

CHAPTER 4

An Illustrative Interlude

Wave Packets in One Dimension

- 4.1 *On the Nature of the Free-Particle State Function*
- 4.2 *Wave Packet Construction for Fun and Profit*
- 4.3 *The Amplitude Function*
- * 4.4 *Fourier Analysis (A Mathematical Detour)*
- 4.5 *An Extended Example: The Gaussian Wave Packet Unmasked*
- 4.6 *Uncertainty Regained*
- 4.7 *(Not Quite) All About Momentum*
- 4.8 *Final Thoughts: A Wealth of Representations*

I dare say that's an idea which
has already occurred to you,
but with the weight of my great mind
behind it, no doubt it strikes
the imagination more forcibly.

—Lord Peter Wimsey
in *Strong Poison*
by Dorothy L. Sayers

Postulates I and II are the first bricks in the foundation of quantum mechanics. The first postulate identifies the basic element of the theory: the wave function. The second postulate interprets this function as a position probability amplitude. As befits the introduction, the discussion in Chap. 3 was general and rather abstract. So in this chapter, we'll take a breather from this development to explore at length a single, simple example: *a microscopic free particle in one dimension*. The physics of this system is especially simple because, as its name implies, such a particle is free of external forces or fields.¹

Aside: Free Particles in the Real World. A free particle is, of course, an idealization; no system is truly isolated from external influences. Nevertheless, the example of this chapter finds wide application in quantum physics. The reason is that in many situations, the external forces that do act on a particle are so weak that we can neglect them. For example, in electron scattering experiments physicists use a beam of non-interacting electrons. Such a beam is, of course, subject to the force of gravity. But we need not take this force into account in a description of its physics, because the effect of this very weak force on the particles in the beam is negligible.

Our objective in this chapter is the wave function $\Psi(x, t)$ of a free particle in one dimension. Ordinarily, we would obtain this function by mathematical machinations—we'd solve the time-dependent Schrödinger Equation [Eq. (3.39)],

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, t). \quad (4.1)$$

Since a free particle experiences no external forces, its potential energy is a constant the value of which I'll set equal to zero:²

$$V(x) = 0 \quad [\text{for a free particle}]. \quad (4.2)$$

So the Schrödinger Equation for a free particle is just (4.1) without the term in $V(x)$.

At this stage in our study, I want to avoid the algebraic chore of solving this second-order partial differential equation—even for so simple a system as the free particle. Instead, I want to lead you to a deeper understanding of the nature of wave functions. So our strategy (in § 4.1 and 4.2) will be to *deduce* rather than derive the state function for a free particle.

What we will find is that this function must be a *complex wave packet*. Wave packets play an important role in quantum mechanics, so we'll spend a little time (in

¹A classical analogue of a free particle in one dimension is a macroscopic bead constrained to move along a (hypothetical) infinite, frictionless wire.

²Recall that the potential energy of a system is arbitrary to within an additive constant, since only *potential differences* are measurable. See Chap. 8 of *Fundamentals of Physics*, 2nd ed., by D. Halliday and R. Resnick (New York: Wiley, 1981).

§ 4.2–4.4) examining the mathematics of their construction via Fourier analysis. But, as always, physics remains paramount, and in § 4.5 we'll discover *uncertainty* in the representation of a state by a wave packet. Finally, in § 4.6–4.7, we'll see a tantalizing glimpse of how to extract information about observables other than position from a wave function. This analysis will hurtle us into Chap. 5, where we tackle momentum.

4.1 ON THE NATURE OF THE FREE-PARTICLE STATE FUNCTION

Always trust the simplest explanation that fits all the facts unless there's a damn good reason not to do so.

— Dr. Stuart Hay
in *Incarnate*
by Ramsey Campbell

What do we know about state functions? In particular, what properties should characterize the state functions of a particle in one dimension? Well, in § 3.5 I argued that such a function must be single-valued, continuous, and—most importantly—normalizable. That is, it must obey the boundary condition (3.29), according to which $\Psi(x, t)$ must go to zero (as $|x| \rightarrow \infty$) rapidly enough that its normalization integral $\int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx$ is finite. Physically, this condition means that the wave function must be *spatially localized*. That's one property.

Another is evident from the Schrödinger Equation (4.1): $\Psi(x, t)$ must be complex. Here's why: the right-hand side of this equation has a multiplicative factor of $i = \sqrt{-1}$ that is absent from the left-hand side. Therefore *no purely real or purely imaginary function can satisfy this equation*. Were $\Psi(x, t)$ purely real, for example, then the left-hand side would be real and the right-hand side would be imaginary—which would violate the equal sign!³

These two properties pertain to the state functions of *any* system. When we turn to the free particle (or any other *isolated system*) we find a third, quite different property: a fundamental symmetry of nature called the *homogeneity of free space*. I want to tell you about this property, which is the topic of the next subsection, to introduce you to the power and beauty of symmetry arguments. From this symmetry property of space itself, we'll derive a condition on the probability density $P = |\Psi|^2$ that *all free-particle state functions* must satisfy. Then we'll use this property—and a little imagination and logic—to deduce the wave function for the free particle in one dimension.

The Homogeneity of Free Space

What's the first step we must take if we want to investigate the physics of a system, be it microscopic or macroscopic? We must define a *reference frame*. The one you're probably most familiar with is the *rectangular (or Cartesian) coordinate system* shown in

³This argument does *not* imply that $\Psi(x, t)$ must be complex at all times; it can be real (or imaginary) at certain, discrete times. But it does imply that the wave function cannot be purely real or imaginary *at all times*.

Fig. 4.1. The directions of the three mutually orthogonal axes that define this reference frame are \hat{e}_x , \hat{e}_y , and \hat{e}_z .⁴ These axes intersect at the origin O .

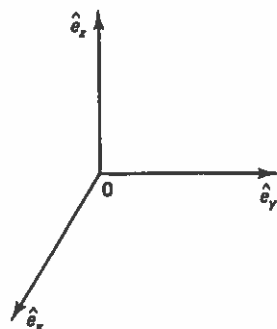


Figure 4.1 A Cartesian coordinate system. Within this system several sets of orthogonal coordinates can be used, among them *rectangular* and *spherical* coordinates.

The decision of where to put the origin of coordinates is very important, because all vectors are referred to this point. But the choice of origin is ours to make. After all, coordinates and reference frames are just mathematical artifices that physicists invent to solve problems.

A Historical Aside. This feature of theoretical physics was noted in 1885 in an essay by Charles Howard Hinton (1853–1907):

To measure, we must begin somewhere, but in space there is no “somewhere” marked out for us to begin at. This measuring is something, after all, foreign to space, introduced by us for our convenience.

And as to dimensions, in order to enumerate and realize the different dimensions, we must fix on a particular line to begin with, and then draw other lines at right angles to this one.

But the first straight line we take can be drawn in an infinite number of directions. Why should we take any particular one?

If we take any particular line, we do something arbitrary, of our own will and decision, not given to us naturally by space.

Hinton’s comments lead us to expect physically measurable properties to be independent of such arbitrary choices. And, indeed, they are.⁵

In practice we have several ways to pick the origin of coordinates. We might choose an origin that will simplify the solution of whatever equations we confront. Or we might select as the origin the location of a measuring apparatus. But most often we look to nature for guidance. For example, we might identify some physical entity—say, a (point) particle in the system or the source of an electromagnetic field—as the origin.

But if the particle is free, then we cannot use the latter gambit, for nothing in free space distinguishes one point over another. That is, nature does not identify a preferred origin for a free particle. In this case we can put O anywhere we wish.

⁴Little hats do a lot of work in quantum mechanics. Throughout this book, a little hat on an e , such as \hat{e}_i , will denote a unit vector in the i direction. (For rectangular coordinates, $i = x, y, z$.) But from Chap. 5 onward, little hats on *other* symbols will denote operators. Be wary.

⁵Hinton was so interesting a character that I can’t resist telling you a little about him. Many consider him one of the great philosophers of hyperspace; he was fascinated by the fourth dimension. No, fascinated is the wrong word; Hinton was obsessed. In an effort to construct a mental image of a four-dimensional universe, he memorized 46,656 one-inch cubes, each of which had been assigned a Latin name. Evidently, this daunting task was not challenging enough for Hinton, who next decided to learn his cubic yard of cubes in each of its twenty-four possible orientations. For more on this eccentric but brilliant mathematician, see Rudy Rucker’s delightful book, *The Fourth Dimension: Toward a Geometry of Higher Reality* (Boston: Houghton Mifflin Co., 1984).

This discussion of the origin of coordinates leads us to the fundamental symmetry property I mentioned above: the **homogeneity of free space**. When we say "free space is homogeneous" we mean that the physical properties of a system in free space are independent of the origin of coordinates. The implications of homogeneity for a physical theory (such as quantum mechanics) are strict indeed:

Rule

All physical quantities we calculate must be independent of the origin of coordinates.

You can see what this means if you imagine picking up the system and *translating* it through space to a new location. According to this rule, all measurable quantities that you calculate from a state descriptor of the system after translation must equal those calculated from the corresponding state descriptor before translation.

Since in quantum mechanics we calculate properties from wave functions, it should come as no surprise that the homogeneity requirement imposes a limitation on wave functions. But be careful—the nature of this limitation is rather subtle. *Homogeneity does not imply that the state function itself must be independent of the coordinate origin, because this function is not measurable.* But all measurable quantities are calculated from the probability density $\Psi^*\Psi$, so *the homogeneity of free space demands that the probability density be independent of the origin of coordinates.* That is, a translation of a microscopic free particle must not alter its probability density. Such a translation appears in Fig. 4.2.

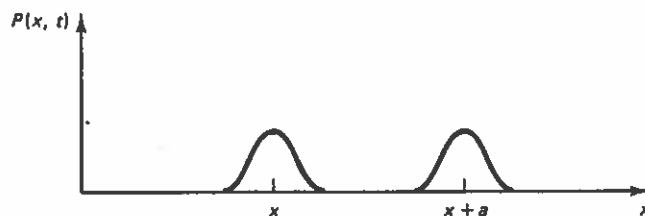


Figure 4.2 The effect on the probability density of the translation of a microscopic system by a distance a in the $+x$ direction. The state function of the system is changed by the translation and so depends on a . But the probability density must be unchanged; i.e., it must be independent of a .

To use this property to deduce the free-particle state function, we'll need a mathematical expression of it. So let's consider translating a system that *before translation* is in a quantum state represented by Ψ . The state function *after translation* will, in general, be some other function of position and time. (We'll assume instantaneous translation, so t does not change.) This function will also depend on the translation distance a . So I'll represent the state after translation by Ψ'_a . Now, the relationship between the state functions of a one-dimensional system before and after translation in the x direction is simply

$$\Psi'_a(x, t) = \Psi(x - a, t) \quad [\text{for translation by } a \text{ in the } +x \text{ direction}]. \quad (4.3)$$

With this notation we can easily write down the homogeneity requirement that the probability densities before and after translation be equal, viz.,

$$\text{homogeneity of free space} \implies |\Psi'_a|^2 = |\Psi|^2. \quad (4.4)$$

We are now ready to tackle the problem of the free particle. But before we begin, let's summarize the properties that the state function of such a particle must obey:

1. Ψ must be spatially localized (normalizable);
2. Ψ must be a complex function of position and time;
3. Ψ must not violate the homogeneity of free space.

Homogeneity and the Free-Particle State Function

To show you how to use the homogeneity requirement (4.4) to check out prospective free-particle state functions, I'll try one that we know is wrong. Consider a free particle in a state with momentum p and energy E .⁶

According to the de Broglie relations (2.16), the wave characteristics of particles in such a state are the associated wavelength $\lambda = h/p$ and frequency $\nu = E/h$, where h is Planck's constant. These relations suggest a *guess* at the wave function of the particle: a real harmonic wave with this wavelength and frequency:

$$f(x, t) = A \cos\left(\frac{2\pi}{\lambda}x - 2\pi\nu t + \alpha\right). \quad \text{real harmonic wave} \quad (4.5)$$

In this generic harmonic wave, the amplitude A and phase constant α are real numbers that, in practice, are determined from the initial conditions on the problem.⁷ In this section we are concerned only with the *functional form* of $f(x, t)$, so for convenience I'll set $\alpha = 0$.

Before proceeding to shoot down this guess, I want to get rid of the unsightly factors of 2π littering Eq. (4.5). Harmonic waves are usually written in terms of the wave number k and angular frequency ω , which are defined by

$$k \equiv \frac{2\pi}{\lambda} \quad \text{wave number} \quad (4.6a)$$

$$\omega \equiv 2\pi\nu \quad \text{angular frequency} \quad (4.6b)$$

The de Broglie relations specify the connection between these fellows and the momentum p and energy E of the state:

$$p = \hbar k \quad (4.7a)$$

$$E = \hbar\omega, \quad (4.7b)$$

where I've introduced the all-purpose 2π -absorber (otherwise known as the "rationalized Planck's constant")

⁶In nature, free-particle states in which energy and momentum can be known precisely don't exist. Statistically speaking, we say that the uncertainties in the energy and momentum are positive for all states: $\Delta E > 0$ and $\Delta p > 0$. But states do exist in which the energy and momentum are very nearly certain (*i.e.*, these uncertainties are very small), and we often approximate such a state by a function with a well-defined E and p .

⁷The initial conditions on $f(x, t)$ are just its values at a particular position and time, usually at $x = 0$ and $t = 0$. We can choose the phase constant α to force the general form (4.5) to agree with any initial conditions. If, for example, $f(0, 0) = A$, we choose $\alpha = 0$. If, on the other hand, $f(0, 0) = 0$, we choose $\alpha = 3\pi/2$. The latter often-used choice, by the way, transforms the cosine function into a sine function, so that the function becomes $f(x, t) = A \sin(kx - \omega t)$. And so forth.

$$\hbar \equiv \frac{h}{2\pi}$$

(4.8)

In its new clothes, our guess (4.5) for a free-particle state function looks like

$$\Psi(x, t) = A \cos(kx - \omega t). \quad (4.9)$$

This function is sketched in Fig. 4.3.

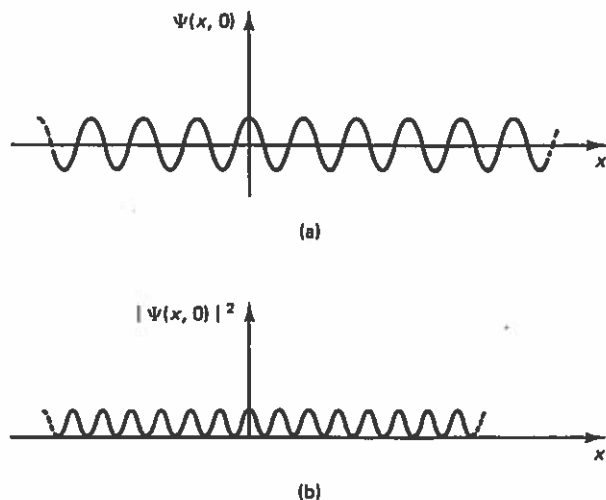


Figure 4.3 (a) The real harmonic wave of Eq. (4.9) at $t = 0$, and (b) its square. This function oscillates throughout space, as suggested by the dotted lines at the fringes of these curves. Consequently it cannot be normalized and is not physically admissible.

Aside: The Dispersion Relation. You probably remember from your study of waves that the angular frequency ω and the wave number k are related via a **dispersion relation**. In quantum mechanics, we can determine the dispersion relation from the relationship between the total energy and the momentum. For example, the energy of a free particle is purely kinetic, so provided its velocity is non-relativistic ($v \ll c$), the total energy E is related to the linear momentum p by the simple formula

$$E = \frac{p^2}{2m}. \quad [\text{for a non-relativistic free particle}] \quad (4.10a)$$

Translating this into a dispersion relation via the definitions (4.7), we get⁸

$$\omega(k) = \frac{\hbar k^2}{2m}. \quad \text{dispersion relation for a free particle} \quad (4.10b)$$

Now we all know why Eq. (4.9) won't do. First, we can see from Fig. 4.3 that for this guess the normalization integral—the area under the probability density curve—is infinite, so this function can't be normalized. Moreover, it's not complex and so couldn't

⁸If the particle is traveling at relativistic velocities, the total energy (including the rest-mass energy) and the linear momentum are related by Eq. (2.14), so (4.10b) is not applicable. For such a particle of rest mass m_0 , the dispersion relation is

$$\omega(k) = \left[c^2 k^2 + \left(\frac{m_0 c^2}{\hbar} \right)^2 \right]^{1/2}$$

satisfy the Schrödinger equation (4.1). But I want to show you yet another reason it won't work: it violates the homogeneity requirement.

Example 4.1. The Real Harmonic Wave and the Homogeneity Requirement

The demonstration is easy: we just determine the probability densities of the state (4.9) before and after translation and see if they're the same. Before translation, the probability is just the squared modulus of the function (4.9),

$$P(x, t) = A^2 \cos^2(kx - \omega t). \quad (4.11)$$

After translation, the wave function is given [a la Eq. (4.3)] by

$$\Psi'_a(x, t) = A \cos[k(x - a) - \omega t], \quad (4.12a)$$

which we can expand (using the handy trig identities in Appendix H) into

$$\Psi'_a(x, t) = A [\cos(kx - \omega t) \cos ka + \sin(kx - \omega t) \sin ka]. \quad (4.12b)$$

So the probability density after translation is

$$\begin{aligned} \Psi'^*_a(x, t) \Psi'_a(x, t) &= A^2 \cos^2(kx - \omega t) \cos^2 ka \\ &+ A^2 [\sin^2(kx - \omega t) \sin^2 ka + 2 \cos ka \sin ka \cos(kx - \omega t) \sin(kx - \omega t)]. \end{aligned} \quad (4.13)$$

Now look carefully at the first term in (4.13). Compare it to (4.11). See? The first of the three terms in the probability density *after translation* is $P(x, t) \cos^2 ka$, the product of the probability density *before translation* and an additional factor! This result proves that a real harmonic wave, in addition to its other faults, violates the homogeneity requirement:

$$P'_a(x, t) \neq P(x, t). \quad [\text{for a real harmonic wave}]. \quad (4.14)$$

This fact *alone* is enough to invalidate this function as a state descriptor for a free particle, for it is inconsistent with a fundamental symmetry property of nature itself. Back to the drawing board.

Question 4-1

As you probably know, any real function can be decomposed into a series of sine and cosine functions. Using this fact, present a brief argument that no real function of x and t can satisfy the homogeneity requirement.

Question 4-2

Show that the linear combination of plane harmonic waves

$$\Psi(x, t) = \cos(kx - \omega t) + i \sin(kx - \omega t) \quad (4.15)$$

does satisfy the homogeneity requirement.

A Second Guess: The Complex Harmonic Wave

Of the three defects of the real harmonic wave, the easiest to repair is its real character. A simple *complex* function that we might nominate as a candidate for the representative of a free-particle state with well-defined energy and momentum is the generalization suggested by Question 4-2: a **complex harmonic wave** of the form

$$\Psi(x, t) = A e^{i(kx - \omega t)}, \quad \text{complex harmonic wave} \quad (4.16)$$

where, as in the real harmonic wave, the frequency and wave number are related by the free-particle dispersion relation⁹ $\omega(k) = \hbar k^2/2m$. Now let's see if this guess satisfies the demanding homogeneity requirement.

Example 4.2. The Complex Harmonic Wave and the Homogeneity Requirement

The state function (4.16) *after translation* is

$$\Psi'_a(x, t) = A e^{i(kx - ka - \omega t)} \quad (4.17a)$$

$$= e^{-ika} [A e^{ik(x - \omega t)}] \quad (4.17b)$$

$$= e^{-ika} \Psi(x, t). \quad (4.17c)$$

I hope you're way ahead of me by now. According to (4.17c), the state function after translation is identical to that before translation except for the multiplicative factor e^{-ika} . So the state function depends on the origin of coordinates only through this *exponential* factor. [Notice that since ka is a constant, this is just a global phase factor (§ 3.5).] When we form the probability density after translation, this factor obligingly goes away:

$$\Psi'^*_a(x, t) \Psi'_a(x, t) = e^{ika} \Psi^*(x, t) e^{-ika} \Psi(x, t) \quad (4.18a)$$

$$= \Psi^*(x, t) \Psi(x, t). \quad (4.18b)$$

So the probability density formed from a complex harmonic wave is unchanged by a translation. We conclude that such a wave does satisfy the homogeneity requirement (4.4). It also satisfies another of our properties: it's complex. That's two out of three. Now, what's wrong with it?

Question 4-3

Verify that the complex harmonic wave (4.16) satisfies the time dependent Schrödinger Equation (4.1) for the free particle.

On the Horns of a Dilemma

Alas, the simple complex harmonic wave (4.16) is not spatially localized. This regrettable property is obvious from its probability density, *which is constant*:

$$P(x, t) = \Psi^*(x, t) \Psi(x, t) = |A|^2. \quad [\text{for a complex harmonic wave}.] \quad (4.19)$$

A constant probability density implies that we're equally likely to detect an electron anywhere in space. That is, the complex harmonic wave would represent a state in which we know *nothing* about the position of the particle; this observable is "infinitely

⁹Eq. (4.16) is the general form of a complex traveling wave that propagates in the $+x$ direction. The corresponding form for a wave propagating in the $-x$ direction is

$$\Psi(x, t) = A e^{-i(kx + \omega t)}.$$

You may be familiar with such waves from your study of electricity and magnetism, where they are used to represent electric and magnetic fields. It is important to remember, however, that complex electromagnetic waves are just problem-solving tools; we ultimately must take the real parts of such functions, because only real electromagnetic waves exist in the laboratory. For more on complex functions in electromagnetic theory, see Chap. 8 of *Introduction to Electrodynamics* by David J. Griffiths (Englewood Cliffs, N. J.: Prentice Hall, 1981).

indeterminate" ($\Delta x = \infty$). So in no sense is a such a state spatially localized. Indeed, it's hard even intuitively to see how we could associate such a wave with a particle.

Question 4-4

Is the infinite position uncertainty for the complex harmonic wave consistent with the Heisenberg Uncertainty Principle? If so, why? If not, why not?

The lack of spatial localization shows up in the normalization integral for the complex harmonic wave, *which is infinite*:

$$\begin{aligned} \int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx \\ = |A|^2 \int_{-\infty}^{\infty} dx = \infty. \quad [\text{for a complex harmonic wave}]. \end{aligned} \quad (4.20)$$

We know from § 3.5 that we cannot normalize such a function and hence must reject it as physically inadmissible to quantum physics.

Let's review. We argued that the free-particle wave function we seek must satisfy three innocent-looking properties: it must be spatially-localized, complex, and consistent with the homogeneity requirement. Our first guess, the real harmonic wave, violated all of these conditions. Our second, the complex harmonic wave, violated only the requirement of spatial localization. But that's not good enough.

Our explorations have not led to the answer—but they have led to valuable clues. The complex harmonic function is so nearly the wave function we seek that it makes sense at this point to try to *construct* a spatially-localized function by adding together a bunch of these harmonic waves with different wave numbers and frequencies. In the next section, we'll do just that: we're going to build a wave packet.

4.2 WAVE PACKET CONSTRUCTION FOR FUN AND PROFIT

Go back to the functions graphed in Fig. 3.1. These are "snapshots" of physically admissible wave functions (taken at times when they happen to be real). Each wave function is characterized by a *single dominant finite region of enhanced position probability*—that is the distinctive feature of spatial localization. The probability density for each of these functions defines a "high probability" region of space, a realm of possible positions at which the particle is likely to be found. Our goal is to construct such a function.

This point of view emphasizes why a single harmonic wave fails: such a wave is monochromatic (*i.e.*, characterized by a single frequency), but *regions of enhanced amplitude arise from the interference of harmonic waves with differing wave numbers and frequencies*. This fact will be our guiding principle as we set out to build a free-particle wave function. And our tool will be superposition.¹⁰

It's not hard to see how to use superposition to build a wave packet. In a superposition of monochromatic harmonic waves, two kinds of interference happen. *Constructive interference* occurs at positions where the interfering waves are *in phase*, leading to an

¹⁰In this section, I'll assume that you're familiar with the mathematical and physical properties of waves at roughly the sophomore undergraduate level. If you need a refresher, try one of the Selected Readings at the end of this chapter.

enhanced amplitude of the total wave. And *destructive interference* occurs where the interfering waves are *out of phase*, leading to a diminished amplitude. We can use these interference phenomena to construct a spatially localized function by forming a linear combination of complex harmonic waves with varying frequencies and amplitudes. Such a linear combination is called a **wave packet**.

Applying these facts about waves to the task of § 4.1, constructing a function that satisfies the three criteria discussed there, we conclude that what we need is a complex wave packet with a single region of enhanced amplitude:

$$\boxed{\text{free particle state function} = \text{a complex wave packet}} \quad (4.21)$$

A Digression: The Pure-Momentum Function

Before we look at such packets we must get out of the way a mundane but important matter of notation. In spite of their defects, plane harmonic waves such as (4.16) are widely used in quantum mechanics, where they are usually written in terms of momentum and energy, as

$$\Psi_p(x, t) = A e^{i(px - Et)/\hbar} \quad (4.22)$$

Such a function is called, sensibly, a **pure momentum function**. Notice that I've appended a subscript p to $\Psi(x, t)$ to remind us what value of momentum we're talking about. Similarly, when discussing the complex harmonic wave written in terms of the wave number k [Eq. (4.16)], I'll sometimes affix to Ψ a subscript k .

Aside: The Mathematics of Waves—Phase Velocity. The most important property of a harmonic wave is its propagation velocity, which is called **phase velocity**. The phase velocity is defined as the velocity of a point of constant phase.¹¹ For a one-dimensional wave the phase velocity is

$$v_{ph} \equiv \left. \frac{\partial x}{\partial t} \right|_{\Psi=\text{constant}} \quad \text{phase velocity} \quad (4.23)$$

For example, the phase velocity of a complex harmonic wave is [see Exercise 4.1]

$$v_{ph} = \lambda \nu = \frac{\omega}{k} = \frac{E}{p}. \quad (4.24)$$

So far I have left one thing in the pure momentum function (4.22) unspecified: the amplitude A . We're at liberty to choose this constant to fit the physical conditions of our problem—and when we get to collision problems (Chap. 8) we'll take advantage of this flexibility. But there is a conventional choice for A that exploits a nifty property of complex plane waves.

If the problem we're solving doesn't suggest a value of A , a good choice for the complex harmonic wave $\Psi_k(x, t)$ is $A = 1/\sqrt{2\pi}$. The resulting function

¹¹If you are a little bit rusty on the meaning of these quantities *please review*. You'll find useful information about phase velocities in such sources as Chap. 7 of *Vibrations and Waves* by A. P. French (New York: Norton, 1966) and in *Waves* by Frank S. Crawford, Jr. (New York: McGraw-Hill, 1968).

$$\Psi_k(x, t) = \frac{1}{\sqrt{2\pi}} e^{i(kx - \omega t)} \quad (4.25)$$

is, for reasons I'll explain in a moment, called a **normalized plane wave**.

For the pure momentum function $\Psi_p(x, t)$, the optimum choice is $A = 1/\sqrt{2\pi\hbar}$. The so-called **normalized pure momentum function** is

$$\Psi_p(x, t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i(px - Et)/\hbar} \quad (4.26)$$

From here on I'll use these choices of A unless there is a good reason to do otherwise.

You'll discover why these choices are desirable as you work with the pure momentum function (see especially § 4.7). Here's a preview: they enable us to take advantage of the fact that complex exponentials form a representation of the *Dirac Delta function*, viz.,¹²

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ik'x} e^{ikx} dx = \delta(k - k'). \quad (4.27)$$

You're probably wondering why I refer to these as "normalized" functions, when we know that a complex harmonic wave can't be normalized. This usage is, indeed, inconsistent. Historically, it entered colloquial parlance (at least among mathematicians) because two "normalized plane waves" satisfy a kind of "pseudo-normalization integral,"

$$\int_{-\infty}^{\infty} \Psi_k^*(x, 0) \Psi_{k'}(x, 0) dx = \delta(k - k'). \quad \text{Dirac Delta function normalization} \quad (4.28)$$

The General Form of a Wave Packet

Equation (4.21) gives us our marching orders: to construct a free-particle wave function, we must add together (superpose) complex plane waves with different wave numbers k . Your first thought might be to try a linear combination of a *finite* number of plane waves with discrete wave numbers k_j and amplitudes A_j , such as

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \sum_{j=1}^N A_j e^{i(k_j x - \omega_j t)}.$$

This reasonable suggestion runs aground on a basic property of waves: *The superposition of a finite number of plane waves with discrete wave numbers has an infinite number of comparable regions of constructive interference. Each of these regions is separated from its neighbor by a region of destructive interference.* This property of wave packets is illustrated in Fig. 4.4 and Problem 4.1.

¹²You may or may not have run across the Dirac Delta function $\delta(x)$ in your studies. Actually, it's not a function at all; it's what mathematicians call a *functional*. You can get an idea what $\delta(x)$ is by envisioning a "spike" that is zero everywhere except the point where its argument is zero, $x = 0$. So in (4.28), $\delta(k - k')$ is zero everywhere except at $k = k'$, where it's infinite. You can find a brief overview of the Dirac Delta function and its properties in Appendix L. For more information, I recommend the introductory treatments found on pp. 53–55 of *Quantum Physics* by R. G. Winter (Belmont, Ca.: Wadsworth, 1979), and in Appendix 2 of *Quantum Mechanics*, Volume I by Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloe (New York: Wiley-Interscience, 1977).

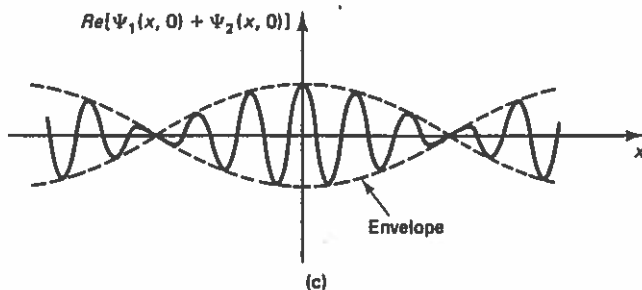
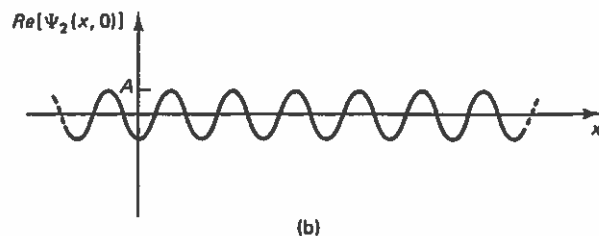
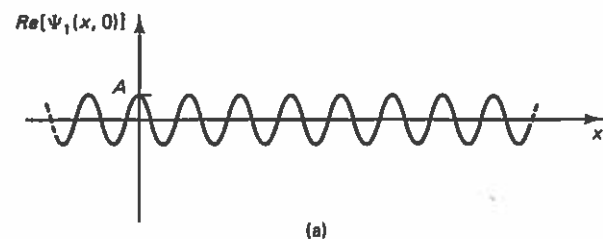


Figure 4.4 A simple (and unsuitable) wave packet constructed by superposing a mere *two* plane harmonic waves. Each wave has equal amplitude, $A(k_1) = A(k_2) = A$, but a different wave number: $k_1 = 12\pi$, $k_2 = 10\pi$. (a) The first wave, $\Psi_1(x, 0)$. (b) The other wave, $\Psi_2(x, 0)$. (c) Their superposition, $\Psi(x, 0) = \Psi_1(x, 0) + \Psi_2(x, 0)$. The spread of wave numbers for the plane waves in $\Psi(x, 0)$ is $\Delta k = 2\pi$. (In this figure, only the real parts of the three waves are shown.)

But we want a packet with one *dominant* region of enhanced amplitude—with a single biggest bump. [Additional regions of secondary amplitude (smaller bumps) are okay.] The solution is to use an infinite number of plane waves:

Rule

To construct a wave packet with a single dominant region of enhanced amplitude we must superpose an infinite number of plane wave functions with infinitesimally differing wave numbers.

Since k is a continuous variable, our wave packet will have the form of an integral over functions of the form $e^{i(kx - \omega t)}$. To control the mixture of complex harmonic waves in the superposition, we'll assign each complex plane wave an "amplitude" $A(k)$. Using the normalized plane-wave functions (4.25), we write the general form for a wave packet as

$$\begin{aligned}\Psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx - \omega t)} dk \\ &= \int_{-\infty}^{\infty} A(k) \Psi_k(x, t) dk\end{aligned}$$

wave packet (4.29)

At present, the amplitude function $A(k)$ is arbitrary; in practice, we define this function to give $\Psi(x, t)$ physical properties that correspond to the quantum state it represents.¹³

Before going any further, I want to emphasize an extremely important point. Equation (4.29) is applicable to many different (one-dimensional) quantum systems; it is not limited to the free particle. In fact, most of the results of this chapter are not limited to the free particle. It is crucial to remember that in constructing wave packets we specify a particular system by our choice of the dispersion relation $\omega = \omega(k)$. For the free particle, the appropriate relation is (4.10b), $\omega(k) = \hbar k^2/2m$. To apply the general form to other systems, we just select the appropriate dispersion relation. Please don't forget this.

Aside: The Mathematician's View. A mathematician would probably interpret Eq. (4.29) as an expansion of $\Psi(x, t)$ in a "complete set" of plane wave functions $\Psi_k(x, t)$, with $A(k)$ the *expansion coefficient* corresponding to the plane wave with wave number k . [The amplitude function $A(k)$ is also sometimes called the *spectral distribution function*.] In Chap. 12 we'll discover the (considerable) advantages to adopting this more formal perspective on superpositions of quantum waves.

Do you understand how the superposition (4.29) forms a spatially localized function? The key is the *phases* $kx - \omega t$ of the constituent plane harmonic waves $\Psi_k(x, t)$. Consider a fixed time—say, $t = 0$. At this time all waves in the packet are *in phase* at one (and only one) point. This value of x is the *the point of total constructive interference*. At this point the probability density $P(x, 0) = |\Psi(x, 0)|^2$ attains its *global maximum*; for this reason, this point is called the *center of the wave packet*. We usually denote the center of the wave packet by x_0 .¹⁴

Now, at any other $x \neq x_0$ the plane waves in the packet are *out of phase*, so some destructive interference occurs. As we move away from the center of the packet (*i.e.*, as $|x - x_0|$ increases), this interference becomes more and more destructive, until eventually the amplitude of the state function becomes negligibly small. This is why a wave packet is spatially localized [c.f., Eq. (3.29)].¹⁵

When we construct a wave packet, we specify the *system* by the dispersion relation $\omega = \omega(k)$. To specify a particular *state* of this system, we choose the amplitude function $A(k)$. This function determines such properties of the packet as its "width"—the spread of values of x encompassed by $\Psi(x, 0)$. Let's see how this works.

¹³There appears to be an inconsistency between the dimensions of the normalized plane wave (4.25), the normalized pure momentum state function (4.26), and the physically admissible state functions of Chap. 3. In one dimension, the latter must have units of inverse square root of length ($1/\sqrt{L}$), because the integral $\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t) dx$ must be dimensionless [c.f., Eq. (3.28a)]. Sure enough, neither $\Psi_k(x, t)$ nor $\Psi_p(x, t)$ has the correct dimensions. But this isn't a problem because these functions appear in wave packets where they are multiplied by amplitude functions that fix the dimensionality of the packet. For example, the units of $A(k)$ in (4.32) are (see § 4.3) \sqrt{L} . Similarly, in § 4.6 we'll construct a wave function out of pure momentum state functions with an amplitude function $\Phi(p)$ that, when multiplied by $\Psi_p(x, t)$, produces a packet with the correct dimensions.

¹⁴Be careful not to confuse the center of the wave packet with the average position, $\langle x \rangle(0)$; for some wave functions, these two points do coincide. But not for all. One other thing: the center of the packet at $t = 0$ need not be the origin of coordinates; we can construct a wave packet with its center at $x_0 \neq 0$ (see § 4.6).

¹⁵The argument I have sketched here is formally known as the *stationary phase condition*. This condition determines where the point of total constructive interference occurs for a superposition of plane waves. You can find a good introductory discussion of the stationary phase condition in § 2.5 of *Introduction to the Quantum Theory*, 2nd ed. by David Park (New York: McGraw-Hill, 1974) and more advanced discussions on p. 51 of *Quantum Mechanics*, Volume I by Albert Messiah (New York: Wiley, 1966) and on p. 19 of *Quantum Mechanics*, Volume I by Kurt Gottfried (Reading, Mass.: Benjamin/Cummings, 1966).

4.3 THE AMPLITUDE FUNCTION

The amplitude function $A(k)$ governs the mixture of plane harmonic waves in a particular wave packet; in this sense $A(k)$ distinguishes one wave packet from another. In practice, we usually determine the amplitude function from the value of the state function at $t = 0$ (§ 4.4). But in this section I'll take the amplitude function as given, because I want to show you—by example—how a superposition of an infinite number of complex harmonic waves with a particular amplitude function produces a wave packet with a single dominant region of enhanced position probability. We'll also examine the subtle relationship between the evolution of a wave packet and the motion of a classical particle and will peek into a laboratory where wave packets are used in collision experiments.

Figure 4.5 shows two typical amplitude functions. The function in Fig. 4.5a is peaked at $k = k_0$, so the dominant plane wave in the packet formed when we insert this function into the general form (4.29) is $\Psi_{k_0}(x, t)$. Plane wave functions $\Psi_k(x, t)$ with wave numbers far from k_0 make negligible contributions to the total packet $\Psi(x, t)$.

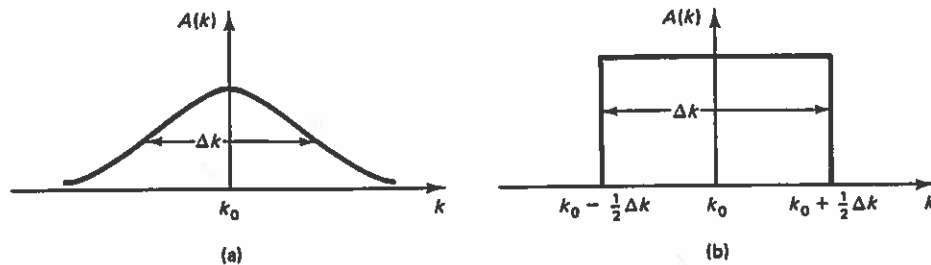


Figure 4.5 Two amplitude functions. Each function is characterized by its center k_0 and width Δk . The function in (a) is a Gaussian and will be discussed in § 4.5; the one in (b) is a square step and is used in Example 4.1. In (b), the value of $A(k_0) = 1/\sqrt{\Delta k}$ produces a properly normalized amplitude function (see § 4.4).

The function in Fig. 4.5b is more equitable: all harmonic waves with wave numbers in the range $k_0 - \frac{1}{2}\Delta k \leq k \leq k_0 + \frac{1}{2}\Delta k$ contribute equally to the resulting wave packet. In Example 4.1 we'll construct a wave packet from this amplitude function. Stay tuned.

Aside: On Complex Amplitude Functions. By the way, the sample amplitude functions in Fig. 4.5 are real. But $A(k)$ can be (and often is) complex. If so, we sometimes choose to write it in terms of a magnitude $|A(k)|$ and a phase $\alpha(k)$, i.e.,

$$A(k) = |A(k)|e^{i\alpha(k)}. \quad (4.30)$$

It's important to not lose sight of the physics amidst all the mathematics of wave packet construction. Try to think about these amplitude functions as controllers of the mixture of *pure momentum states* in the quantum state represented by the wave packet $\Psi(x, t)$. After all, each function $\Psi_k(x, t)$ in such a packet is associated (via the de Broglie relation) with a particular value of the momentum, $p = \hbar k$. This way of looking at the superposition $\int_{-\infty}^{\infty} A(k)\Psi_k(x, t) dx$ reveals that *the momentum of a quantum state represented by a wave packet is uncertain, i.e.,*

$$\Delta p > 0. \quad [\text{for a wave packet}]. \quad (4.31)$$

This connection between the amplitude function $A(k)$ and the momentum uncertainty Δp is no accident, and we'll return to it in § 4.6 and 4.7.

Question 4-5

What amplitude function $A(k)$ would produce a packet with a well-defined momentum (i.e., with $\Delta p = 0$)? What's wrong with the function $\Psi(x, t)$ you would get were you to insert this amplitude function into Eq. (4.29)?

Example 4.3. Construction of a Valid State Function

Let's see what sort of wave packet we get when we use the amplitude function of Fig. 4.5b,¹⁶

$$A(k) = \begin{cases} \frac{1}{\sqrt{\Delta k}} & k_0 - \frac{1}{2}\Delta k \leq k \leq k_0 + \frac{1}{2}\Delta k \\ 0 & \text{otherwise} \end{cases} \quad (4.32)$$

For simplicity, we'll consider only $t = 0$.

With this amplitude function, the wave packet (4.29) becomes a simple finite integral over the region of wave number where $A(k)$ is non-zero:

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk \quad (4.33a)$$

$$= \frac{1}{\sqrt{2\pi} \Delta k} \int_{k_0 - \frac{1}{2}\Delta k}^{k_0 + \frac{1}{2}\Delta k} e^{ikx} dk. \quad (4.33b)$$

Perusing our integral tables (Appendix I), we find the desired integral and easily derive

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi} \Delta k} e^{ik_0 x} \frac{2}{x} \sin\left(x \frac{\Delta k}{2}\right). \quad (4.34)$$

The corresponding probability density,

$$P(x, 0) = \frac{1}{2\pi \Delta k} \frac{4}{x^2} \sin^2\left(x \frac{\Delta k}{2}\right), \quad (4.35)$$

appears in Fig. 4.6.

Question 4-6

Evaluate the normalization integral for the state function (4.34).

The wave function (4.34) has an infinite number of local maxima. Still, this function doesn't violate the requirement of spatial localization, because the peak values of these humps decrease as x increases in either direction from $x = 0$. [This causes the *envelope* of the wave packet to die away to zero as $|x| \rightarrow \infty$.] Consequently the probability density defines only one *dominant* region of enhanced position probability, as desired.

Nevertheless, the position of a particle in an ensemble of particles represented by this state function is clearly uncertain: the function in Fig. 4.6 has a non-zero width ($\Delta x > 0$). Not surprisingly, the momentum is also uncertain ($\Delta p > 0$). This result follows from the Heisenberg Uncertainty Principle or, putting it mathematically, from the spread of wave numbers that characterizes the amplitude function (4.32).

Example 4.1 illustrates important features of the wave packets used in quantum physics. To summarize: *A wave packet is a normalizable function that is peaked about*

¹⁶I chose the value of the constant $A(k) = 1/\sqrt{\Delta k}$ so that the amplitude function would be normalized, i.e., so that $\int_{-\infty}^{\infty} A^*(k)A(k) dk = 1$. That $A(k)$ satisfy this condition isn't mathematically essential, but it is convenient (see § 4.4), and it takes care of the dimensionality problem noted in footnote 13.

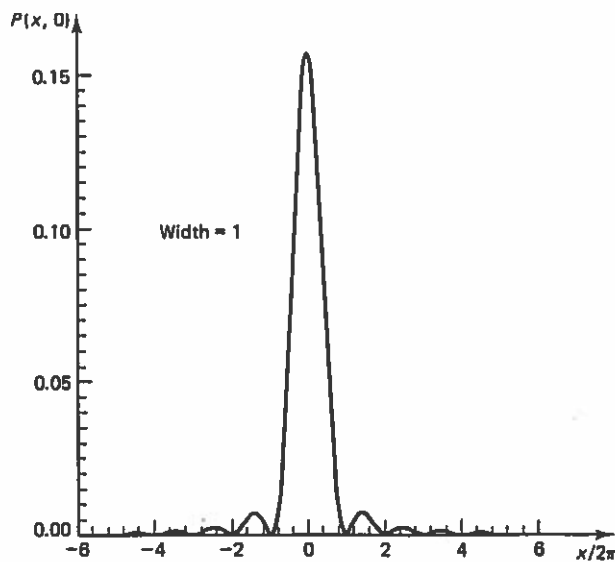


Figure 4.6 The position probability density $P(x, 0)$ for the wave packet erected in Example 4.3. This function is physically admissible because (among its other virtues) it is spatially localized.

a point of total constructive interference, its center. This function is characterized by a non-zero but finite spread in the variables x and k .

Wave Packet Motion and the Correspondence Principle

In Example 4.1 we considered a wave packet at a fixed time. The way such packets evolve as time goes by is the subject of Chap. 6 (especially § 6.7). But I want to show you one feature of wave packet motion now, because it illustrates the quaint and curious relationship between quantum mechanics and classical physics, a pervasive theme of this book.

Each of the monochromatic traveling waves that makes up a wave packet has a phase velocity $v_{ph} = \omega/k$. But the propagation velocity of the packet is, by definition, the velocity of its center. From your study of waves, you probably remember that this quantity is the **group velocity** and that (in one dimension) it is defined as

$$v_{gr} \equiv \left. \frac{d\omega}{dk} \right|_{k=k_0} \quad \text{group velocity} \quad (4.36)$$

In words: we can calculate v_{gr} by evaluating the first derivative of the dispersion relation $\omega = \omega(k)$ at the center of the amplitude function, $k = k_0$.¹⁷

We can easily figure out the group velocity of a free particle from the dispersion relation $\omega(k) = \hbar k^2/(2m)$. Applying the definition (4.36), we find that for the (general) wave packet (4.29),

$$v_{gr} = \frac{\hbar k_0}{m} = \frac{p_0}{m} \quad [\text{for a free particle}]. \quad (4.37a)$$

¹⁷With the passing of time, most wave packets disperse (spread). But this phenomenon is not described by v_{gr} , which provides information only about the propagation of the packet. Eventually, a packet may spread so much that it loses its definition; if this happens, the group velocity is no longer meaningful.

Does this result look familiar? It should: it's the *classical* velocity that a particle of mass m would have if its momentum was p_0 :

$$v_{\text{classical}} = \left. \frac{dE}{dp} \right|_{p=p_0} = \frac{p_0}{m}. \quad [\text{classical physics}] \quad (4.37b)$$

Isn't *that* interesting?

Be careful about how you interpret this little demonstration. It's very easy to be seduced by the similarity in Eqs. (4.37) into concluding that classical physics *does* pertain to microscopic particles. But this conclusion is not correct. What Eqs. (4.37) say is that a free particle wave packet with an amplitude function $A(k)$ peaked about $k = k_0$ evolves in such a way that *the position of its center*, the peak of the dominant region of enhanced probability, changes at a speed identical to that of a classical particle with the same mass and momentum $\hbar k_0$. It's important to note that (4.37b) pertains to a particle with a definite momentum, p_0 , while the wave packet from which we calculated (4.37a) has an indeterminate momentum ($\Delta p > 0$).

This correspondence between the motion of a quantum-mechanical wave packet and the dynamics of a (related) classical particle is a manifestation of the *Correspondence Principle* (Chap. 2), according to which the predictions of quantum physics must reduce to those of classical physics "in the classical limit." "But where," I hear you wonder, "is 'the classical limit' in all this?"

Splendid question. Look, a classical particle has a well-defined position and momentum, so one way to take a wave packet to the classical limit is to reduce the position and momentum uncertainties to zero:

$$\Delta x \rightarrow 0 \quad \text{and} \quad \Delta p \rightarrow 0. \quad \text{classical limit of a wave packet} \quad (4.38)$$

In this limit, the wave packet reduces to a probability amplitude that represents a state in which the position of the particle and its momentum are definite at each time [in fact, $\Psi(x, t)$ reduces to a Dirac Delta function]. What we showed in Eqs. (4.37) is that this point moves through space at the speed predicted by classical physics.¹⁸

This insight is but a glimmer of a far more profound result we'll discover in Chap. 11. There we'll explore the classical limit of the *laws of motion of quantum physics* and will find that in the classical limit the expectation value $\langle x \rangle(t)$ for a quantum state obeys Newton's Second Law, *i.e.*, the wave packet for a *macroscopic* particle follows that particle's classical trajectory.

Wave Packets in the Laboratory

Do you feel as if you're drowning, getting deeper and deeper into mathematics, leaving physics forever behind? Do you find it ominous that the next section is subtitled "A Mathematical Detour"? If so, don't fret. As we master all this mathematics we're really learning the language of quantum physics. But perhaps we should stop by the lab to see how an experimental physicist might produce a beam of free particles in a state that could be represented by a wave packet.

¹⁸The uncertainties in (4.38) are related by the Heisenberg Uncertainty Principle $\Delta x \Delta p \geq \hbar/2$. From this relation, we could argue that the classical limit is that in which \hbar is negligible and can hence be approximated by zero. This limit is sometimes written $\hbar \rightarrow 0$ —an expression that is probably perplexing, since \hbar is not zero at all; it's a *constant* equal to 1.0546×10^{-34} J sec. If you want to read more about the correspondence principle, see the excellent discussion in Chap. 8 of *Introduction to Quantum Mechanics* by R. H. Dicke and J. P. Wittke (Reading, Mass.: Addison-Wesley, 1960).

Such a beam would most likely be used in a collision experiment like the one sketched in Fig. 4.7. The *source* emits a beam of nearly mono-energetic particles—here, electrons—with energy E_0 and momentum $p_0 = \sqrt{2m_0E_0}$, where m_0 is the rest mass of the projectile. (For an electron, $m_0 = m_e = 9.109 \times 10^{-31}$ kg.) The resulting beam travels a finite (but large) distance to the target, which might be a gas cell or a second beam directed at right angles to the electron beam. Scattered projectiles travel a finite (but large) distance to the detector, which we can move through space so as to sample the scattered particles at any angle.

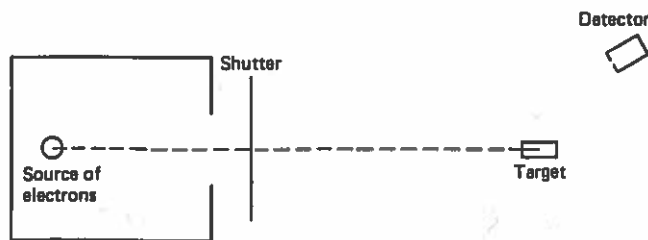


Figure 4.7 A (rather crude) schematic of a collision experiment. The target in this experiment is fixed. As described in the text, by judicious use of the shutter we can produce a *pulse* of electrons in a state represented by a wave packet with a known width Δx .

If the density of the beam is low enough that to a good approximation the particles don't interact and if the source "prepares" them so that all are in the same quantum state, then the beam is an ensemble (see Chap. 3). But what is the wave function that represents the particles in the beam?

The nature of some collision experiments permits us to *approximate* this wave function by a plane wave (as the limit of an extremely fat wave packet; see § 6.9 and 8.3). But in some experiments, the beam is "chopped"—rather like pepperoni.

We could generate a chopped beam of electrons by, for example, placing a movable shutter in front of the opening in the source, as in Fig. 4.7. By rapidly raising, then lowering the shutter, we generate a *pulse* of electrons of length L . (The value of L is determined by the energy of the electrons and by how long the shutter is open.) This pulse is an ensemble of free particles whose state is represented by a wave packet.

From the physical conditions in the laboratory, we can infer several features of this packet. For one thing, the position uncertainty of the particles in this beam is non-zero; in fact, Δx is roughly equal to the dimension of the beam: $\Delta x \approx L$. Consequently the momentum of the particles is not well-defined; rather, the state is characterized by a distribution of momenta that is peaked about p_0 . According to the Heisenberg Uncertainty Principle, the momentum uncertainty is roughly $\Delta p \approx \hbar/(2L)$. All of these features conform to our understanding of the nature of a wave packet.

Aside: Wave Packets for Three-Dimensional Systems. In general, we must treat a wave packet in the lab as a three-dimensional function. The three-dimensional extension of the general form (4.29) is

$$\Psi(\mathbf{r}, t) = \frac{1}{\sqrt{(2\pi)^3}} \int A(\mathbf{k}) e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} d\mathbf{k}, \quad (4.39a)$$

where $d\mathbf{k}$ is a volume element in "momentum space" (e.g., in rectangular coordinates, $d\mathbf{k} = dk_x dk_y dk_z$). The center of this packet, $\mathbf{r}_0(t)$, propagates at the group velocity,

which is a vector determined by taking the gradient of the dispersion relation, viz., $\omega = \omega(\mathbf{k})$ at $\mathbf{k} = \mathbf{k}_0$, i.e.

$$\mathbf{v}_{\text{gr}} = \nabla_{\mathbf{k}} \omega(\mathbf{k}) \Big|_{\mathbf{k}=\mathbf{k}_0}. \quad (4.39b)$$

Fortunately, we usually need not consider explicitly two of the three dimensions of the packet's motion. This bit of legerdemain will be explained in Chap. 8.

The details of how to construct such a wave function are interesting, but discussing them would take us too far afield. But before we leave this section, I should note that in a real collision experiment, we can set the mean values and uncertainties of the position and momentum of the incident particles, to the precision allowed by nature and human fallibility. These characteristics *define* the wave packet that represents the state of the projectiles. And that is how we create and use wave packets in laboratory quantum physics.

*4.4 FOURIER ANALYSIS (A MATHEMATICAL DETOUR)

In § 4.2, we wrote down the general form (4.32) of a wave packet,

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx - \omega t)} dk. \quad (4.40a)$$

At $t = 0$, this equation takes on a form that may be familiar:

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk. \quad (4.40b)$$

Equation (4.40b) reveals that *the amplitude function $A(k)$ is the Fourier transform of the state function $\Psi(x, t)$ at $t = 0$* . That is, the amplitude function is related to the wave function at $t = 0$ by a Fourier integral.¹⁹

Fourier analysis—the generation and deconstruction of Fourier series and integrals—is the mathematical method that underlies the construction of wave packets by superposition. Fourier analysis is a vital element of our quantum mechanics' tool kit, for we can use it to zip back and forth between the amplitude function and the corresponding state function. Moreover, the study of Fourier analysis leads to a deeper understanding of waves *per se*. When this method is applied to *probability waves*—i.e., to state functions—it leads to important, sometimes astonishing physical principles (see § 4.6). For all these reasons, we're going to take a short sojourn into Fourier analysis.

Mathematicians commonly use Fourier analysis to rip functions apart, representing them as sums or integrals of simple component functions, each of which is characterized by a single frequency. This method can be applied to any function $f(x)$ that is *piecewise continuous*—i.e., that has at most a finite number of finite discontinuities. Wave functions, which must be continuous (see § 3.5), satisfy this condition and so are prime candidates for Fourier analysis. Moreover, Fourier analysis is a preview of an extremely powerful mathematical technique: the method of eigenfunction expansion (Chap. 12).

Whether we represent $f(x)$ via a Fourier series or a Fourier integral depends on whether or not this function is *periodic*. Any function that repeats itself is said to be

¹⁹If you already figured this out and don't feel the need of a review of Fourier series and integrals, skip to § 4.5. (You may, however, want to read the last subsection—on the definition of the width of a function.) If you've never studied Fourier analysis, you'll find a list of good references at the end of this chapter.

periodic. More precisely, if there exists a finite number L such that $f(x + L) = f(x)$, then $f(x)$ is periodic with period L . Perhaps the most familiar periodic functions are $\sin(2\pi x/L)$, $\cos(2\pi x/L)$, and $\exp(2\pi i x/L)$. We can write any function that is periodic (or that is defined on a finite interval) as a *Fourier series*. But if $f(x)$ is non-periodic or is defined on the infinite interval from $-\infty$ to $+\infty$, we must use a *Fourier integral*.

Fourier Series

Fourier series are not mere mathematical devices; they can be generated in the laboratory. For example, a *spectrometer* decomposes an electromagnetic wave into spectral lines, each of which has a different frequency and amplitude (intensity). Thus, a spectrometer decomposes a periodic function in a fashion analogous to the Fourier series. But our present concern is with the mathematics.

Suppose we want to write a periodic, piecewise continuous function $f(x)$ as a series of simple functions. Let L denote the period of $f(x)$, and choose as the origin of coordinates the midpoint of the interval defined by this period, $-L/2 \leq x \leq L/2$. (This choice allows us to exploit the symmetry (if any) of $f(x)$.)

The particular functions that appear in the Fourier series expansion of a periodic function are sines and cosines. Letting a_n and b_n denote (real) expansion coefficients, we write this series as²⁰

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left[a_n \cos\left(2\pi n \frac{x}{L}\right) + b_n \sin\left(2\pi n \frac{x}{L}\right) \right]. \quad \text{real Fourier series} \quad (4.41)$$

We calculate the coefficients in (4.41) from the function $f(x)$ as

$$a_0 = \frac{1}{L} \int_{-L/2}^{L/2} f(x) dx \quad (4.42a)$$

$$a_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \cos\left(2\pi n \frac{x}{L}\right) dx \quad (n = 1, 2, \dots) \quad (4.42b)$$

$$b_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(2\pi n \frac{x}{L}\right) dx \quad (n = 1, 2, \dots) \quad (4.42c)$$

Notice that the summation in (4.41) contains *an infinite number of terms*. In practice we retain only a finite number of these terms—this approximation is called **truncation**. Truncation is viable, of course, only if the sum converges to whatever accuracy we want *before* we chop it off.

A Mathematical Aside: On Truncation. Truncation is not as extreme an act as it may seem. If $f(x)$ is normalizable, then the expansion coefficients in (4.41) decrease in magnitude with increasing n , *i.e.*,

$$|a_n| \rightarrow 0 \text{ and } |b_n| \rightarrow 0 \text{ as } n \rightarrow \infty.$$

Under these conditions, which are satisfied by physically admissible wave functions, the sum (4.41) can be truncated with impunity at some finite maximum value n_{\max} of the index n . Of course, a certain amount of trial and error is required to determine the value of n_{\max} that is required for the desired accuracy.

²⁰*Beware:* the precise form of the Fourier series (and integral) representations of a function depend on the interval of periodicity; many authors choose the limits of this interval to be $-L$ and $+L$.

Truncation is not the only simplification one stumbles across in working with Fourier series. If $f(x)$ is particularly simple, all but a small, finite number of terms in (4.41) may be zero. And you should always look for coefficients that are zero before you start grinding out integrals. This advice leads to the question: how can we spot such coefficients without evaluating them? That is, what (other than an accident) could make an expansion coefficient zero?

The Power of Parity

In Example 3.4, we saw that parity arguments can render integral evaluation trivial if the integrand is an odd function of the variable of integration. The same thing is true of the integrals in the expansion coefficients (4.42): they call for integration over a symmetric integral (from $-L/2$ to $+L/2$) of an integrand that involves trigonometric functions with well-known parity properties:²¹

$$\sin(-x) = -\sin x \quad (\text{odd}) \quad (4.43a)$$

$$\cos(-x) = +\cos x \quad (\text{even}) \quad (4.43b)$$

From Eqs. (4.43) it follows that if $f(x)$ has definite parity, then either the integrand in a_n or that in b_n will be odd:

Rule

If $f(x)$ is even or odd, then half of the expansion coefficients in its Fourier series are zero.

If, for example, $f(x)$ is *odd* [i.e., $f(-x) = -f(x)$], then all the coefficients a_n are zero, and we're left with a series involving only the "sine coefficients" b_n . Such a series is called a *Fourier sine series*. The constant coefficient a_0 in (4.41) is zero for any function of definite parity. So if $f(x)$ is such a function, there are two possibilities:

$$\begin{array}{l} f(x) \text{ is odd } [f(-x) = -f(x)] \implies \\ \left\{ \begin{array}{l} a_n = 0 \quad (n = 1, 2, \dots) \\ f(x) = \sum_{n=1}^{\infty} b_n \sin\left(2\pi n \frac{x}{L}\right) \end{array} \right. \end{array} \quad \begin{array}{l} \text{Fourier sine series} \\ (4.44a) \end{array}$$

$$\begin{array}{l} f(x) \text{ is even } [f(-x) = +f(x)] \implies \\ \left\{ \begin{array}{l} b_n = 0 \quad (n = 1, 2, \dots) \\ f(x) = \sum_{n=1}^{\infty} a_n \cos\left(2\pi n \frac{x}{L}\right) \end{array} \right. \end{array} \quad \begin{array}{l} \text{Fourier cosine series} \\ (4.44b) \end{array}$$

²¹For more on parity in Fourier analysis, see § 5.10 of *Advanced Calculus for Applications* by F. B. Hildebrand (Englewood Cliffs, N.J.: Prentice Hall, 1962).

Aside: Functions That Don't Have Definite Parity. The Fourier sine and cosine expansions may come in handy even if $f(x)$ does not have definite parity, because we can easily write *any* function as the sum of an even function and an odd function. Suppose $f(x)$ is neither even nor odd [i.e., $f(-x) \neq \pm f(x)$]. Let's define two new functions $g(x)$ and $h(x)$ as

$$g(x) = \frac{1}{2} [f(x) + f(-x)]$$

$$h(x) = \frac{1}{2} [f(x) - f(-x)].$$

By definition, $g(x)$ is even and $h(x)$ is odd. Using these definitions, we can write the function $f(x)$ as [see the next Question]

$$f(x) = \underbrace{g(x)}_{\text{even}} + \underbrace{h(x)}_{\text{odd}}.$$

So for the rest of this section, I'll assume that $f(x)$ is either even or odd.

Question 4-7

Write down the functions $g(x)$ and $h(x)$ for

$$f(x) = \frac{1}{2}e^{-x^2} + 7x$$

and prove that each has definite parity.

Fourier and His Series: A Historical-Mathematical Aside. As a brief respite from all this math, let's look back in time. The method of representing functions by series (or integrals) of sine and cosine functions was derived by a Frenchman named Jean Baptiste Joseph Fourier (1768–1830). When young, Fourier dreamed of serving in the French army. (Had these dreams not been dashed, Fourier might not have become much older.) But he was too adept at mathematics for the French government to let him become cannon fodder, so Fourier had to settle for a career as a world-renowned mathematician. In the early 1800's, Fourier set out to find a way to represent functions in terms of sines and cosines.

To develop a series representation of a periodic function $f(x)$, Fourier used a rather standard optimization technique. His first step was to write the function he wanted to represent as a *finite* series of the form

$$f_K(x) = a_0 + \sum_{n=1}^K \left[a_n \cos\left(2\pi n \frac{x}{L}\right) + b_n \sin\left(2\pi n \frac{x}{L}\right) \right].$$

The subscript K in this expansion indicates the number of terms included in it. Fourier then asked: what choices for the coefficients a_n and b_n lead to a function $f_K(x)$ that *most closely approximates* $f(x)$ —i.e., to the “best” such representation? His answer: the function with coefficients that *minimize the mean square deviation*,²²

$$\frac{1}{2L} \int_{-L/2}^{+L/2} [f(x) - f_K(x)]^2 dx.$$

Fourier easily implemented that minimization via the *orthogonality relations* for the sine and cosine:

$$\int_{-L/2}^{L/2} \cos\left(2\pi n \frac{x}{L}\right) \sin\left(2\pi m \frac{x}{L}\right) dx = 0 \quad (4.45a)$$

²²We have met this sort of beast before (in § 3.3); it is just a measure of the extent to which the series representation $f_K(x)$ differs from $f(x)$ over the interval $[-L/2, +L/2]$.

$$\int_{-L/2}^{L/2} \cos\left(2\pi n \frac{x}{L}\right) \cos\left(2\pi m \frac{x}{L}\right) dx = \int_{-L/2}^{L/2} \sin\left(2\pi n \frac{x}{L}\right) \sin\left(2\pi m \frac{x}{L}\right) dx$$

$$= \begin{cases} 0, & \text{if } m \neq n; \\ 1, & \text{if } m = n. \end{cases} \quad (4.45b)$$

What he found—the optimum expansion coefficients—are those of Eqs. (4.42).

Following this signal success, Fourier went on to write a classic study of heat (which he believed to be vital to man's health) and then died tumbling down a flight of stairs. But his theory lives on.

The Fourier series is by no means the only way to expand a function. (You probably know about the most common alternative, a Taylor series.) But its value derives in part from its wide applicability. Moreover, evaluation of the Fourier coefficients is usually comparatively easy. Because the integrals (4.42) involve sines and cosines, they can often be dug out of integral tables. Even if $f(x)$ is sufficiently nasty that the required integrals are too complicated to evaluate analytically, we can always dump them on the nearest computer. (Computers love sines and cosines.)

The Complex Fourier Series

If $f(x)$ does not have a definite parity, we can expand it in a **complex Fourier series**. To derive this variant on the Fourier series (4.41), we just combine the coefficients a_n and b_n so as to introduce the complex exponential function $e^{i2\pi nx/L}$; viz.,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L}. \quad \text{Complex Fourier Series} \quad (4.46)$$

Note carefully that in the complex Fourier series (4.46) the summation runs from $-\infty$ to ∞ . The expansion coefficients c_n for the complex Fourier series are

$$c_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x) e^{-i2\pi nx/L} dx. \quad (4.47)$$

As you might expect, in general these coefficients are complex.

Question 4-8

Derive Eqs. (4.46) and (4.47) and thereby determine the relationship of the coefficients c_n of the complex Fourier series of a function to the coefficients a_n and b_n of the corresponding real series.

Fourier Integrals

I have emphasized that only a *periodic* function (or one defined on a finite interval) can be expanded in a Fourier series. To represent a *non-periodic* function in terms of sines and cosines, we resort to an integral: *any normalizable function can be expanded in an infinite number of sine and cosine functions that have infinitesimally differing arguments*. Such an expansion is called a **Fourier integral**.²³

The Fourier integral representation of a non-periodic function looks a little like the complex Fourier series representation (4.46) of a periodic function. Its general form is

²³A function $f(x)$ can be represented by a Fourier integral provided the integral $\int_{-\infty}^{\infty} |f(x)| dx$ exists. All wave functions satisfy this condition, for they are normalizable.

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

inverse Fourier transform (Fourier integral) (4.48)

The function $g(k)$ in (4.48) plays the role analogous to that of the expansion coefficients c_n in the complex series (4.46). The relationship of $g(k)$ to $f(x)$ is more clearly exposed by the inverse of (4.48),

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

Fourier transform (4.49)

In mathematical parlance, $f(x)$ and $g(k)$ are said to be Fourier transforms of one another. More precisely, $g(k)$ is the **Fourier transform** of $f(x)$, and $f(x)$ is the **inverse Fourier transform** of $g(k)$. When convenient, I'll connote these relationships by the shorthand notation

$$g(k) = \mathcal{F}[f(x)] \quad \text{and} \quad f(x) = \mathcal{F}^{-1}[g(k)]. \quad (4.50a)$$

Our immediate application of Fourier transform theory is to the wave packet $\Psi(x, 0)$ and its amplitude function $A(k)$. If we translate the relationship (4.40b) between these functions into our new notation, we have

$$A(k) = \mathcal{F}[\Psi(x, 0)] \quad \text{and} \quad \Psi(x, 0) = \mathcal{F}^{-1}[A(k)]. \quad (4.50b)$$

Many useful relationships follow from the intimate relationship between $f(x)$ and $g(k)$. For our purposes, the most important is the so-called **Bessel-Parseval relationship**:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |g(k)|^2 dk. \quad \text{Bessel-Parseval relationship} \quad (4.51)$$

[Don't forget the absolute value bars in (4.51); they are essential if $f(x)$ is complex.] Among the many applications of this relationship in quantum mechanics is the *normalization of the amplitude function* (§ 4.7).

Question 4-9

Use the properties of the Dirac Delta function to prove the Bessel-Parseval relationship (4.51).

How Wide Is My Wave Function? (A Short Discourse on Widths)

Mathematicians, scientists, and engineers often talk about the "width" of a function. Unfortunately, these folk have been unable to agree on precisely what they mean by "the width of a function," so in your reading you may come across diverse definitions of this quantity.

But the idea is simple and the name appropriate: The "width" w_x of a function $f(x)$ is just a quantitative measure of its spread, its spatial extent. We have already seen (in several examples) that the width of any normalizable function is finite and non-zero: i.e., $0 < w_x < \infty$. But beyond this observation, confusion reigns. In Fig. 4.8 you'll find some widely used definitions of w_x .

To avoid further confusion, I want to get my definition up front right now. *In this book I shall define the width of a function $f(x)$ to be the standard deviation of its position,*

as defined in § 3.3 [see Eq. (3.25)]. Hence the width of a state function $\Psi(x, t)$ is its position uncertainty Δx , as illustrated in Fig. 4.8c.

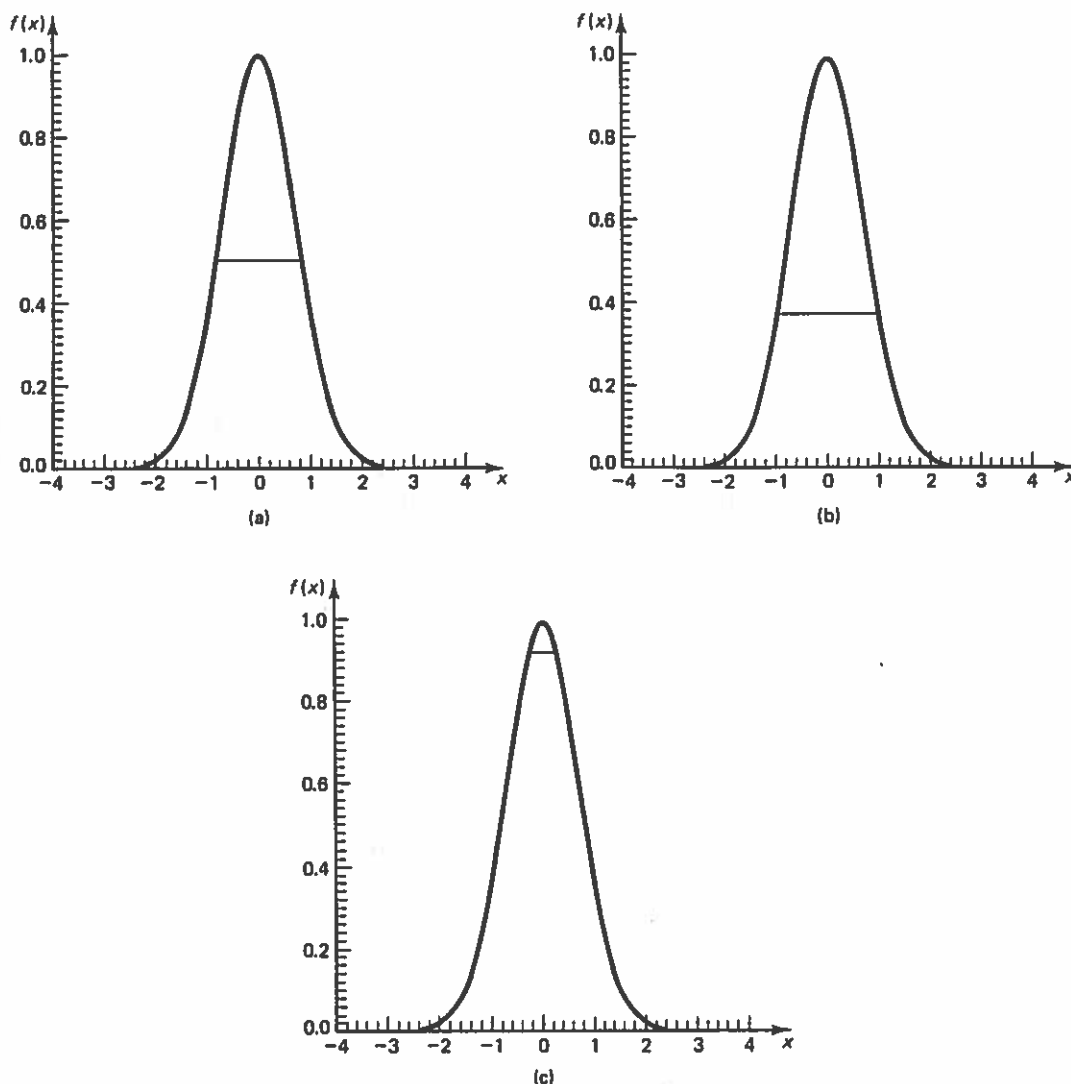


Figure 4.8 A cornucopia of definitions of the width w_x of a function $f(x)$. The function at hand is $f(x) = e^{-x^2}$. (a) The full-width-at-half-maximum, $w_x = 1.665$. (b) The extent of the function at the special point where $f(x) = [f(x)]_{\max}/e$. The function e^{-x^2} is equal to $1/e$ of its maximum value at $x = \pm 1$, so this definition gives $w_x = 1.736$. (c) My definition: the standard deviation of x ; for this function, $w_x = \Delta x = 0.560$.

We can define a width for any function; for example, the width w_k of the amplitude function $A(k)$ is a measure of its extent in the variable k (see § 4.7). And, not surprisingly, if two functions are related, so may be their widths. For instance, there is an “inverse correlation” between the width w_x of a function $f(x)$ and the width w_k of its Fourier transform: the wider the function $f(x)$, the narrower its Fourier transform $g(k)$. From an analysis of the Fourier integral (4.48), mathematicians have shown that

$$f(x) = \mathcal{F}^{-1}[g(k)] \implies w_x w_k \approx 1. \quad (4.52a)$$

Question 4-10

Explain briefly why Eq. (4.52a) is true. Base your argument on the amount of destructive interference in the wave packet as the distance from the point of *total constructive interference* increases.

Although Eq. (4.52a) is useful, it expresses this inverse relationship only qualitatively. But the *precise* value of the product $w_x w_k$ depends on the precise definition of w_x and w_k . With my definition of w_x and w_k as the standard deviations of position and wavenumber, this relation takes on the form

$$w_x w_k = \Delta x \Delta k \geq \frac{1}{2} \quad (4.52b)$$

In § 4.6, we'll translate this relationship into a principle (which you can probably guess now) that relates a critical physical property of a state function and its amplitude function.

4.5 AN EXTENDED EXAMPLE: THE GAUSSIAN WAVE PACKET UNMASKED

In Example 4.1 we used a known amplitude function $A(k)$ to construct a free-particle wave packet (at $t = 0$) as a superposition of complex harmonic waves. Mathematically speaking, we were *calculating the wave function as the inverse Fourier transform of the amplitude function*:

$$\Psi(x, 0) = \mathcal{F}^{-1}[A(k)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk. \quad (4.53a)$$

In quantum physics, we usually want to go the other way, to *calculate the amplitude function as the Fourier transform of the wave function at the initial time $t = 0$* :

$$A(k) = \mathcal{F}[\Psi(x, 0)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dx. \quad (4.53b)$$

In this section I want to illustrate this technique by examining an extremely important type of state function: the Gaussian function. In particular, we'll generate the amplitude function for a simple Gaussian function and then look at its width. What we discover when we do so will carry us back into the physics of the Heisenberg Uncertainty Principle (§ 4.6).

Example 4.4. The Amplitude Function for a Gaussian

The Gaussian function is a wave packet with a well-defined center and a single peak. Its amplitude function, which we're going to calculate, has the same properties. In § 6.7 we'll watch the time development of a Gaussian function; here we consider only $t = 0$. The Gaussian function contains one parameter, a real number L that governs its width.

The most general form of such a function has a center at $x_0 \neq 0$ and corresponds to an amplitude function that is centered at $k_0 \neq 0$:

$$\Psi(x, 0) = \left(\frac{1}{2\pi L^2} \right)^{1/4} e^{ik_0 x} e^{-[(x-x_0)/(2L)]^2}. \quad (4.54)$$

But for simplicity, I want to consider a Gaussian centered at $x_0 = 0$ with an amplitude function centered at $k_0 = 0$, i.e.,

$$\Psi(x, t = 0) = \left(\frac{1}{2\pi L^2} \right)^{1/4} e^{-x^2/(4L^2)}. \quad (4.55)$$

In Fig. 4.9, you'll find two such wave packets (with different values of L). Each exhibits the characteristic shape of a Gaussian function: each has a single peak and decreases rather rapidly as x increases from zero. But because the Gaussian function decays *exponentially*, it never actually equals zero for finite x . (It is, nonetheless, normalizable.) You'll also find in Fig. 4.9 the probability density $|\Psi(x, 0)|^2$ for a Gaussian. This figure illustrates one of the special properties of a Gaussian wave function: its probability is also a Gaussian function, one that has the same center but is narrower than the state function from which it is calculated.

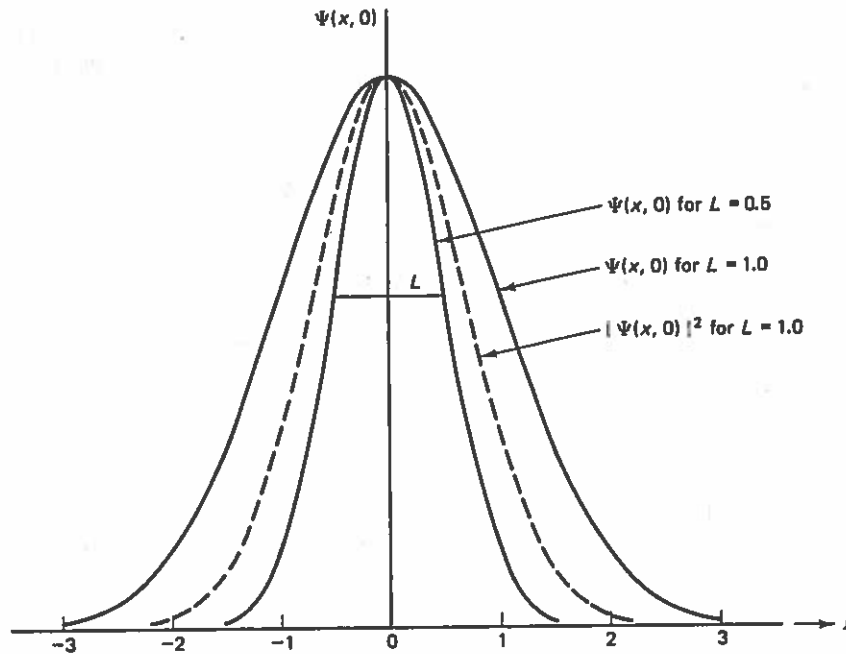


Figure 4.9 Two Gaussian wave packets of the form (4.55); the parameter L for these functions takes on the values $L = 0.5$ and $L = 1.0$ (solid curves). The corresponding probability density for $L = 1.0$ is shown as a dashed curve.

Question 4-11

Verify that the state function (4.55) is normalized.

To see precisely how individual plane harmonic waves $\Psi_k(x, t)$ combine to form a Gaussian wave packet, let's evaluate the amplitude function $A(k)$. We begin by substituting the state function (4.55) into the general expression (4.53b) for the amplitude function, viz.,

$$A(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi L^2} \right)^{1/4} \int_{-\infty}^{\infty} \exp \left[-\frac{1}{4L^2} x^2 - ikx \right] dx. \quad (4.56)$$

This rather nasty-looking integral is a standard (if perhaps unfamiliar) form:²⁴

$$\int_{-\infty}^{\infty} e^{-\alpha x^2 - \beta x} dx = \sqrt{\frac{\pi}{\alpha}} e^{\beta^2/(4\alpha)}. \quad (\alpha > 0) \quad (4.57)$$

This handy form is just what we need to conquer the integral in (4.56). Letting $\alpha = 1/(4L^2)$ and $\beta = ik$ in this expression, we obtain

$$A(k) = \left(\frac{2}{\pi} L^2\right)^{1/4} e^{-k^2 L^2}. \quad [\text{for a Gaussian with } x_0 = 0]. \quad (4.58)$$

Compare carefully the *mathematical form* of the amplitude function (4.58) and the (initial) wave function (4.55). Lo and behold: *the Fourier transform of a Gaussian function of the variable x is a Gaussian of the variable k .* (Please don't generalize: this reciprocity is not a general property of functions and their Fourier transforms; it is a special feature of the Gaussian function.)

The Gaussian $\Psi(x, 0)$ and its amplitude function are graphed in Fig. 4.10. As advertised above, the center of $A(k)$ —the value of the wave number at the peak of the amplitude function—is at $k_0 = 0$. Both the wave function and the amplitude function have a non-zero width, and from the (Fourier transform) relationship these functions bear to one another, it's not surprising that their widths are inversely related²⁵ [c.f., Eqs. (4.52)]: $w_x w_k \approx 1$.

Normalization of the Amplitude Function

In Question 4-11 I asked you to verify that the Gaussian wave function is normalized. Happily, we need not explicitly normalize the amplitude function calculated from this wave function, because a property of Fourier transforms—the Bessel-Parseval relationship (4.51)—guarantees that *the Fourier transform of a normalized function is normalized*:

$$\int_{-\infty}^{\infty} |A(k)|^2 dk = \int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx = 1. \quad (4.59)$$

²⁴Gaussian functions occur so often in quantum physics and chemistry that most of their mathematical properties have been derived and tabulated. You'll find enough information to work the problems in this book in Appendix J, which is based on the Appendix in *Elementary Quantum Mechanics* by David S. Saxon (San Francisco: Holden-Day, 1968). To find everything you could conceivably want to know about Gaussian functions (and more) get a copy of "The Gaussian Function in Calculations of Statistical Mechanics and Quantum Mechanics," which appears in *Methods of Computational Physics*, Volume 2, edited by B. Alder, S. Fernbach, and M. Rotenberg (New York: Academic Press, 1963).

²⁵A word about widths of Gaussian functions: The conventional value of the width of a Gaussian function of the form (4.54) is $w_x = L/\sqrt{2}$. This differs from what my definition gives, $w_x = \Delta x = L$. The difference arises because many authors use L as the width not of the *wave function* but rather of the *probability density*. I further need to alert you that many authors define the Gaussian function in a slightly different fashion than I have, using $L/\sqrt{2}$ everywhere that I have used L . In a book that adopts this form, you'll see, instead of Eq. (4.54), the function

$$\Psi(x, t = 0) = \left(\frac{1}{\pi L^2}\right)^{1/4} e^{-x^2/(2L^2)}.$$

Both forms are OK—after all, it's the x -dependence of this function that identifies it as a Gaussian. I prefer (4.54) because it leads to simple expressions for the position and momentum uncertainties. But this multiplicity of conventional forms should cause no difficulty: you can regain our equations from those in a book that adopts this alternate form by replacing L everywhere by $L/\sqrt{2}$.

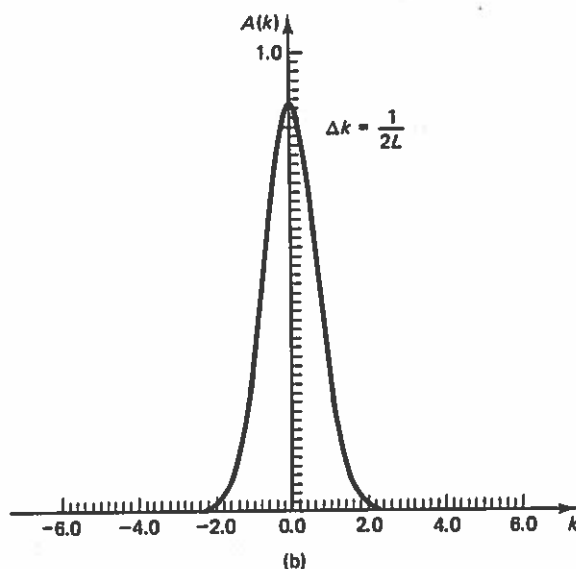
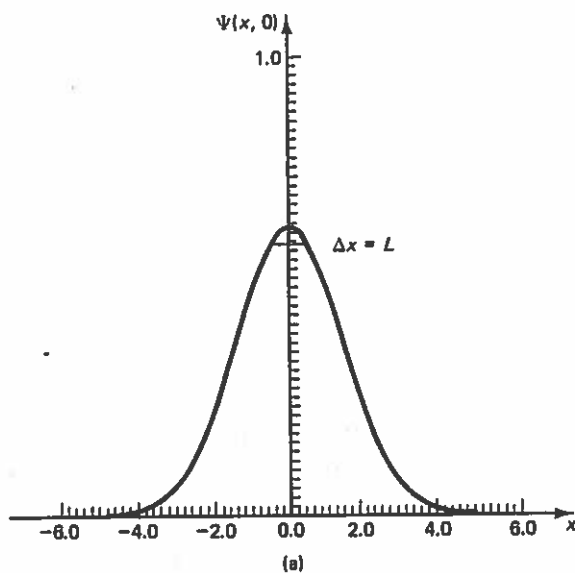


Figure 4.10 (a) A Gaussian wave packet and (b) its Fourier transform. Note that the two functions have the same *mathematical form* [see Eq. (4.58)]. Also note that the constant $1/(2L)$ plays the same role in $A(k)$ that L does in $\Psi(x, 0)$.

Of course, the Bessel-Parseval equality applies to any wave function and its amplitude function—not just to a Gaussian. And Eq. (4.59) comes in handy in problem solving, as a way to check the (sometimes considerable) algebra required to evaluate an amplitude function: you can be pretty sure that if you made a mistake in the evaluation of $A(k)$, then the resulting function will not be normalized. Consider this a hint.

The Width of a Gaussian and Its Amplitude Function

Before leaving the Gaussian wave function, I want to probe further the relationship between its width and that of its amplitude function. According to my definition, the widths

of these Gaussian functions, w_x and w_k , respectively, are just the standard deviations Δx and Δk we calculate according to the expressions of § 3.3.

Example 4.5. The Product of the Widths

Consider a Gaussian of the form (4.55) with $L = 1$. Evaluating the standard deviation of such a function is quite easy (see Example 3.5), viz.,

$$\Delta x = 1 \quad \text{for} \quad \Psi(x, 0) = \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4}. \quad (4.60)$$

So all we need is Δk .

To evaluate this quantity from $A(k)$, we just generalize Eq. (3.45) for Δx to a function whose independent variable is k instead of x :

$$(\Delta k)^2 = \langle k^2 \rangle - \langle k \rangle^2. \quad (4.61a)$$

The mean values in this expression are

$$\langle k \rangle = \int_{-\infty}^{\infty} A^*(k) k A(k) dk \quad (4.61b)$$

$$\langle k^2 \rangle = \int_{-\infty}^{\infty} A^*(k) k^2 A(k) dk. \quad (4.61c)$$

Now, substituting the amplitude function (4.58) with $L = 1$ into these equations and performing a little simple algebra, we find

$$\Delta k = \frac{1}{2} \quad \text{for} \quad \Psi(x, 0) = \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4}. \quad (4.62)$$

Combining this result with (4.59) for the width of the wave function, we obtain the product

$$\Delta x \Delta k = \frac{1}{2} \quad \text{for} \quad \Psi(x, 0) = \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4}. \quad (4.63)$$

This result is a special case of Eq. (4.52b), according to which the product of the widths of two wave packets of any form is *greater than or equal to* $1/2$. In fact, the Gaussian function is the *only* mathematical form for which this product *equals* $1/2$. In qualitative terms, Eq. (4.63) just illustrates a familiar property of wave packets (§ 4.4): *the greater the spread of the amplitude function, the narrower the extent of the wave function and position probability density for the state.*

Question 4-12

The amplitude function for the *general form* of the Gaussian, Eq. (4.54), is

$$A(k) = \left(\frac{2}{\pi} L^2\right)^{1/4} e^{-ix_0 k} e^{-(k-k_0)^2 L^2}.$$

Prove that the standard deviations in x and k for the general form of a Gaussian packet—(4.54) with arbitrary L —are

$$\Delta x = L \quad \text{and} \quad \Delta k = \frac{1}{2L}.$$

Although I promised to wait until Chap. 6 to deal with the time development of wave functions, I can't resist showing you how easily we can write down a general form for $\Psi(x, t)$ once we have in hand the amplitude function. This function appears in the general form of a wave packet [Eq. (4.29)]:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx - \omega t)} dk. \quad (4.64)$$

Since the amplitude function doesn't depend on t , we just insert it into (4.64) and voilà: we've got an integral form of the wave function at any time. My point in showing you this is to suggest an important connection between the initial wave function and its subsequent form, a connection that *can* be made through the medium of the amplitude function:

$$\boxed{\Psi(x, 0) \quad \Rightarrow \quad A(k) \quad \Rightarrow \quad \Psi(x, t)} \quad (4.65)$$

Notice, by the way, that to generate $\Psi(x, t)$ from $A(k)$ we must know the dispersion relation $\omega(k)$ for the system.

Question 4-13

Write down the state function $\Psi(x, t)$ that has a Gaussian with $L = 1$ as its initial value at $t = 0$.

In Chap. 12, we'll discover lurking in the connection (4.65) a powerful problem solving strategy, one that can be applied to a wide variety of systems to bypass the task of solving the Schrödinger Equation.

4.6 UNCERTAINTY REGAINED

One of the defining characteristics of a wave packet

$$\Psi(x, t) = \int_{-\infty}^{\infty} A(k) \Psi_k(x, t) dk \quad (4.66)$$

is its non-zero (but finite) standard deviation: $\Delta x > 0$. If the packet represents a state of a particle at time t , then this mathematical fact has an important physical interpretation: the position of the particle is uncertain.

Similarly, the amplitude function $A(k)$, the Fourier transform of $\Psi(x, 0)$, is characterized by a non-zero (finite) standard deviation Δk . And, as I emphasized in § 4.3, this mathematical fact has important consequences for the momentum: this observable is necessarily uncertain [Eq. (4.31)]: $\Delta p = \hbar \Delta k > 0$. Notice that this conclusion pertains to *any* state of *any* system, provided the state is represented by a wave packet. Were we to measure the momentum on an ensemble of particles in such a state, we'd obtain results that fluctuate around the mean value $\langle p \rangle$.

This summary illustrates how in quantum physics mathematical properties of waves translate into physical characteristics of particles in quantum states represented by wave functions. The lexicon of the simplest such translations is the two de Broglie relations $p = \hbar k$ and $E = \hbar \omega$.

Let's see what happens if we use these relations to translate the fundamental wave property that relates the standard deviations of a wave packet and its Fourier transform.

Return of the Heisenberg Uncertainty Principle

The standard deviations Δx and Δk are related by [Eq. (4.52b)] $\Delta x \Delta k \geq 1/2$. Translating these standard deviations into position and (via $p = \hbar k$) momentum uncertainties, we trivially regain the Heisenberg Uncertainty Principle (HUP):²⁶

$$\Delta x \Delta p \geq \frac{1}{2} \hbar. \quad (4.67)$$

In quantum mechanics, we calculate the position uncertainty Δx from the state function $\Psi(x, t)$ and the momentum uncertainty Δp from the amplitude function $A(k)$ as

$$\Delta x = \sqrt{(\Delta x)^2} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \quad (4.68a)$$

$$\Delta p = \hbar \sqrt{(\Delta k)^2} = \hbar \sqrt{\langle k^2 \rangle - \langle k \rangle^2} \quad (4.68b)$$

Note carefully the inequality in Eq.(4.67). Only one wave packet gives equality in Eq. (4.67), the Gaussian function of § 4.4:

$$\Delta x \Delta p = \frac{1}{2} \hbar \quad (\text{Gaussian wave packet}) \quad (4.69)$$

For this reason a Gaussian is sometimes referred to as the *minimum uncertainty wave packet*.²⁷

Our derivation of the HUP is so straightforward that you may be tempted to overlook its profound implications. Equation (4.67) appears here as an inevitable consequence of our decision (Postulate I) to represent quantum states by wave functions that (Postulate II) are interpreted as position probability amplitudes (and hence must be spatially localized). I hope this derivation convinces you once and for all that *uncertainty relations are intrinsic to the quantum-mechanical description of the microverse and as such are wholly unrelated to experimental error or defects in measuring apparatus*. Note also the generality of our argument: it shows that the HUP is not limited to a particular microscopic system or quantum state. This is heady stuff, and I suggest you pause and ponder the subtle and beautiful interplay of mathematics and physics in the remarkably simple derivation of Heisenberg's profound principle.

Aside: The Uncertainty Principle in Three Dimensions. For a particle in three dimensions with wave function $\Psi(\mathbf{r}, t)$, the rectangular components of position and momentum—the components of \mathbf{r} and \mathbf{p} along the orthogonal axes \hat{e}_x , \hat{e}_y , and \hat{e}_z —obey uncertainty relations like (4.67):

²⁶Because these uncertainties have explicit definitions, some authors call Eq. (4.67) "the precise uncertainty principle." Whatever you call it, this inequality is a special case of the *Generalized Uncertainty Principle* (the GUP). The GUP, which we'll meet in § 11.4, is an indeterminacy relationship between the uncertainties of any two observables that cannot simultaneously be measured to infinite precision. As noted in Chap. 2, two such observables are *complementary* in the sense that the more we know about one, the less we can know about the other.

²⁷You can prove this assertion by minimizing the product $\Delta x \Delta p$. For the details, see § 10.9 of *Quantum Theory* by David Bohm (Englewood Cliffs, N. J.: Prentice Hall, 1953).

$$\begin{aligned}
\Delta x \Delta p_x &\geq \frac{1}{2} \hbar \\
\Delta y \Delta p_y &\geq \frac{1}{2} \hbar \\
\Delta z \Delta p_z &\geq \frac{1}{2} \hbar.
\end{aligned}
\tag{4.70}$$

Fig. 4.11 summarizes graphically the correlation between the position and momentum uncertainties that is expressed mathematically in the HUP (4.67). For a narrow state function (Fig. 4.11a), the *position* of the particle is rather well-defined (*i.e.*, Δx is small). But, inevitably, the corresponding amplitude function $A(k) = \mathcal{F}[\Psi(x, 0)]$ encompasses a wide range of pure momentum states (Fig. 4.11b). So we know very little about the *momentum* of the particle in such a state, and Δp is large. On the other hand, a broad state function (Fig. 4.11c) implies a more precise knowledge of momentum (Fig. 4.11d).

With the translation of wave properties of the Fourier transform $A(k)$ of $\Psi(x, 0)$ into physical statements concerning momentum, we have broadened our insight into the physical content of the state function. Back in Chap. 3, we considered this function solely as a source of information about *position*. But in this chapter we've discovered how to extract statistical information concerning a *momentum measurement* (the uncertainty $\Delta p = \hbar \Delta k$) from the state function via its amplitude function. But this is not the only momentum information that lies hidden in $A(k)$; in the next section we'll see how to dig out detailed probabilistic information about a measurement of this observable.

4.7 (NOT QUITE) ALL ABOUT MOMENTUM

As you've doubtless deduced, there is buried in the amplitude function a wealth of physical information about momentum. In fact, we can determine from this function probabilistic and statistical information about momentum that is analogous to the information about position we can extract from $\Psi(x, t)$. To show you how, I first want to rewrite the general form (4.29) of the wave packet,

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx - \omega t)} dk, \tag{4.71}$$

in terms of the *pure momentum state functions* I introduced in § 4.2 [Eq. (4.26)]:

$$\Psi_p(x, t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i(px - Et)/\hbar}. \tag{4.72}$$

To do so requires only a simple change of variable—but even so simple a task can hide traps for the unwary.

Changing Variables in the Amplitude Function

At first, the necessary variable change seems trivial. The de Broglie relation $p = \hbar k$ shows us how to change from wave number to momentum, so to write $\Psi(x, t)$ as an integral over p we first define a new function—say, $\Phi(p)$ —that is proportional to the amplitude function $A(k)$. We then just write the Fourier transform relation (4.71) as an integral over $\Phi(p)\Phi_p(x, t)$ expressing the differential volume element dk as $dk = dp/\hbar$. This is a good plan, but I'm going to vary it slightly so as to minimize later anguish.

I'll define the function $\Phi(p)$ in terms of the amplitude function $A(k)$ as

$$\Phi(p) \equiv \frac{1}{\sqrt{\hbar}} A\left(\frac{p}{\hbar}\right). \quad \text{momentum probability amplitude} \tag{4.73}$$

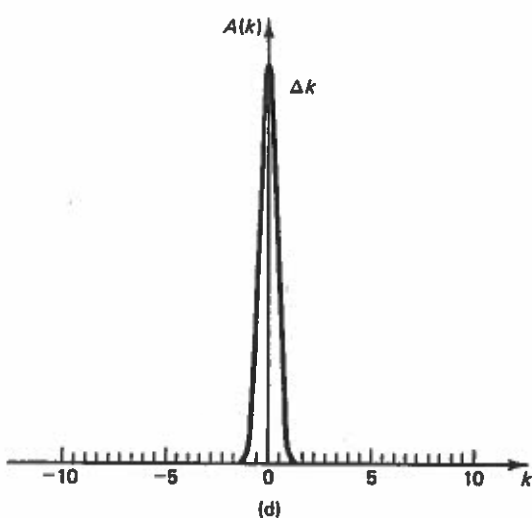
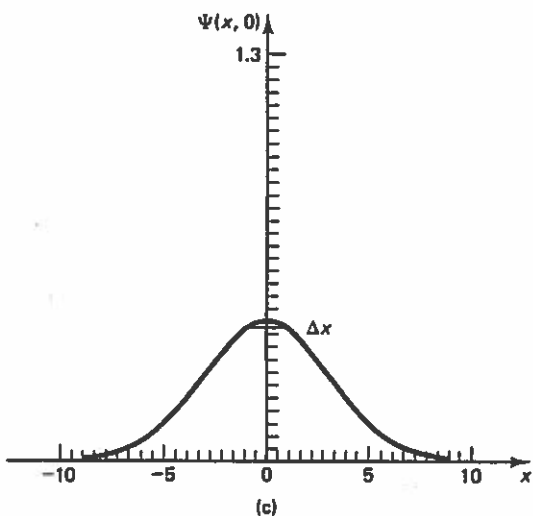
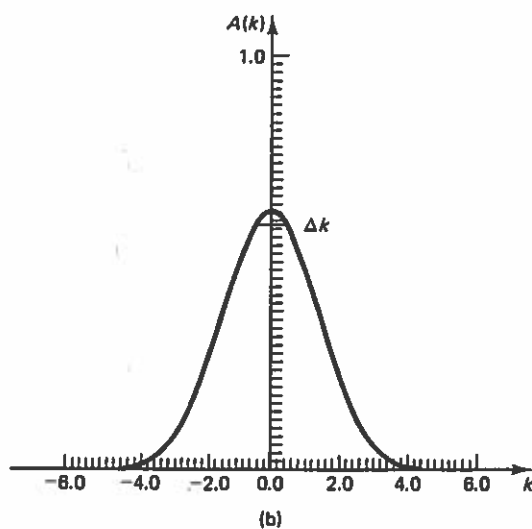
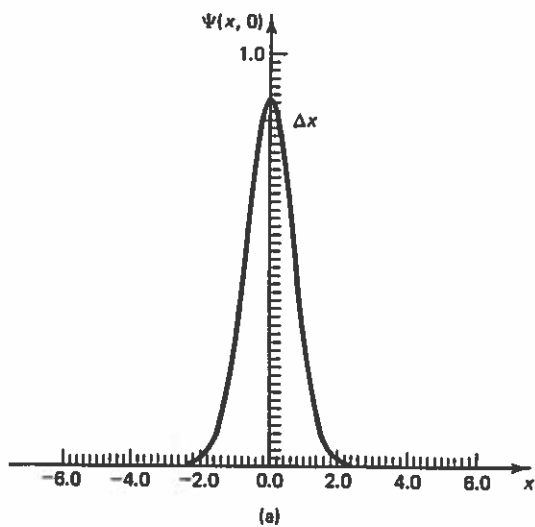


Figure 4.11 Illustrations of the inverse relationship between the widths of $\Psi(x, 0)$ and $A(k)$. Because of this relationship, the momentum uncertainty in the state represented by $\Psi(x, 0)$ is inversely correlated with the position uncertainty Δx via the HUP, Eq. (4.67).

Notice that, by analogy with the position probability amplitude $\Psi(x, t)$, I've dubbed $\Phi(p)$ the **momentum probability amplitude**.

In terms of this function, the wave packet (4.71) at $t = 0$ becomes the momentum integral

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp. \quad (4.74)$$

[Don't fret about the peculiar factors of $1/\sqrt{\hbar}$ in Eqs. (4.73) and (4.74); I'll explain what I am doing in the next aside.]

The inverse of (4.74), the expression for $\Phi(p)$ as an integral with respect to x of $\Psi(x, 0)$, follows easily from the definition (4.73):

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ipx/\hbar} dx. \quad (4.75)$$

We find, not unexpectedly, that *the momentum probability amplitude is the Fourier transform of the position probability amplitude*, with x and p rather than x and k as the transformation variables:

$$\begin{aligned} \Psi(x, 0) &= \mathcal{F}^{-1}[\Phi(p)] \\ \Phi(p) &= \mathcal{F}[\Psi(x, 0)] \end{aligned}$$

(4.76)

I prefer Eqs. (4.76) to the Fourier relationships of § 4.5 for $\Psi(x, 0)$ and $A(k)$, these equations emphasize the physically important variables position and momentum. So unless I tell you otherwise, please understand the shorthand relations (4.76) to refer to Eqs. (4.74) and (4.75) [see the summary in Fig. 4.12].

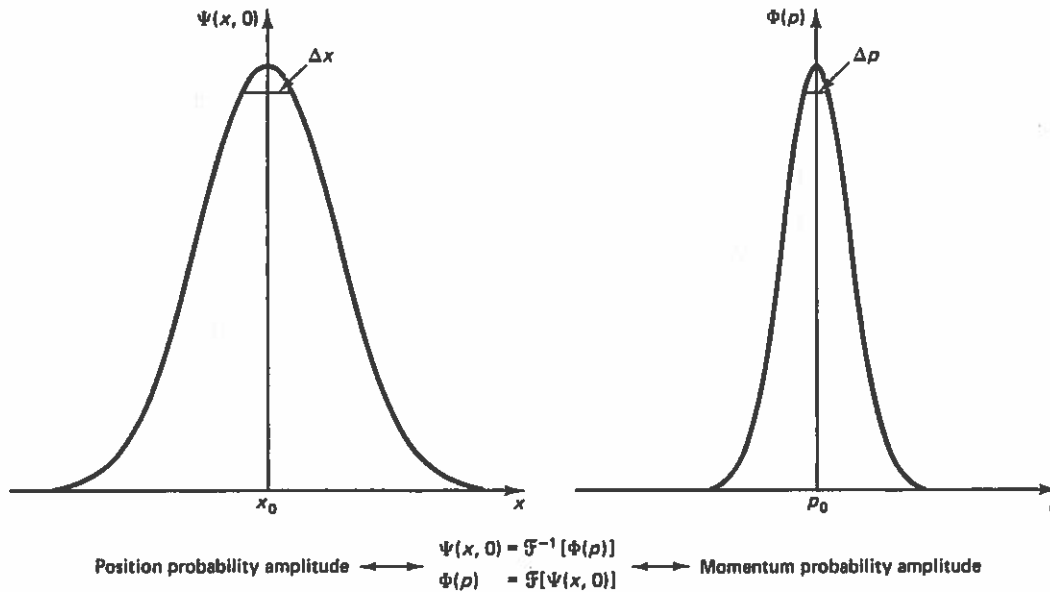


Figure 4.12 Summary of the Fourier relationships between a state function $\Psi(x, 0)$ and the corresponding momentum probability amplitude $\Phi(p)$.

We can generalize the momentum-integration form of the wave packet, (4.74), to arbitrary time, just as we did to obtain the wave-number-integration form in Eq. (4.64) of § 4.5:

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{i(p x - E t)/\hbar} dp \quad (4.77a)$$

$$= \int_{-\infty}^{\infty} \Phi(p) \Psi_p(x, t) dp. \quad (4.77b)$$

Of course, to apply Eqs. (4.77) to a particular system, we must relate ω and k via the appropriate dispersion relation. Once we have done so, we can express any state function as a superposition of pure momentum functions $\Psi_p(x, t)$. Notice, by the way, that the momentum probability amplitude $\Phi(p)$ does not depend on time.²⁸

Aside: Defining the Momentum Probability Amplitude. You may be wondering why I defined the momentum probability amplitude in (4.73) with an extra factor of $1/\sqrt{\hbar}$, rather than as simply $A(p/\hbar)$. Well, when we change variables from k to p , we have to somehow deal with the factor of $1/\hbar$ that arises from the differential relationship $dk = dp/\hbar$; this $1/\hbar$ appears in the expression for the wave packet as an integral over momentum. By including a factor of $1/\sqrt{\hbar}$ in the definition (4.73) and absorbing the other $1/\sqrt{\hbar}$ in the prefactors in the Fourier transform relations (4.74) and (4.75), we preserve a useful property of the amplitude function: automatic normalization.

Recall (§ 4.4) that, courtesy of the Bessel-Parseval relation (4.51), an amplitude function $A(k)$ determined from a *normalized* state function $\Psi(x, 0)$ is automatically normalized with respect to integration over k [c.f., Eq. (4.59)]. This means that in problem solving, we need normalize only $\Psi(x, 0)$. With the definition (4.73) of $\Phi(p)$, automatic normalization is assured for the momentum probability amplitude—applying our change of variables to (4.59), we find

$$\int_{-\infty}^{\infty} |\Phi(p)|^2 dp = \int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx = 1. \quad (4.77c)$$

The Interpretation of $\Phi(p)$: Born Again

My appellation for $\Phi(p)$ —the *momentum probability amplitude*—strongly suggests an analogy to the *position probability amplitude* $\Psi(x, 0)$. In fact, these functions are different ways of representing the same quantum state (§ 4.7) that highlight information about different observables:

$$\left. \begin{array}{ll} \Psi(x, t) \longrightarrow \text{position} \\ \Phi(p) \longrightarrow \text{momentum} \end{array} \right\} \text{ same quantum state}$$

This analogy suggests that we interpret $\Phi(p)$ for momentum like we interpreted $\Psi(x, t)$ for position. To jog your memory, here's the Born interpretation of $\Psi(x, t)$ as a position probability amplitude (Postulate II):

Interpretation of $\Psi(x, t)$: If the members of an ensemble are in a quantum state represented by the wave function $\Psi(x, t)$, then

$$P(x, t)dx = |\Psi(x, t)|^2 dx$$

is the probability that in a position measurement at time t a particle will be detected in the infinitesimal region from x to $x + dx$.

²⁸Some applications of quantum mechanics are based on a time-dependent momentum probability amplitude $\Phi(p, t)$. This function is defined, as you might have guessed, as the inverse Fourier transform of the wave function at time t :

$$\Phi(p, t) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x, t) e^{-ipx/\hbar} dx$$

In practice, a time-dependent momentum amplitude is useful only in a very small number of cases—because the integral in its definition is quite ferocious. You can find a good discussion of these time-dependent momentum amplitudes in *Elementary Quantum Mechanics* by David S. Saxon (San Francisco: Holden-Day, 1968).

Now, a reasonable generalization of this idea to the momentum amplitude $\Phi(p)$, which represents the same quantum state as $\Psi(x, t)$, is²⁹

Interpretation of $\Phi(p)$: If the members of an ensemble are in a quantum state that is represented by a wave function $\Psi(x, t)$ with Fourier transform $\Phi(p) = \mathcal{F}[\Psi(x, 0)]$, then

$$P(p) dp = |\Phi(p)|^2 dp = \Phi^*(p)\Phi(p) dp$$

is the probability that in a momentum measurement at time t a particle's momentum will be found to have a value in the infinitesimal region from p to $p + dp$.

This generalization is the key to calculating *probabilistic information about momentum* from a wave function $\Psi(x, t)$. And it buttresses the extension of our definitions of the statistical properties $\langle x \rangle$ and Δx to momentum, viz.,

$\begin{aligned}\langle p \rangle &\equiv \int_{-\infty}^{\infty} p P(p) dp \\ &= \int_{-\infty}^{\infty} \Phi^*(p) p \Phi(p) dp\end{aligned}$	Expectation Value of Momentum	(4.78)
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$\begin{aligned}\Delta p &\equiv \sqrt{(\Delta p)^2} \\ &= \left[\langle (p - \langle p \rangle)^2 \rangle \right]^{1/2} \\ &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2}\end{aligned}$	Momentum Uncertainty	(4.79)
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In (4.79), the expectation value of p^2 , which we need to evaluate the momentum uncertainty, is just

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Phi^*(p) p^2 \Phi(p) dp. \quad (4.80)$$

To illustrate the application of these extensions, I've gathered our results (from § 4.6) for a sample Gaussian wave function $\Psi(x, 0)$ and its Fourier transform, suitably expressed them in terms of x and p , and tabulated the whole thing in Table 4.1.

Question 4-14

Write the expressions for $\Psi(x, 0)$ and for $\Phi(p)$ in Table 4.1 in terms of Δx and Δp respectively (instead of L). Your results show the important dependence of the Gaussian function and its Fourier transform on their (initial) widths—a feature of the Gaussian to which we'll return in § 6.7.

²⁹In more formal treatments of quantum mechanics, such as befits a graduate course, Postulate II is stated abstractly as a way to interpret the quantum state descriptor in terms of an arbitrary observable. To see how this goes, see *Quantum Mechanics*, Vol. I by C. Cohen-Tannoudji, B. Diu, and F. Laloë (New York: Wiley-Interscience, 1977).

TABLE 4.1 POSITION AND MOMENTUM INFORMATION FOR A GAUSSIAN STATE FUNCTION WITH $L = 1.0$, $x_0 = 0$, AND $p_0 = 0$

Position	Momentum
$\Psi(x, 0) = \left(\frac{1}{2\pi L^2}\right)^{1/4} e^{-x^2/(4L^2)}$ $\langle x \rangle = 0$ $\Delta x = L$	$\Phi(p) = \left(\frac{2L^2}{\pi \hbar^2}\right)^{1/4} e^{-p^2 L^2/\hbar^2}$ $\langle p \rangle = 0$ $\Delta p = \frac{1}{2L} \hbar$

Question 4-15

We understand the existence of a center x_0 of a wave packet $\Psi(x, t)$ as due to constructive interference in the superposition of complex harmonic waves that is the packet. For a symmetric packet this point coincides with the expectation value at $t = 0$, i.e., $x_0 = \langle x \rangle(0)$. Provide a similar explanation of the existence of the center $p_0 = \hbar k_0 = \langle p \rangle$ of the momentum probability amplitude.

With this generalization to $\Phi(p)$ of the expressions for the expectation value and the uncertainty, we've developed machinery for calculating all we are permitted to know about momentum from this probability amplitude. And an impressive menu it is: We can work out the probabilities of each possible outcome of an ensemble measurement of momentum as well as statistical quantities that characterize all the results of the measurement: the mean value ($\langle p \rangle$) and the extent to which individual results fluctuate about the mean (Δp). Underlying this scheme are a few basic principles: the de Broglie relation $p = \hbar k$, the Born interpretation of a state function as a probability amplitude, and basic properties of waves.

Still, the momentum probability amplitude $\Phi(p)$ is but one avenue to momentum information about a quantum state. There are others—which is good news, because in some applications, determining $\Phi(p)$ as the Fourier transform of the wave function $\Psi(x, 0)$ is an algebraic nightmare. But fear not. Chap. 5 is in the offing.

4.8 FINAL THOUGHTS: A WEALTH OF REPRESENTATIONS

Our quest for a free-particle state function, which began in § 4.1 with the complex harmonic wave and culminated in § 4.2–4.3 with the wave packet, has taken us deep into the mysteries of momentum. But before I bring this observable center stage, in the next chapter, I want to reinforce the physics that underlies the mathematics of Fourier analysis—which led us into the world of momentum amplitudes in the first place.

Underlying the application of Fourier analysis to the construction and deconstruction of wave packets are physical principles familiar from Chaps. 2 and 3. Predominant among these is the omnipresent *Principle of Superposition*, which we saw reflected in our imagining a wave packet as a superposition of pure momentum states. Second, *wave-particle duality* is implicit in our use of the mathematics of waves to build and analyze functions that represent states of microscopic particles, as it is in our use of the de Broglie relations to interpret these states. And finally, *uncertainty* appeared naturally, almost as an afterthought, from our mathematical machinations.

This subtle interplay of the mathematics of complex functions and the physics of the microworld is one of the marvels of quantum physics. No one really knows *why* this mathematical artifice of man's mind happens to describe the real world so well; this is a question for philosophers and metaphysicists.³⁰

The principal results of this chapter were the general form (4.29) of the wave packet, the Fourier transform relations (4.76) between the position and probability amplitudes, and our finding (§ 4.7) that a state function yields (probabilistic and statistical) information about position or about momentum—depending on how we treat it. The algebraic procedures we use to extract position information from $\Psi(x, 0)$ and momentum information from $\Phi(p)$ are identical; only the variables are changed. This powerful analogy is summarized in Table 4.2.

TABLE 4.2 POSITION AND MOMENTUM REPRESENTATIONS OF A QUANTUM STATE OF A PARTICLE IN ONE DIMENSION

	Position	Momentum
Observable	x	p
State function	$\Psi(x, 0)$	$\Phi(p)$
Probability density	$P(x, 0) = \Psi(x, 0) ^2$	$P(p) = \Phi(p) ^2$
Expectation value	$\langle x \rangle (0) = \int_{-\infty}^{\infty} \Psi^*(x, 0) x \Psi(x, 0) dx$	$\langle p \rangle = \int_{-\infty}^{\infty} \Phi^*(p) p \Phi(p) dp$
Uncertainty	$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$	$\Delta p = \sqrt{\langle (p - \langle p \rangle)^2 \rangle}$
	$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$	$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$

In more advanced formulations of quantum mechanics, the position and momentum amplitudes $\Psi(x, t)$ and $\Phi(p)$ are but two of an infinite number of “representations” of a more abstract state descriptor, the *state vector*. A state vector is not a function. Neither is it a vector in our geometrical space, \mathbb{R}^3 . Instead, it lives in an abstract vector space called a *Hilbert space*, where it is ruled by the mathematics of *linear algebra*. The state vector is usually denoted by the symbol $|\Psi(t)\rangle$.

Our wave function $\Psi(x, t)$ is the representation of this critter in (one-dimensional) “position space,” where the coordinate is x . Our momentum probability amplitude $\Phi(p)$ is its representation in “momentum space,” where the coordinate is p . In fact, one can devise an *infinite number of different representations of a quantum state*. Each representation corresponds to a different observable: there is an energy representation, an angular momentum representations, and so forth.

This more abstract formulation was developed by P. A. M. Dirac.³¹ Although later in this volume I'll show you a wonderfully convenient shorthand notation Dirac introduced for integrals, I won't show you quantum mechanics from his powerful but austere vantage point. At this stage, I want to keep matters as concrete as possible.

³⁰But if you're curious to read a physicist's thoughts on the matter, you should read Eugene Wigner's fascinating essay on the interconnections between mathematics and physics. It is reprinted as Chap. 17 of his collection *Symmetry and Reflections* (Cambridge, Mass.: MIT Press, 1970).

³¹Dirac's exposition of quantum mechanics, *The Principles of Quantum Theory*, 4th ed. (Oxford: Clarendon Press, 1958)—which is now available in paperback—is a genuine classic that eventually should be read and re-read by every serious student of quantum theory.

Before we leave the matter of incarnations of the state vector, I want to make one final important point:

Rule

No representation of a state contains any more (or less) physical information than any other.

This being the case, our decision to represent a state by $\Psi(x, 0)$ or by $\Phi(p)$ or by a function of some other variable becomes a matter of personal proclivity. In practice, the choice of representation is guided by expediency: we can usually find a representation that is particularly appropriate to the problem at hand (*i.e.*, that saves us work).

ANNOTATED SELECTED READINGS

Waves

You probably studied waves in a freshman or sophomore general physics course or in a separate course devoted solely to this topic. If not, you should have a look at one of the following excellent texts (arranged in order of increasing difficulty):

1. French, A. P., *Vibrations and Waves* (New York: W. W. Norton, 1961) (available in paperback). This book contains an especially good treatment of *superposition* in Chap. 2 and of interference phenomena in Chap. 8.
2. Crawford, Frank S. Jr., *Waves: Berkeley Physics Course*, Volume 3 (New York: McGraw-Hill, 1968). An exhaustive treatment of waves that emphasizes their applications to nearly every area of physics. For interesting discussions of dispersion and the group velocity of de Broglie waves, see Supplementary Topics 2 and 4.
3. Elmore, W. C., and Mark A. Heald, *The Physics of Waves* (New York: McGraw-Hill, 1969).

Wave Packets and Uncertainty

One of the most intriguing things to emerge from our discussions of wave packets was the uncertainty principle. For a more detailed analysis of the relationship between this important physical principle and the mathematics of state functions, look in nearly any graduate-level quantum book, such as

4. Rabinowitz, A., *Quantum Mechanics* (New York: Elsevier, 1968), § 30 and 31.
 5. Bohm, David, *Quantum Theory* (Englewood Cliffs, N. J.: Prentice Hall, 1953), § 10.9.
- The same A. P. French who wrote the book on waves I recommended above has also co-authored an excellent quantum mechanics text (at a slightly lower level than this one):
6. French, A. P., and Edwin F. Taylor, *An Introduction to Quantum Physics* (New York: Norton, 1978) (available in paperback). This whole book is readable, insightful, and worth your time; but I particularly recommend their discussion of wave packets (§ 8.7).

Fourier Analysis

Fourier series and integrals are so important to the mathematics of science and engineering that any "math methods" book worth its salt will contain an exposition of this topic, usually with lots of illustrations. A treatment that is particularly oriented towards students of physics, albeit at a rather advanced level, is the one in