Chapter 2
Mathematical Preliminaries

Anyone taking a course in quantum mechanics usually has had several semesters of calculus and some additional advanced courses in mathematics and mathematical physics. In this chapter I review briefly some of the mathematical concepts we will need in our study of quantum mechanics.

2.1 Complex Function of a Real Variable

Since the wave function in quantum mechanics is complex, I will often be dealing with complex functions. If $\psi(x)$ is a complex function of a real variable x, then it can be written as

$$\psi(x) = u(x) + iv(x) \tag{2.1a}$$

$$= |\psi(x)|\, e^{i\phi(x)}, \tag{2.1b}$$

where the real functions,

$$u(x) = \mathrm{Re}\,[\psi(x)]\,; \tag{2.2a}$$

$$v(x) = \mathrm{Im}\,[\psi(x)]\,, \tag{2.2b}$$

are related to the *magnitude* $|\psi(x)|$ and *argument* $\phi(x)$ of $\psi(x)$ by

$$|\psi(x)| = \sqrt{[u(x)]^2 + [v(x)]^2}, \tag{2.3a}$$

$$\phi(x) = \tan^{-1}\,[v(x)/u(x)]\,, \tag{2.3b}$$

P.R. Berman, *Introductory Quantum Mechanics*, UNITEXT for Physics,
https://doi.org/10.1007/978-3-319-68598-4_2

with $-\pi/2 \leq \phi(x) \leq \pi/2$.[1] The *complex conjugate* of $\psi(x)$, denoted by $\psi^*(x)$, is defined as

$$\psi^*(x) = u(x) - iv(x). \tag{2.4}$$

Some equations that you will find useful are

$$|\psi(x)|^2 = \psi(x)\psi^*(x) = [u(x)]^2 + [v(x)]^2, \tag{2.5a}$$

$$e^{i\theta} = \cos\theta + i\sin\theta, \tag{2.5b}$$

$$\left|e^{i\theta}\right| = 1, \qquad \theta \text{ real}; \tag{2.5c}$$

$$e^{2\pi in} = 1, \qquad n \text{ integer}; \tag{2.5d}$$

$$e^{\pi in} = (-1)^n, \qquad n \text{ integer}. \tag{2.5e}$$

I assume that you are familiar with complex functions of a real variable, but include some review problems at the end of the chapter.

2.2 Functions and Taylor Series

In physics, we are always making approximations. Most potentials can be approximated as quadratic in a region near a potential minimum. Often we want to know the value of a function in the region of a particular point. To be able to get this information, we must know the value of the function at the point and the values of the derivatives of the function at the point. The more derivatives we know, the better we can approximate the function.

2.2.1 Functions of One Variable

This is the simplest case and the one with which you are most familiar. Consider the function shown in Fig. 2.1.

Suppose we know the value $f(x')$ at $x' = b$ and want to approximate the function at $x' = x$, when $x \approx b$. If the function were a straight line between the two points, then a knowledge of the slope of the line would be sufficient to calculate $f(x)$. One can get a better and better approximation to $f(x)$ by approximating the function between the points as a polynomial—the higher the order of the polynomial, the

[1] The restriction of $\phi(x)$ to values $-\pi/2 \leq \phi(x) \leq \pi/2$ corresponds to what is known as the *principal value* of $\tan^{-1}$. In some problems, such as those to be encountered in scattering theory, $\phi(x)$ can correspond to a physical quantity that should not be restricted to these limits.

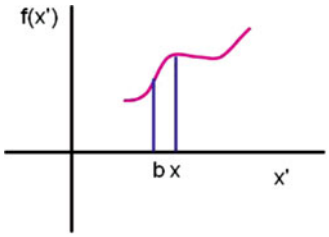

Fig. 2.1 Approximating a function $f(x')$ near $x' = b$

better the approximation. In effect, each time we add a power to the polynomial fit, we need to know one higher derivative of the function in the vicinity of $x' = b$. To proceed formally one writes

$$f^{(n-1)}(x) - f^{(n-1)}(b) = \int_b^x f^{(n)}(x'')\, dx'', \tag{2.6}$$

where $f^{(n)}(x)$ is the nth derivative of $f(x)$ and $f^{(n)}(b)$ is a shorthand notation for $f^{(n)}(x)$ evaluated at $x = b$. If you change the x to x' in this equation and integrate both sides with respect to x' from b to x, you can obtain

$$f^{(n-2)}(x) - f^{(n-2)}(b) - (x-b) f^{(n-1)}(b) = \int_b^x dx' \int_b^{x'} f^{(n)}(x'')\, dx''. \tag{2.7}$$

This procedure can be repeated to arrive at

$$\begin{aligned} &f^{(n-3)}(x) - f^{(n-3)}(b) - (x-b) f^{(n-2)}(b) - \frac{(x-b)^2}{2!} f^{(n-1)}(b) \\ &\quad = \int_b^x dx_3 \int_b^{x_3} dx_2 \int_b^{x_2} f^{(n)}(x_1)\, dx_1. \end{aligned} \tag{2.8}$$

Continuing up to n integrations, I find

$$\begin{aligned} &f(x) - f(b) - (x-b) f^{(1)}(b) \\ &\quad - \frac{(x-b)^2}{2!} f^{(2)}(b) - \cdots - \frac{(x-b)^{n-1}}{(n-1)!} f^{(n-1)}(b) \\ &\quad = \int_b^x dx_n \ldots \int_b^{x_4} dx_3 \int_b^{x_3} dx_2 \int_b^{x_2} f^{(n)}(x_1)\, dx_1. \end{aligned} \tag{2.9}$$

Solving Eq. (2.9) for $f(x)$, I obtain

$$f(x) = f(b) + (x-b) f^{(1)}(b) + \frac{(x-b)^2}{2!} f^{(2)}(b) + \cdots + \frac{(x-b)^{n-1}}{(n-1)!} f^{(n-1)}(b), \tag{2.10}$$

with a remainder that is of order $\frac{(x-b)^n}{(n)!}f^{(n)}(b)$. Equation (2.10) is known as Taylor's theorem and the sum on the right-hand side of the equation is a Taylor series of the function $f(x)$ about $x = b$. One can set $b \to y$ and $x \to y + a$ in Eq. (2.10) to write Taylor's theorem in the form

$$f(y+a) = f(y) + af^{(1)}(y) + \frac{a^2}{2!}f^{(2)}(y) + \cdots \frac{a^{n-1}}{(n-1)!}f^{(n-1)}(y), \tag{2.11}$$

with a remainder that is of order $\frac{a^n}{(n)!}f^{(n)}(y)$. In general, Eq. (2.10) converges only for $|x-b| < r_c(b)$ and Eq. (2.11) only for $|a| < r_c(y)$, where r_c is the *radius of convergence*.

As an example, I can approximate $\sqrt{27}$ by taking $b = 25$, $x = 27$, and $f(x) = \sqrt{x}$ in Eq. (2.10). If I keep only three terms in the series, I find

$$\sqrt{27} \approx \sqrt{25} + \frac{2}{2\sqrt{25}} + \frac{4}{2!}\left(-\frac{1}{2}\right)\frac{1}{2}\frac{1}{25^{3/2}} = 5.196, \tag{2.12}$$

with an expected error of order $\frac{8}{3!}\frac{1}{2}\frac{1}{2}\frac{3}{2}\frac{1}{25^{5/2}} = 0.00016$. The exact value is 5.19615 so the error is 0.00015, in agreement with the estimate of the error. The Taylor series of $\sqrt{25+x}$ converges for $|x-25| < 25$.

2.2.2 Scalar Functions of Three Variables

Next I consider scalar functions of the form $f(\mathbf{r})$. What does this mean? In this expression, $\mathbf{r} = x\mathbf{u}_x + y\mathbf{u}_y + z\mathbf{u}_z$ is the coordinate vector (I use a notation in which $\mathbf{u}_j$ is a unit vector in the j direction). If one specifies (x, y, z), then $f(\mathbf{r}) \equiv f(x, y, z)$ gives a prescription for evaluating the value of the function at that point. For example, the scalar potential associated with a point charge q located at position $\mathbf{a} = a_x\mathbf{u}_x + a_y\mathbf{u}_y + a_z\mathbf{u}_z$ is

$$V(\mathbf{r}) = V(x, y, z) = \frac{q}{4\pi\epsilon_0}\frac{1}{\sqrt{(x-a_x)^2 + (y-a_y)^2 + (z-a_z)^2}}. \tag{2.13}$$

Taylor's theorem can be extended to functions of three variables, such as $V(\mathbf{r})$. To generalize the one variable result, I use a "trick." The trick is to express the function at the new point in terms of a *single dependent variable*, as one does when writing a parametric equation for a line in terms of a single variable [e.g., $x = at, y = bt^2$]. Thus I write

$$f(\mathbf{r} + \mathbf{a}) = f(x + a_x, y + a_y, z + a_z) = f(x + \alpha t, y + \beta t, z + \gamma t), \tag{2.14}$$

where

$$a_x = \alpha t, \quad a_y = \beta t, \quad a_z = \gamma t. \tag{2.15}$$

Now I can consider $f(\mathbf{r}+\mathbf{a})$ as a function of a single variable t and use the chain rule to obtain

$$f(\mathbf{r}+\mathbf{a}) = f(\mathbf{r}) + \left.\frac{df}{dt}\right|_{t=0} t + \frac{1}{2!}\left.\frac{d^2f}{dt^2}\right|_{t=0} t^2 + \cdots, \tag{2.16}$$

where

$$\begin{aligned}\left.\frac{df}{dt}\right|_{t=0} &= \left[\begin{array}{c}\frac{\partial f}{\partial(x+\alpha t)}\frac{d(x+\alpha t)}{dt} + \frac{\partial f}{\partial(y+\beta t)}\frac{d(y+\beta t)}{dt} \\ + \frac{\partial f}{\partial(z+\gamma t)}\frac{d(z+\gamma t)}{dt}\end{array}\right]_{t=0} \\ &= \frac{\partial f}{\partial x}\alpha + \frac{\partial f}{\partial y}\beta + \frac{\partial f}{\partial z}\gamma. \end{aligned} \tag{2.17}$$

Similarly,

$$\begin{aligned}\left.\frac{d^2f}{dt^2}\right|_{t=0} &= \left[\frac{\partial f'}{\partial(x+\alpha t)}\alpha + \frac{\partial f'}{\partial(y+\beta t)}\beta + \frac{\partial f'}{\partial(z+\gamma t)}\gamma\right]_{t=0} \\ &= \frac{\partial^2 f}{\partial x^2}\alpha^2 + \frac{\partial^2 f}{\partial x\partial y}\beta\alpha + \frac{\partial^2 f}{\partial x\partial z}\gamma\alpha + \frac{\partial^2 f}{\partial y\partial x}\alpha\beta + \frac{\partial^2 f}{\partial y^2}\beta^2 \\ &\quad + \frac{\partial^2 f}{\partial y\partial z}\gamma\beta + \frac{\partial^2 f}{\partial z\partial x}\alpha\gamma + \frac{\partial^2 f}{\partial z\partial y}\beta\gamma + \frac{\partial^2 f}{\partial z^2}\gamma^2. \end{aligned} \tag{2.18}$$

Combining all terms and using Eq. (2.15), I obtain

$$\begin{aligned} f(\mathbf{r}+\mathbf{a}) &= f(\mathbf{r}) + \frac{\partial f}{\partial x}a_x + \frac{\partial f}{\partial y}a_y + \frac{\partial f}{\partial z}a_z \\ &\quad + \frac{1}{2!}\left[\begin{array}{c}\frac{\partial^2 f}{\partial x^2}a_x^2 + \frac{\partial^2 f}{\partial y^2}a_y^2 + \frac{\partial^2 f}{\partial z^2}a_z^2 \\ +2\frac{\partial^2 f}{\partial x\partial y}a_xa_y + 2\frac{\partial^2 f}{\partial x\partial z}a_xa_z + 2\frac{\partial^2 f}{\partial z\partial y}a_za_y\end{array}\right] + \cdots. \end{aligned} \tag{2.19}$$

It is easy to generate higher order terms. Note that the first derivative terms can be written as $\nabla f \cdot \mathbf{a}$ and can be used to *define* the gradient in arbitrary coordinate systems.

2.2.3 Vector Functions of Three Variables

Quantities such as scalars, vectors, tensors are often defined in terms of their transformation properties under some symmetry operation. For example, a scalar function under rotation is one that is unchanged as the coordinate axes are rotated. A vector function such as the electric field $\mathbf{E}(\mathbf{r})$ consists of *three* scalar functions $[E_x(\mathbf{r}), E_y(\mathbf{r}), E_z(\mathbf{r})]$ whose components change in a prescribed manner under a

rotation of the coordinate axes. If you want to make a Taylor series expansion of a vector function, you must expand *each* of the component functions in a Taylor series. Thus,

$$\begin{aligned}\mathbf{E}(\mathbf{r}+\mathbf{a}) \simeq \mathbf{E}(\mathbf{r}) &+ \left[\frac{\partial E_x}{\partial x}a_x + \frac{\partial E_x}{\partial y}a_y + \frac{\partial E_x}{\partial z}a_z\right]\mathbf{u}_x + \\ &+ \left[\frac{\partial E_y}{\partial x}a_x + \frac{\partial E_y}{\partial y}a_y + \frac{\partial E_y}{\partial z}a_z\right]\mathbf{u}_y \\ &+ \left[\frac{\partial E_z}{\partial x}a_x + \frac{\partial E_z}{\partial y}a_y + \frac{\partial E_z}{\partial z}a_z\right]\mathbf{u}_z \\ &= \mathbf{E}(\mathbf{r}) + (\mathbf{a}\cdot\nabla)\,\mathbf{E}(\mathbf{r}). \end{aligned} \tag{2.20}$$

The vector form in the last line is useful only in rectangular coordinates. Note that if you write $\mathbf{E}(\mathbf{r})$ using spherical or cylindrical coordinates and make a Taylor's expansion, you must make a Taylor's expansion of *both* the components *and* the unit vectors, since the unit vectors depend on the coordinates.

2.3 Vector Calculus

Most of you are familiar with the divergence or Gauss theorem and Stokes theorem. There are generalized versions of these theorems that I will need at some later time. The generalized Gauss and Stokes theorems can be stated as:

Generalized Gauss theorems:

$$\oint_S d\mathbf{a} = \int_V d\tau\nabla; \tag{2.21a}$$

$$\oint_S d\mathbf{a} f(\mathbf{r}) = \int_V d\tau\nabla f(\mathbf{r}); \tag{2.21b}$$

$$\oint_S d\mathbf{a}\cdot\mathbf{F}(\mathbf{r}) = \int_V d\tau\nabla\cdot\mathbf{F}(\mathbf{r}); \tag{2.21c}$$

$$\oint_S d\mathbf{a}\times\mathbf{F}(\mathbf{r}) = \int_V d\tau\nabla\times\mathbf{F}(\mathbf{r}), \tag{2.21d}$$

where $\oint_S$ implies a surface integral containing the volume V and $d\mathbf{a}$ is an outward normal to the surface. The differential da is an element of surface area and $d\tau$ is a volume element.

Generalized Stokes theorems:

$$\oint_C d\mathbf{l} = \int_S (d\mathbf{a} \times \boldsymbol{\nabla}) \,; \tag{2.22a}$$

$$\oint_C d\mathbf{l} f(\mathbf{r}) = \int_S (d\mathbf{a} \times \boldsymbol{\nabla}) f(\mathbf{r}); \tag{2.22b}$$

$$\oint_C d\mathbf{l} \cdot \mathbf{F}(\mathbf{r}) = \int_S (d\mathbf{a} \times \boldsymbol{\nabla}) \cdot \mathbf{F}(\mathbf{r}) = \int_S d\mathbf{a} \cdot [\boldsymbol{\nabla} \times \mathbf{F}(\mathbf{r})] \,; \tag{2.22c}$$

$$\oint_C d\mathbf{l} \times \mathbf{F}(\mathbf{r}) = \int_S (d\mathbf{a} \times \boldsymbol{\nabla}) \times \mathbf{F}(\mathbf{r}), \tag{2.22d}$$

where $\oint_C$ implies a line integral containing the surface area S and $d\mathbf{l}$ is a differential element tangent to the line. Note that $d\mathbf{a} \times \boldsymbol{\nabla}$ takes on a simple form only in rectangular coordinates.

We will often encounter expressions that involve taking the gradient or Laplacian of exponential functions, namely

$$\boldsymbol{\nabla} e^{iax} = iae^{iax} \mathbf{u}_x; \tag{2.23a}$$

$$\begin{aligned} \boldsymbol{\nabla} e^{i\mathbf{a}\cdot\mathbf{r}} &= \boldsymbol{\nabla} e^{i(a_x x + a_y y + a_z z)} \\ &= i \left(a_x \mathbf{u}_x + a_y \mathbf{u}_y + a_z \mathbf{u}_z \right) e^{i\mathbf{a}\cdot\mathbf{r}} = i\mathbf{a} e^{i\mathbf{a}\cdot\mathbf{r}}; \end{aligned} \tag{2.23b}$$

$$\nabla^2 e^{iax} = -a^2 e^{iax}; \tag{2.23c}$$

$$\nabla^2 e^{i\mathbf{a}\cdot\mathbf{r}} = -\left(a_x^2 + a_y^2 + a_z^2 \right) e^{i\mathbf{a}\cdot\mathbf{r}} = -a^2 e^{i\mathbf{a}\cdot\mathbf{r}}, \tag{2.23d}$$

where

$$\boldsymbol{\nabla} = \mathbf{u}_\mathbf{x} \frac{\partial}{\partial x} + \mathbf{u}_y \frac{\partial}{\partial y} + \mathbf{u}_z \frac{\partial}{\partial z} \tag{2.24}$$

is the gradient operator,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{2.25}$$

is the Laplacian operator, and $\mathbf{u}_j$ is a unit vector in the j direction.

2.4 Probability Distributions

You are all familiar with elementary concepts of probability theory. If you throw one die, there is a probability of $1/6$ that any number comes up. If you increase the number of sides of the die to 3 million, then the probability for any side to

come up is $1/\left(3\times10^6\right)$ (welcome to the lottery). As the number of sides increases without limit, the probability for any *specific* event to occur goes to zero, even if we know one event must occur on each trial. In the limit of the number of sides going to infinity, the probability of individual events is replaced by what is called the *probability density* $P(x)$ for an event to occur.

To illustrate the concept of a probability density, consider the probability that a point chosen at random on a line having length L is at the midpoint of the line. Of course, this probability is zero, as it is to obtain any single point in a single measurement. On the other hand, we can ask for the probability that a point chosen at random lies between x and $x+dx$. This probability is no longer equal to zero, but is given by

$$P(x)dx = dx/L, \tag{2.26}$$

since

$$P(x) = \begin{cases} 1/L & 0 \le x \le L \\ 0 & \text{otherwise} \end{cases} \tag{2.27}$$

is the probability density for a uniform distribution of points on the line.

I limit the discussion to one dimension, but extensions to higher dimensions are obvious. The probability distribution is *normalized* such that

$$\int_{-\infty}^{\infty} P(x)dx = 1. \tag{2.28}$$

The nth moment of the distribution is defined as

$$\langle x^n\rangle = \int_{-\infty}^{\infty} P(x)x^n dx. \tag{2.29}$$

The *average value* of x is the first moment,

$$\langle x\rangle = \bar{x} = \int_{-\infty}^{\infty} P(x)xdx, \tag{2.30}$$

while the *variance* of x is defined as

$$\Delta x^2 = \left\langle (x-\langle x\rangle)^2\right\rangle = \int_{-\infty}^{\infty} P(x)\left(x-\langle x\rangle\right)^2 dx = \left\langle x^2\right\rangle - \langle x\rangle^2 = \overline{x^2} - \bar{x}^2. \tag{2.31}$$

The *standard deviation* of x, denoted by Δx, is the square root of the variance. Often, but not always, the standard deviation is a measure of the width of the distribution about its mean value.

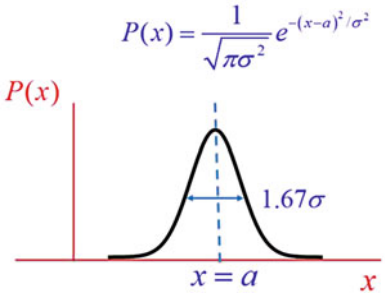

Fig. 2.2 Gaussian probability distribution

One of the most important probability distributions is the *Gaussian* or *normal* distribution defined by

$$P(x) = Ne^{-(x-a)^2/\sigma^2}, \tag{2.32}$$

where N is a normalization factor (see Fig. 2.2). To determine N, I require that

$$\int_{-\infty}^{\infty} Ne^{-(x-a)^2/\sigma^2} dx = 1. \tag{2.33}$$

The only way to evaluate *any* integral is to already know the answer—that is, you guess a solution and see if it works.[2] Fortunately, there are tables of integrals and built-in functions in computer programs that allow you to benefit from the collected guesses of many mathematicians and physicists. In this case, you will find that

$$\int_{-\infty}^{\infty} Ne^{-(x-a)^2/\sigma^2} dx = N\sigma\sqrt{\pi}, \tag{2.34}$$

which, when combined with Eqs. (2.32) and (2.33), leads to the normalized distribution

$$P(x) = \frac{1}{\sqrt{\pi}\sigma} e^{-(x-a)^2/\sigma^2}. \tag{2.35}$$

The mean or average value of x is

$$\bar{x} = \frac{1}{\sqrt{\pi}\sigma} \int_{-\infty}^{\infty} xe^{-(x-a)^2/\sigma^2} dx = a, \tag{2.36}$$

[2]Of course, you have undoubtedly learned many techniques for evaluating integrals, but these are all based on guesses that work.

as should be obvious from Fig. 2.2. The variance is

$$\Delta x^2 = \frac{1}{\sqrt{\pi}a}\int_{-\infty}^{\infty} e^{-(x-a)^2/\sigma^2}\,(x-a)^2\,dx = \frac{\sigma^2}{2}, \tag{2.37}$$

so $\Delta x = \sigma/\sqrt{2}$.

I can calculate the half-width at half maximum (HWHM) or full-width at half maximum (FWHM) of this distribution by solving the equation

$$\left|f(x_{1/2})\right|^2 = |f(\bar{x})|^2/2 = |f(a)|^2/2 \tag{2.38}$$

or

$$\frac{1}{\sqrt{\pi}\sigma}e^{-\left(x_{1/2}-a\right)^2/\sigma^2} = \frac{1}{2\sqrt{\pi}\sigma}. \tag{2.39}$$

The solution of this equation is

$$\left|x_{1/2}-a\right| = \sigma\sqrt{\ln 2} \approx 0.8326\sigma. \tag{2.40}$$

The HWHM is equal to 0.8326σ and the FWHM is equal to 1.665σ.

There can be some confusion as to the meaning of the "width" of a probability distribution. For a smooth distribution such as a Gaussian, one can define the "width" as either the HWHM or FWHM. For other distributions, the HWHM and FWHM may have no significance at all. On the other hand, the standard deviation of a probability distribution is always defined as the square root of the variance of the distribution. For some distributions, such as a Gaussian, the standard deviation and HWHM are not all that different, but for other distributions, they can differ dramatically. Some examples will help to illustrate this point.

For a uniform probability distribution

$$P(x) = \begin{cases} 1 & |x| \le 1/2 \\ 0 & \text{otherwise} \end{cases}, \tag{2.41}$$

(x is now taken as a dimensionless variable), the HWHM is equal to $1/2$, while $\Delta x = 1/\sqrt{12} = 0.29$. For a Gaussian probability distribution

$$P(x) = \frac{1}{\pi^{1/2}}e^{-x^2}, \tag{2.42}$$

the HWHM is equal to 0.83, while $\Delta x = 1/\sqrt{2} = 0.707$. For both the uniform and Gaussian distributions the HWHM's and standard deviations are comparable. However, for the *Lorentzian* probability distribution

$$P(x) = \frac{1}{\pi}\frac{1}{x^2+1}, \tag{2.43}$$

the HWHM is equal to 1, while $\Delta x = \infty$. Finally if I take $P(x)$ as the sum of two Gaussian distributions,

$$P(x) = \frac{1}{2\pi^{1/2}}\left(e^{-(x-10)^2} + e^{-(x+10)^2}\right), \tag{2.44}$$

the HWHM has no real meaning [although you could talk about the HWHM of *each* term in Eq. (2.44)], while $\Delta x = \sqrt{201/2}$. Thus, although I will often use the terms "width" and "standard deviation" interchangeably, they need not be the same at all.

2.5 Fourier Transforms

In quantum mechanics, we often need to use Fourier transforms. The wave functions in coordinate space and momentum space are Fourier transforms of one another. This topic is covered in most textbooks on mathematical physics, so I will just sketch a few of the results. The functions $f(x)$ and $a(k)$ are Fourier transforms of one another if

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} a(k)e^{ikx}dk, \tag{2.45}$$

$$a(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx, \tag{2.46}$$

assuming that these integrals exist. We can also talk about frequency-time Fourier transforms defined by

$$g(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} b(\omega)e^{-i\omega t}d\omega, \tag{2.47a}$$

$$b(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(t)e^{i\omega t}dt. \tag{2.47b}$$

In essence, the Fourier transform of a spatial function is an expansion in functions having different wavelengths or propagation constants k, while the Fourier transform of a time-dependent function is an expansion in terms of its frequency components (including negative frequencies).

There are many properties of Fourier transforms that are derived in standard textbooks. The most important property that we will encounter relates the variances Δx^2 and Δk^2. Let $f(x)$ and $a(k)$ be Fourier transforms of one another and define

$$\bar{x} = \int_{-\infty}^{\infty} x\,|f(x)|^2\,dx, \tag{2.48a}$$

$$\Delta x^2 = \int_{-\infty}^{\infty} (x-\bar{x})^2\,|f(x)|^2\,dx, \tag{2.48b}$$

$$\bar{k} = \int_{-\infty}^{\infty} k\,|a(k)|^2\,dk, \tag{2.48c}$$

$$\Delta k^2 = \int_{-\infty}^{\infty} \left(k-\bar{k}\right)^2\,|a(k)|^2\,dk. \tag{2.48d}$$

It then follows that

$$\Delta x \Delta k = \sqrt{\Delta x^2 \Delta k^2} \geq \frac{1}{2}, \tag{2.49}$$

provided all these quantities exist and the normalization is such that

$$\int_{-\infty}^{\infty} |f(x)|^2\,dx = 1. \tag{2.50}$$

I will prove Eq. (2.49) in Chap. 5. In essence, $|f(x)|^2$ can be considered to be a probability distribution in coordinate space and $|a(k)|^2$ a probability distribution in k-space. The quantities $\bar{x}$ and $\bar{k}$ are the average values or mean of the functions $|f(x)|^2$ and $|a(k)|^2$, respectively, and Δx^2 and Δk^2 are the variances in coordinate and k-space, respectively, while

$$\Delta x = \sqrt{\Delta x^2}; \qquad \Delta k = \sqrt{\Delta k^2} \tag{2.51}$$

are the standard deviations in coordinate and k-space, respectively. Thus the narrower the distribution is in k space, the wider it is in coordinate space and visa versa.

As a simple example, consider

$$f(x) = \frac{1}{(\pi\sigma^2)^{1/4}} e^{-x^2/2\sigma^2} e^{ik_0 x}, \tag{2.52}$$

for which

$$|f(x)|^2 = \frac{1}{(\pi\sigma^2)^{1/2}} e^{-x^2/\sigma^2} \tag{2.53}$$

is a Gaussian having full-width at half maximum (FWHM) equal to 1.67σ. The Fourier transform of $f(x)$ is

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) \exp(-ikx)$$
$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} dx\, e^{-x^2/2\sigma^2} e^{-i(k-k_0)x}. \tag{2.54}$$

The integral is tabulated or can be evaluated using contour integration. Explicitly, one finds

$$a(k) = \left(\frac{\sigma^2}{\pi}\right)^{1/4} e^{-(k-k_0)^2\sigma^2/2}; \tag{2.55}$$

$$|a(k)|^2 = \left(\frac{\sigma^2}{\pi}\right)^{1/2} e^{-(k-k_0)^2\sigma^2}. \tag{2.56}$$

The k-space distribution, $|a(k)|^2$, is *also* a Gaussian, centered at $k = k_0$, having FWHM equal to $1.67/\sigma$.

The variance of x is

$$\Delta x^2 = \int_{-\infty}^{\infty} dx\, x^2 |\psi(x,0)|^2 = \frac{\sigma^2}{2} \tag{2.57}$$

and the variance of k is

$$\Delta k^2 = \left\langle (k-k_0)^2 \right\rangle = \int_{-\infty}^{\infty} dk\ (k-k_0)^2 |a(k)|^2 = \frac{1}{2\sigma^2}, \tag{2.58}$$

such that

$$\Delta x \Delta k = \frac{1}{2}, \tag{2.59}$$

the minimum possible value.

Similarly, in the time domain for the distributions $|g(t)|^2$ and $|b(\omega)|^2$, one finds

$$\Delta\omega \Delta t \geq \frac{1}{2}, \tag{2.60}$$

which is known as the frequency-time uncertainty relation. The narrower the bandwidth (frequency spread) of a pulse, the wider is its time extent. As we shall see, the coordinate—k-space uncertainty relation follows from the postulates of quantum mechanics, but this is *not* the case for the frequency-time uncertainty relation. In effect, there is no probability distribution that can be associated with the time in quantum mechanics.

2.6 Dirac Delta Function

The Dirac delta function appears in many branches of physics. It is not difficult to understand why this is the case. For example, what is the density of a point charge having total charge q? Clearly, the charge density $\rho(\mathbf{r})$ equals zero everywhere but at the location of the charge. Since the volume of a point equals zero, the density at the position of the charge must be infinite. This leads us to define a function in three dimensions, $\delta(\mathbf{r})$, such that for a point charge,

$$\rho(\mathbf{r}) = q\delta(\mathbf{r}), \tag{2.61}$$

where

$$\delta(\mathbf{r}) = 0 \text{ if } \mathbf{r} \neq 0; \tag{2.62a}$$

$$\delta(\mathbf{r}) = \infty \text{ if } \mathbf{r} = 0; \tag{2.62b}$$

$$\int \delta(\mathbf{r})d\mathbf{r} = 1 \text{ if the origin is inside the integration volume;} \tag{2.62c}$$

$$\int \delta(\mathbf{r})d\mathbf{r} = 0 \text{ if the origin is outside the integration volume.} \tag{2.62d}$$

With this definition

$$\int \rho(\mathbf{r})d\mathbf{r} = q \tag{2.63}$$

as required, provided the charge is in the integration volume. Note that $\delta(\mathbf{r})$ has units of inverse volume.

The Dirac delta function is usually defined by its *integral* properties. That is, for any analytic function $f(\mathbf{r})$, it is defined by

$$\int f(\mathbf{r})\delta(\mathbf{r})d\mathbf{r} = f(0). \tag{2.64}$$

In other words, the Dirac delta function picks out the value of the function at the point where the argument of the delta function is equal to zero. The definitions given in Eqs. (2.62) and (2.64) are consistent.

I will first consider the one-dimensional Dirac delta function and then briefly discuss the Dirac delta function in two and three dimensions. The Dirac delta function in one dimension can be defined by

$$\delta(x) = 0 \text{ if } x \neq 0; \tag{2.65a}$$

$$\delta(x) = \infty \text{ if } x = 0; \tag{2.65b}$$

$$\int \delta(x)dx = 1 \text{ if the origin is inside the integration volume;} \tag{2.65c}$$

$$\int \delta(x)dx = 0 \text{ if the origin is outside the integration volume;} \tag{2.65d}$$

or by

$$\int f(x)\delta(x)dx = f(0), \tag{2.66}$$

where $f(x)$ is an arbitrary analytic function. Note that $\delta(x)$ has units of inverse length.

The Dirac delta function $\delta(x)$ is an infinitely narrow function of x centered at $x = 0$. The area under the function is equal to unity. Perhaps the easiest way to envision the Dirac delta function is the limit of a Gaussian having unit area whose height goes to infinity and width goes to zero,

$$\delta(x) = \lim_{a\to 0} \frac{1}{\sqrt{\pi a^2}} e^{-x^2/a^2}. \tag{2.67}$$

This function has all the required properties. Other representations of the Dirac delta function are

$$\delta(x) = \frac{1}{\pi} \lim_{a\to 0} \frac{a}{x^2 + a^2}, \tag{2.68}$$

$$\delta(x) = \lim_{K\to\infty} \frac{\sin(Kx)}{\pi x}, \tag{2.69}$$

and

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk. \tag{2.70}$$

Equations (2.67) and (2.68) are obvious representations of a narrow function having area equal to unity, but what about Eqs. (2.69) and (2.70)? These equations do not define "proper" mathematical functions and are meaningful only when integrated with functions that vanish as $|x| \sim \infty$. Equation (2.70) is interesting in that the Dirac delta function can be defined as the Fourier transform of a constant. One way of seeing that this works is to write

$$\delta(x) = \lim_{K\to\infty} \frac{1}{2\pi} \int_{-K}^{K} e^{ikx} dk = \lim_{K\to\infty} \frac{\sin(Kx)}{\pi x}. \tag{2.71}$$

As K gets larger, the width of the central peak gets narrower and its height grows as K/π. With increasing K, the function oscillates so rapidly outside the central

peak that, when integrated with an analytic function $f(x)$, any contributions to the integral average to zero, except near the central peak. Equation (2.70) is one that you will encounter many times in this course and other physics courses. Don't forget it! For any variable $\varnothing$ (e.g. $\varnothing = x$, $\varnothing = x - x_0$, etc.),

$$\delta(\varnothing) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik\varnothing} dk. \tag{2.72}$$

Some useful properties of the Dirac delta function are:

$$\delta(-x) = \delta(x); \tag{2.73a}$$

$$\int_{-\infty}^{\infty} dx' f(x')\delta(x - x') = f(x); \tag{2.73b}$$

$$\delta(ax) = \frac{\delta(x)}{|a|}; \tag{2.73c}$$

$$\delta\left[g(x)\right] = \sum_i \frac{\delta(x - x_i)}{|g'(x_i)|}; \tag{2.73d}$$

$$\delta\left(x^2 - a^2\right) = \frac{1}{2\,|a|}\left[\delta(x - a) + \delta(x + a)\right]; \tag{2.73e}$$

$$\int_{-\infty}^{\infty} dx' f(x')\frac{d\delta(x - x')}{dx'} = -f'(x). \tag{2.73f}$$

The sum over i is over all the roots of $g(x_i) = 0$. The proofs are left to the problems.

The Dirac delta function can be used to derive the inverse Fourier transform. Given

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} a(k')e^{ik'x} dk', \tag{2.74}$$

I can multiply this equation by e^{-ikx} and integrate over x to arrive at

$$\begin{aligned}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx f(x)e^{-ikx} &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk'\, a(k')\int_{-\infty}^{\infty} dx\, e^{i(k'-k)x} \\ &= \int_{-\infty}^{\infty} dk'\, a(k')\delta\left(k' - k\right) = a(k),\end{aligned} \tag{2.75}$$

where I used

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k'-k)x} = \delta\left(k' - k\right), \tag{2.76}$$

which follows from Eq. (2.72).

In fact, if $f(x)$ and $a(k)$ are Fourier transforms of one another, then

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k) e^{ikx} dk = \int_{-\infty}^{\infty} dx' \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')} \right] f(x'), \tag{2.77}$$

from which it follows that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')} = \delta\left(x - x'\right). \tag{2.78}$$

In other words, the existence of Fourier transforms leads us to the representation of the Dirac delta function given by Eq. (2.70). You can also use Eq. (2.70) to show that

$$\int_{-\infty}^{\infty} dx \ |f(x)|^2 = \int_{-\infty}^{\infty} dk \ |a(k)|^2, \tag{2.79}$$

which is known as *Parseval's theorem*.

In two dimensions, the Dirac delta function is

$$\delta(\boldsymbol{\rho} - \boldsymbol{\rho}') = \delta\left(x - x'\right) \delta\left(y - y'\right) = \frac{1}{\rho} \delta\left(\rho - \rho'\right) \delta\left(\varphi - \varphi'\right) \tag{2.80}$$

[ρ and ϕ are cylindrical coordinates] and, in three dimensions, it is given by

$$\begin{aligned} \delta(\mathbf{r} - \mathbf{r}') &= \delta\left(x - x'\right) \delta\left(y - y'\right) \delta\left(z - z'\right) \\ &= \frac{1}{r^2} \delta\left(r - r'\right) \delta\left(\cos\theta - \cos\theta'\right) \delta\left(\varphi - \varphi'\right) \end{aligned} \tag{2.81}$$

[r, θ, and ϕ are spherical coordinates].

2.7 Problems

Note: Problems with two or more problem numbers are an indication that the problem might take longer to solve than an average problem.

1. Evaluate $e^{i\pi}$, $e^{i\pi/2}$, and $e^{2.3i}$. If

$$\psi(x) = \frac{e^{iax} e^{-gx^2/2}}{x + ib} = u + iv = re^{i\theta},$$

find u, v, r, θ, assuming that x, a, b, g, r, θ are real. Evaluate $|\psi(x)|^2$.

2. Given the function

$$f(x) = \frac{N}{b^2 + x^2},$$

find N such that $f^2(x)$ is normalized; that is, find N such that

$$\int_{-\infty}^{\infty} f^2(x)dx = 1,$$

assuming that b is real. Find the Fourier transform $a(k)$ of $f(x)$. Evaluate

$$\Delta x^2 = \int_{-\infty}^{\infty} (x - \bar{x})^2 f^2(x)dx$$
$$\Delta k^2 = \int_{-\infty}^{\infty} \left(k - \bar{k}\right)^2 |a(k)|^2 dk$$

and the product $\Delta x \Delta k$. Does $\Delta x \Delta k = 1/2$ for these functions? To evaluate the integrals, you can use integral tables or Mathematica, Maple, or Matlab.

3–4. Suppose that the k space amplitude for a free particle in quantum mechanics is given by

$$a(k) = \begin{cases} 1/\sqrt{2k_0} & -k_0 \leq k \leq k_0 \\ 0 & \text{otherwise} \end{cases}.$$

The wave function $\psi(x, 0)$ is the Fourier transform of $a(k)$. Plot both $k_0 |a(k)|^2$ as a function of k/k_0 and $|\psi(x, 0)|^2 / k_0$ as a function of $k_0 x$. By "eyeballing" the graphs, estimate Δx, Δk, and their product. Now calculate Δk analytically and show that Δx is infinite.

5. If the functions $f(x)$ and $a(k)$ are Fourier transforms of one another, prove Parseval's Theorem,

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |a(k)|^2 dk.$$

6. Prove

$$\delta(ax) = \frac{\delta(x)}{|a|}$$
$$\delta\left(x^2 - a^2\right) = \frac{1}{2|a|}\left[\delta(x - a) + \delta(x + a)\right]$$
$$\int_{-\infty}^{\infty} dx' f(x') \frac{d\delta(x - x')}{dx'} = -f'(x).$$

7. Given the probability distribution

$$P(x) = \begin{cases} 1 & 0 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}.$$

Calculate $\bar{x}$ and Δx. If the probability distribution is shifted so it is centered at $x = 0$, do $\bar{x}$ and Δx change?

8. Use Taylor's theorem to estimate $29^{1/3}$ correct to order 0.001. Compare your answer with the exact value.

9. Show that $\int_0^\infty dx \frac{d\delta(x)}{dx}$ is not well defined. To do this use the definition of the delta function as the limit of a Gaussian,

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

to show that the integral diverges as $a \to 0$.