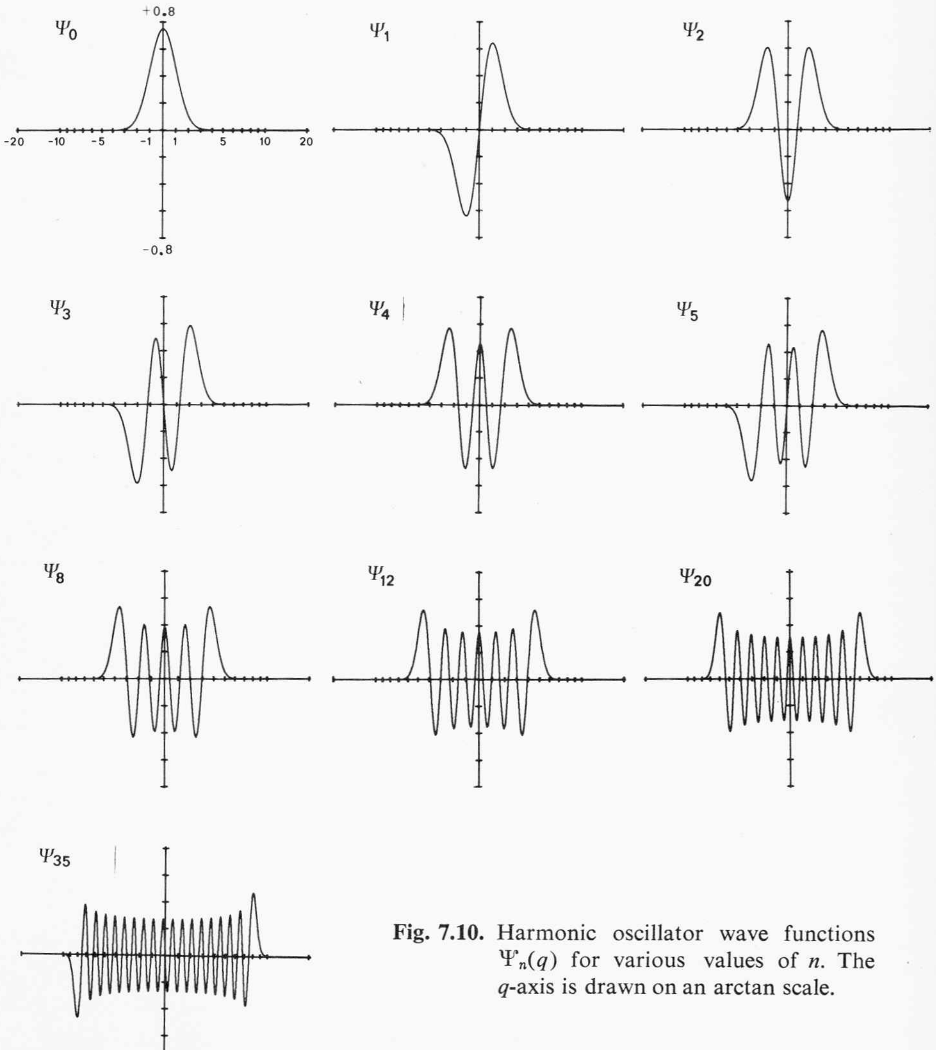

Fig. 7.10. Harmonic oscillator wave functions $\Psi_n(q)$ for various values of n. The q-axis is drawn on an arctan scale.

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

$$
\begin{aligned}
\Psi_n(q) &:= (n!)^{-1/2}(\mathbb{Z}^\dagger)^n\Psi_0(q)\\
&= (n!\,2^n)^{-1/2}\left(q - \frac{d}{dq}\right)^n \Psi_0(q)\\
&= (n!\,2^n\pi^{1/2})^{-1/2}\left(q - \frac{d}{dq}\right)^n \exp(-q^2/2)\\
&= (n!\,2^n\pi^{1/2})^{-1/2}(-1)^n \exp(q^2/2)d^n/dq^n \exp(-q^2)\\
&=: (n!\,2^n\pi^{1/2})^{-1/2}H_n(q)\exp(-q^2/2).
\end{aligned}
\tag{7.166}
$$

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:

$$(\mathbb{F}\Psi_n)(q) = \exp(-i\pi n/2)\Psi_n(q). \tag{7.167}$$

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

$$\mathbb{Z}^\dagger\Psi_n = (n!)^{-1/2}(\mathbb{Z}^\dagger)^{n+1}\Psi_0 = (n+1)^{1/2}\Psi_{n+1}. \tag{7.168}$$

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

$$\begin{aligned}\mathbb{Z}\mathbf{\Psi}_n &= (n!)^{-1/2}\mathbb{Z}(\mathbb{Z}^\dagger)^n\mathbf{\Psi}_0 \\ &= (n!)^{-1/2}\{(\mathbb{Z}^\dagger)^n\mathbb{Z} + [\mathbb{Z}, (\mathbb{Z}^\dagger)^n]\}\mathbf{\Psi}_0 \\ &= (n!)^{-1/2}n(\mathbb{Z}^\dagger)^{n-1}\mathbf{\Psi}_0 = n^{1/2}\mathbf{\Psi}_{n-1};\end{aligned} \tag{7.169}$$

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

$$\begin{aligned}\mathbb{N}\Psi_n(q) &:= \mathbb{Z}^\dagger\mathbb{Z}\Psi_n(q) = n^{1/2}\mathbb{Z}^\dagger\Psi_{n-1}(q) = n\Psi_n(q) \\ &= \frac{1}{2}\left(q - \frac{d}{dq}\right)\left(q + \frac{d}{dq}\right)\Psi_n(q) = \frac{1}{2}\left(-\frac{d^2}{dq^2} + q^2 - 1\right)\Psi_n(q) \\ & \qquad n = 0, 1, 2, \ldots .\end{aligned} \tag{7.170}$$

We shall call $\mathbb{N}$ the *number* operator for the set $\{\mathbf{\Psi}_n\}_{n=0}^\infty$. 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 $\mathbf{\Psi}_n$ is an eigenfunction of $\mathbb{N}$ corresponding to an eigenvalue n, (7.172) implies that $\mathbb{Z}^\dagger\mathbf{\Psi}_n$ and $\mathbb{Z}\mathbf{\Psi}_n$ 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:

$$\mathbb{J}_+ := \tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2) + \frac{i}{4}(\mathbb{QP} + \mathbb{PQ}) = -\tfrac{1}{2}(\mathbb{Z}^\dagger)^2 =: \mathbb{J}_1 + i\mathbb{J}_2, \tag{7.174b}$$

$$\mathbb{J}_- := \tfrac{1}{4}(\mathbb{P}^2 - \mathbb{Q}^2) - \frac{i}{4}(\mathbb{QP} + \mathbb{PQ}) = -\tfrac{1}{2}\mathbb{Z}^2 = \mathbb{J}_+{}^\dagger =: \mathbb{J}_1 - i\mathbb{J}_2, \tag{7.174c}$$

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

$$\mathbb{J}_\pm\Psi_n = d_n{}^\pm\Psi_{n\pm 2}, \qquad 4|d_n{}^+|^2 = (n+1)(n+2), \qquad 4|d_n{}^-|^2 = n(n-1), \tag{7.177}$$

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., $q^m d^n \Upsilon_r(q)/dq^n \to 0$ 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 $\Upsilon_n(q)$'s is equivalent to the zero function. The denumerable set $\{\Upsilon_n(q)\}_{n=0}^\infty$ thus constitutes an *orthonormal basis* for $\mathscr{L}^2(\mathscr{R})$. To this end, we construct a *generating function* of the set:

$$\begin{aligned} G_\psi(x, q) &:= \sum_{n=0}^{\infty} (n!)^{-1/2}(x/2^{1/2})^n \Upsilon_n(q) \\ &= \pi^{-1/4} \exp(q^2/2) \sum_{n=0}^{\infty} (n!)^{-1}(-x/2)^n d^n/dq^n \exp(-q^2) \\ &= \pi^{-1/4} \exp(-q^2/2 + qx - x^2/4) \\ &= \exp(x^2/4)\Upsilon_0(q - x), \end{aligned} \tag{7.178}$$

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

$$0 = (G_\psi(x, \cdot), \mathbf{f}) = \exp(x^2/4) \int_{-\infty}^{\infty} dq \Upsilon_0(q - x) f(q), \tag{7.179}$$

which means that $(\Upsilon_0 * f)(x) = 0$. The Fourier transform of this restriction is $\Upsilon_0(y)\tilde{f}(y) = 0$, 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

$$f(q) = \sum_{n=0}^{\infty} f_n{}^\Psi \Upsilon_n(q), \tag{7.180a}$$

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 $\mathbb{V}^2$ 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:

$$\mathbb{T}_a\Psi_n(q) = \Psi_n(q + a) = \sum_{m=0}^{\infty} T_{mn}(a)\Psi_m(q), \tag{7.181a}$$

$$T_{mn}(a) = (\boldsymbol{\Psi}_m, \mathbb{T}_a\boldsymbol{\Psi}_n) = (\mathbb{T}_{-a}\boldsymbol{\Psi}_m, \boldsymbol{\Psi}_n). \tag{7.181b}$$

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:

$$\begin{aligned} T(x, y) &:= \sum_{m,n=0}^{\infty} (m!\, n!)^{-1/2}(x/2^{1/2})^m (y/2^{1/2})^n T_{mn}(a) \\ &= \int_{-\infty}^{\infty} dq G_\psi(x, q) G_\psi(y, q + a) \\ &= \pi^{-1/2} \exp[-(x^2 + y^2)/4 + ay - a^2/2] \\ &\quad \times \int_{-\infty}^{\infty} dq \exp[-q^2 + q(x + y - a)] \\ &= \exp(-a^2/4) \exp[(xy + ay - ax)/2]. \end{aligned} \tag{7.183a}$$

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)

$$\nabla^{\psi}_{mn} := \frac{\partial}{\partial a} T_{mn}(a)\big|_{a=0} = \delta_{m,n-1}(n/2)^{1/2} - \delta_{m,n+1}[(n+1)/2]^{1/2} \tag{7.185a}$$

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):

$$\begin{aligned}(\boldsymbol{\Upsilon}_c, \boldsymbol{\Upsilon}_{c'}) &= \exp[(c^{*2} + c'^2)/2](\mathbb{T}_{-2^{1/2}c}\boldsymbol{\Psi}_0, \mathbb{T}_{-2^{1/2}c'}\boldsymbol{\Psi}_0)\\ &= \exp[(c^{*2} + c'^2)/2](\boldsymbol{\Psi}_0, \mathbb{T}_{2^{1/2}c^* - 2^{1/2}c'}\boldsymbol{\Psi}_0)\\ &= \exp[(c^{*2} + c'^2)/2]T_{00}(2^{1/2}c^* - 2^{1/2}c')\\ &= \exp[(c^{*2} + c'^2)/2]\exp[-(c^* - c')^2/2] = \exp(c^*c'). \end{aligned} \quad (7.189)$$

In Part IV we shall show that the set of coherent states $\{\boldsymbol{\Upsilon}_c\}_{c\in\mathscr{C}}$ 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 $\boldsymbol{\Psi}$ partial-wave coefficients of a linear combination of functions are the linear combination of their partial-wave coefficients. (b) The functions of the $\boldsymbol{\Psi}$-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 $\boldsymbol{\Psi}$ 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 $\boldsymbol{\Psi}$ coefficients of $qf(q)$ can be found in terms of those of $f(q)$ as in Table 7.4. (g) The role of $\mathbb{V}$ 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 $\boldsymbol{\Psi}$ coefficients f_n^ψ, those of $(-d^2/dq^2 + q^2)\cdot f(q)$ will be $(2n + 1)f_n^\psi$. (h) The $\boldsymbol{\Psi}$ 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),

$$(\mathbb{F}\mathbf{\Psi}_n)(q) = \exp(-i\pi n/2)\Psi_n(q) = \exp[-\tfrac{1}{2}i\pi(\mathbb{H}^h - \tfrac{1}{2})]\Psi_n(q). \tag{7.196}$$

The last term is an exponentiated operator with the action of the Fourier transform on all elements of the $\mathbf{\Psi}$-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 $q\,d/dq$, 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 $\chi_\lambda(q) = \exp[\zeta(q)]v_\lambda(q)$ 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,

$$\mathbb{H}^r\chi_\lambda(q) = -\frac{1}{2}\exp(cq^2)\left[\frac{d^2}{dq^2} + 4cq\frac{d}{dq} + 2c + (4c^2 + 1)q^2\right]v_\lambda(q). \tag{7.199}$$

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.,

$$\left[2\sigma i p \frac{d}{dp} + p^2 - (2\lambda - \sigma i)\right]\tilde{v}_\lambda(p) = 0. \tag{7.201b}$$

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

$$p_+ := \begin{cases} p, & p > 0, \\ 0, & p \leqslant 0, \end{cases} \qquad p_- := \begin{cases} 0, & p \geqslant 0, \\ -p, & p < 0. \end{cases} \tag{7.202b}$$

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:

$$\chi_\lambda{}^{\pm}(q) = C_\lambda \exp(iq^2/2) \sum_{n=0}^{\infty} [\pm 2\exp(3i\pi/4)q]^n \Gamma(n/2 - i\lambda/2 + \tfrac{1}{4})/n!, \tag{7.203b}$$

$$C_\lambda := \exp[i(\pi/8 - \tfrac{1}{2}\lambda \ln 2)] \cdot 2^{-3/2}\pi^{-1} \exp(\pi\lambda/4). \tag{7.203c}$$

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)]):

$$\chi_\lambda{}^{\pm}(q) = C'_\lambda D_{i\lambda - 1/2}(\mp 2^{1/2}\exp(3i\pi/4)q), \tag{7.203d}$$

$$C'_\lambda := \exp(i\pi/8)2^{-3/4}\pi^{-1}\exp(\pi\lambda/4)\Gamma(1/2 - i\lambda). \tag{7.203e}$$

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 $\chi_\lambda{}^{\pm}(q) \sim$

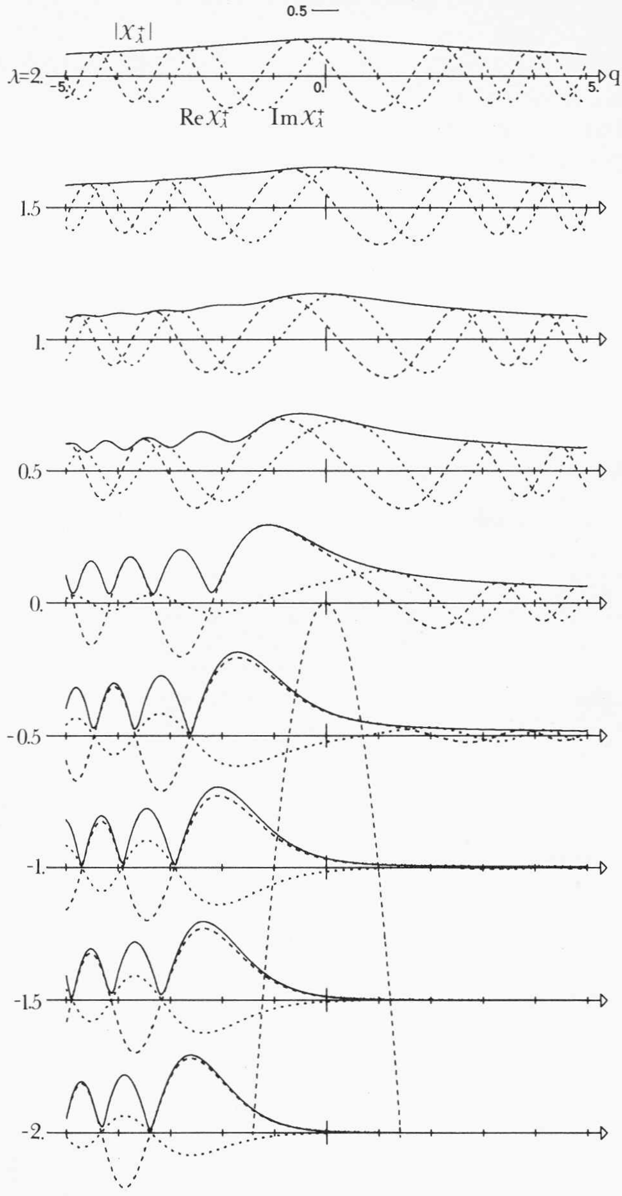

Fig. 7.11. Repulsive oscillator wave functions $\chi_\lambda{}^+(q)$ for values of λ between 2 (top) and -2 (bottom). We show the real, imaginary, and absolute values of this function by heavy dotting, light dotting, and continuous plot. The dotted parabola extending downward from $\lambda = 0$ represents 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 $p_\mp^{-1/2-i\lambda}$ 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 $p_\mp^{-1/2-i\lambda}$ 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

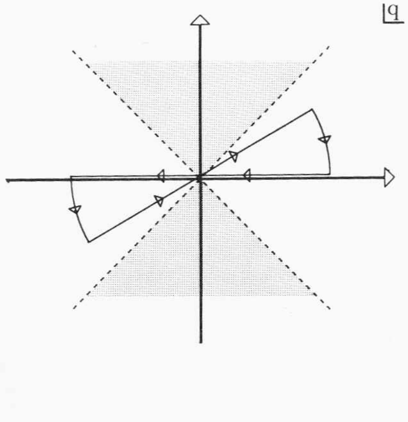

Fig. 7.12. "Bow-tie" contour deformation. Shaded areas indicate the quadrants where the Gaussian integrand diverges for $|q| \to \infty$.

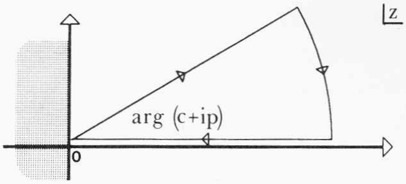

Fig. 7.13. "Sector" contour deformation. Shaded half-plane indicates asymptotic divergence.

in (7.202b). To avoid integration contours at the edges of the convergence regions, we shall first multiply the function $q_+{}^\tau$ by a decreasing exponential $\Theta_c(q) := \exp(-cq)$ and $q_-{}^\tau$ 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 $y \to 0^-$,

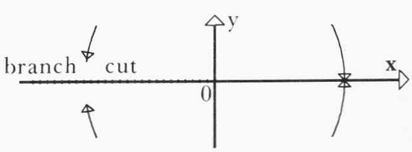

Fig. 7.14. Real limits of the complex power function. A branch cut extends along the negative real axis.

$\arg(x + iy) \to -\pi$; 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),

$$\begin{aligned}\chi_\lambda{}^\pm(q) &= 2^{i\lambda/2}\exp(iq^2/2)(\mathbb{F}^{-1}\tilde{\upsilon}_\lambda{}^\pm)(q) \\ &= 2^{1/2+i\lambda/2}\exp(i\pi/4)\exp(iq^2/2)[\mathbb{F}^{-1}(p_\pm^{-1/2-i\lambda}\mathbf{G}_{2i})](q) \\ &= 2^{i\lambda/2}(2\pi)^{-1/2}\exp(iq^2/2)[(\mathbb{F}^{-1}p_\pm^{-1/2-i\lambda}) * \mathbf{G}_{1/2i}](q).\end{aligned} \tag{7.211}$$

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,

$$(\mathbb{F}\boldsymbol{\chi}_\lambda{}^\pm)(p) = 2^{i\lambda/2}(2\pi)^{1/2}\exp(i\pi/4)[\mathbb{F}(\mathbf{G}_i\cdot\mathbb{F}^{-1}\tilde{\mathbf{v}}_\lambda{}^\pm)](p)$$
$$= 2^{i\lambda/2}(\mathbf{G}_{1/i} * \tilde{\mathbf{v}}_\lambda{}^\pm)(p)$$
$$= 2^{i\lambda/2}(2\pi)^{-1}\exp(i\pi/4)\int_{-\infty}^{\infty} dp'p'^{-1/2-i\lambda}_\pm$$
$$\times \exp[i(-p^2/2 + pp' - p'^2/4)]. \tag{7.213}$$

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* $\boldsymbol{\chi}_\lambda{}^\pm$ *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 $\boldsymbol{\chi}_\lambda{}^\pm = \mathbb{F}^{-1/2} q_\pm^{-1/2-i\lambda}$. 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 $(\boldsymbol{\chi}_\lambda{}^\pm, \boldsymbol{\chi}_{\lambda'}^\pm) = 0$ 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 $(\boldsymbol{\chi}_\lambda{}^\pm, \boldsymbol{\chi}_{\lambda'}^\mp) = 0$.

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($\mathbf{f}$) $\times$ 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

$$\overline{q^r} := \left[\int_{-\infty}^{\infty} dq q^r |f(q)|^2\right] \Big/ \left[\int_{-\infty}^{\infty} dq\, |f(q)|^2\right]. \tag{7.216}$$

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.,

$$\begin{aligned} \Delta_f &:= \left[\int_{-\infty}^{\infty} dq (q - \overline{q^1})^2 |f(q)|^2\right] \Big/ \left[\int_{-\infty}^{\infty} dq\, |f(q)|^2\right] \\ &= \|(\mathbb{Q} - \overline{q^1})\mathbf{f}\|^2/\|\mathbf{f}\|^2. \end{aligned} \tag{7.217}$$

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 **f** is in $\mathscr{L}^2(\mathscr{R})$ and $\overline{q^1} = 0$ for **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*:

$$W_f := \int_{-\infty}^{\infty} dq f(q)/f(0). \tag{7.222}$$

[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 $\|\boldsymbol{\psi}\| = 1$ 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 $\boldsymbol{\psi}$ is $\bar{s} = (\boldsymbol{\psi}, \mathbb{S}\boldsymbol{\psi})$. (e) There is a *dispersion* in the results of measurements on S given by $\Delta_\psi(S) := \|(\mathbb{S} - \bar{s})\boldsymbol{\psi}\|^2$. Note that if $\boldsymbol{\psi}$ 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,

$$\Delta_\psi(S)\cdot\Delta_\psi(R) = \|\mathbb{S}\boldsymbol{\psi}\|^2\|\mathbb{R}\boldsymbol{\psi}\|^2 \geqslant |(\mathbb{S}\boldsymbol{\psi}, \mathbb{R}\boldsymbol{\psi})|^2 \geqslant \tfrac{1}{4}|(\boldsymbol{\psi}, [\mathbb{S}, \mathbb{R}]\boldsymbol{\psi})|^2. \qquad (7.224)$$

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 $\boldsymbol{\psi}$.

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 $\boldsymbol{\psi}$, 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).