(c) If you differentiate an nth-order polynomial, you get a polynomial of order $(n-1)$. For the Hermite polynomials, in fact,

$$\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi). \quad [2.88]$$

Check this, by differentiating H_5 and H_6.

(d) $H_n(\xi)$ is the nth z-derivative, at $z = 0$, of the **generating function** $\exp(-z^2 + 2z\xi)$; or, to put it another way, it is the coefficient of $z^n/n!$ in the Taylor series expansion for this function:

$$e^{-z^2+2z\xi} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi). \quad [2.89]$$

Use this to rederive H_0, H_1, and H_2.

2.4 THE FREE PARTICLE

We turn next to what *should* have been the simplest case of all: the free particle ($V(x) = 0$ everywhere). Classically this would just mean motion at constant velocity, but in quantum mechanics the problem is surprisingly subtle and tricky. The time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad [2.90]$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \quad [2.91]$$

So far, it's the same as inside the infinite square well (Equation 2.21), where the potential is also zero; this time, however, I prefer to write the general solution in exponential form (instead of sines and cosines), for reasons that will appear in due course:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}. \quad [2.92]$$

Unlike the infinite square well, there are no boundary conditions to restrict the possible values of k (and hence of E); the free particle can carry *any* (positive) energy. Tacking on the standard time dependence, $\exp(-iEt/\hbar)$,

$$\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}. \quad [2.93]$$

Now, *any* function of x and t that depends on these variables in the special combination $(x \pm vt)$ (for some constant v) represents a wave of fixed profile, traveling in the $\mp x$-direction, at speed v. A fixed point on the waveform (for example, a maximum or a minimum) corresponds to a fixed value of the argument, and hence to x and t such that

$$x \pm vt = \text{constant}, \quad \text{or} \quad x = \mp vt + \text{constant}.$$

Since every point on the waveform is moving along with the same velocity, its *shape* doesn't change as it propagates. Thus the first term in Equation 2.93 represents a wave traveling to the *right*, and the second represents a wave (of the same energy) going to the *left*. By the way, since they only differ by the *sign* in front of k, we might as well write

$$\Psi_k(x, t) = A e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}, \tag{2.94}$$

and let k run negative to cover the case of waves traveling to the left:

$$k \equiv \pm \frac{\sqrt{2mE}}{\hbar}, \quad \text{with} \begin{cases} k > 0 \Rightarrow & \text{traveling to the right,} \\ k < 0 \Rightarrow & \text{traveling to the left.} \end{cases} \tag{2.95}$$

Evidently the "stationary states" of the free particle are propagating waves; their wavelength is $\lambda = 2\pi/|k|$, and, according to the de Broglie formula (Equation 1.39), they carry momentum

$$p = \hbar k. \tag{2.96}$$

The speed of these waves (the coefficient of t over the coefficient of x) is

$$v_{\text{quantum}} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}. \tag{2.97}$$

On the other hand, the *classical* speed of a free particle with energy E is given by $E = (1/2)mv^2$ (pure kinetic, since $V = 0$), so

$$v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2v_{\text{quantum}}. \tag{2.98}$$

Apparently the quantum mechanical wave function travels at *half* the speed of the particle it is supposed to represent! We'll return to this paradox in a moment—there is an even more serious problem we need to confront first: *This wave function is not normalizable.* For

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2(\infty). \tag{2.99}$$

In the case of the free particle, then, the separable solutions do not represent physically realizable states. A free particle cannot exist in a stationary state; or, to put it another way, *there is no such thing as a free particle with a definite energy.*

But that doesn't mean the separable solutions are of no use to us, for they play a *mathematical* role that is entirely independent of their *physical* interpretation. The general solution to the time-dependent Schrödinger equation is still a linear combination of separable solutions (only this time it's an *integral* over the continuous variable k, instead of a *sum* over the discrete index n):

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} \, dk. \qquad [2.100]$$

(The quantity $1/\sqrt{2\pi}$ is factored out for convenience; what plays the role of the coefficient c_n in Equation 2.17 is the combination $(1/\sqrt{2\pi})\phi(k)\,dk$.) Now *this* wave function *can* be normalized (for appropriate $\phi(k)$). But it necessarily carries a *range* of k's, and hence a range of energies and speeds. We call it a **wave packet**.[32]

In the generic quantum problem, we are *given* $\Psi(x,0)$, and we are asked to *find* $\Psi(x,t)$. For a free particle the solution takes the form of Equation 2.100; the only question is how to determine $\phi(k)$ so as to match the initial wave function:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} \, dk. \qquad [2.101]$$

This is a classic problem in Fourier analysis; the answer is provided by **Plancherel's theorem** (see Problem 2.20):

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} \, dk \Longleftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} \, dx. \qquad [2.102]$$

$F(k)$ is called the **Fourier transform** of $f(x)$; $f(x)$ is the **inverse Fourier transform** of $F(k)$ (the only difference is in the sign of the exponent). There is, of course, some restriction on the allowable functions: The integrals have to *exist*.[33] For our purposes this is guaranteed by the physical requirement that $\Psi(x,0)$ itself

[32] Sinusoidal waves extend out to infinity, and they are not normalizable. But *superpositions* of such waves lead to interference, which allows for localization and normalizability.

[33] The necessary and sufficient condition on $f(x)$ is that $\int_{-\infty}^{\infty} |f(x)|^2 dx$ be *finite*. (In that case $\int_{-\infty}^{\infty} |F(k)|^2 dk$ is also finite, and in fact the two integrals are equal.) See Arfken (footnote 24), Section 15.5.

be normalized. So the solution to the generic quantum problem, for the free particle, is Equation 2.100, with

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0) e^{-ikx} \, dx.} \quad [2.103]$$

Example 2.6 A free particle, which is initially localized in the range $-a < x < a$, is released at time $t = 0$:

$$\Psi(x, 0) = \begin{cases} A, & \text{if } -a < x < a, \\ 0, & \text{otherwise,} \end{cases}$$

where A and a are positive real constants. Find $\Psi(x, t)$.

Solution: First we need to normalize $\Psi(x, 0)$:

$$1 = \int_{-\infty}^{\infty} |\Psi(x, 0)|^2 \, dx = |A|^2 \int_{-a}^{a} dx = 2a|A|^2 \Rightarrow A = \frac{1}{\sqrt{2a}}.$$

Next we calculate $\phi(k)$, using Equation 2.103:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx} \, dx = \frac{1}{2\sqrt{\pi a}} \frac{e^{-ikx}}{-ik} \Big|_{-a}^{a}$$
$$= \frac{1}{k\sqrt{\pi a}} \left(\frac{e^{ika} - e^{-ika}}{2i} \right) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k}.$$

Finally, we plug this back into Equation 2.100:

$$\Psi(x, t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m} t)} \, dk. \quad [2.104]$$

Unfortunately, this integral cannot be solved in terms of elementary functions, though it can of course be evaluated numerically (Figure 2.8). (There are, in fact, precious few cases in which the integral for $\Psi(x, t)$ (Equation 2.100) *can* be calculated explicitly; see Problem 2.22 for a particularly beautiful example.)

It is illuminating to explore the limiting cases. If a is very small, the starting wave function is a nicely localized spike (Figure 2.9(a)). In this case we can use the small angle approximation to write $\sin(ka) \approx ka$, and hence

$$\phi(k) \approx \sqrt{\frac{a}{\pi}};$$

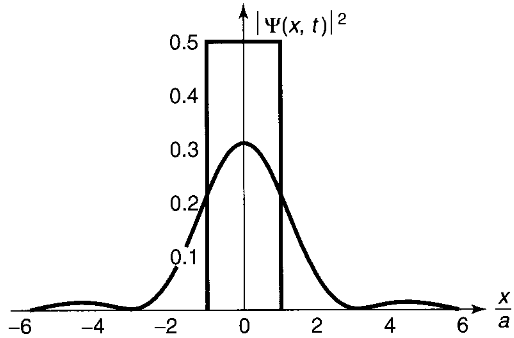

FIGURE 2.8: Graph of $|\Psi(x,t)|^2$ (Equation 2.104) at $t = 0$ (the rectangle) and at $t = ma^2/\hbar$ (the curve).

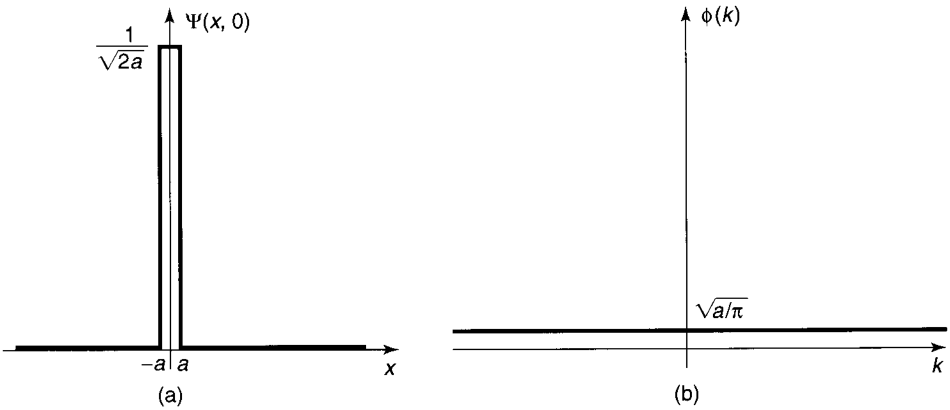

FIGURE 2.9: Example 2.6, for small a. (a) Graph of $\Psi(x, 0)$. (b) Graph of $\phi(k)$.

it's *flat*, since the k's cancelled out (Figure 2.9(b)). This is an example of the uncertainty principle: If the spread in *position* is small, the spread in *momentum* (and hence in k—see Equation 2.96) must be large. At the other extreme (*large* a) the spread in position is broad (Figure 2.10(a)) and

$$\phi(k) = \sqrt{\frac{a}{\pi}}\frac{\sin(ka)}{ka}.$$

Now, $\sin z/z$ has its maximum at $z = 0$, and drops to zero at $z = \pm\pi$ (which, in this context, means $k = \pm\pi/a$). So for large a, $\phi(k)$ is a sharp spike about $k = 0$ (Figure 2.10(b)). This time it's got a well-defined momentum but an ill-defined position.

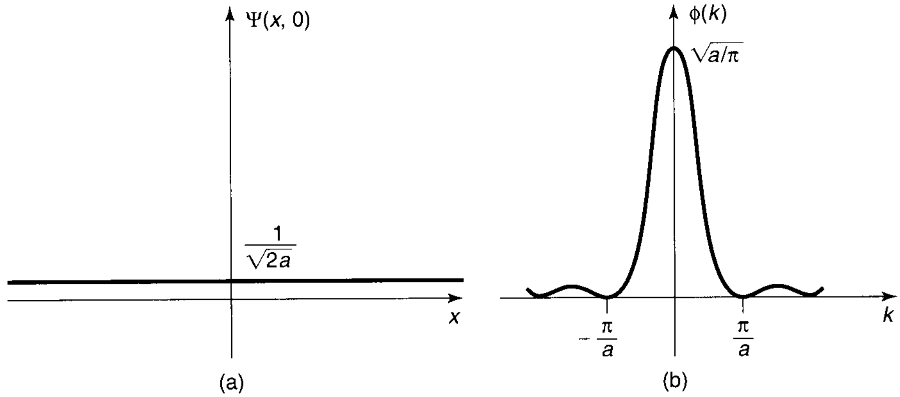

FIGURE 2.10: Example 2.6, for large a. (a) Graph of $\Psi(x,0)$. (b) Graph of $\phi(k)$.

I return now to the paradox noted earlier: the fact that the separable solution $\Psi_k(x,t)$ in Equation 2.94 travels at the "wrong" speed for the particle it ostensibly represents. Strictly speaking, the problem evaporated when we discovered that Ψ_k is not a physically realizable state. Nevertheless, it is of interest to discover how information about velocity *is* contained in the free particle wave function (Equation 2.100). The essential idea is this: A wave packet is a superposition of sinusoidal functions whose amplitude is modulated by ϕ (Figure 2.11); it consists of "ripples" contained within an "envelope." What corresponds to the particle velocity is not the speed of the individual ripples (the so-called **phase velocity**), but rather the speed of the envelope (the **group velocity**)—which, depending on the nature of the waves, can be greater than, less than, or equal to, the velocity of the ripples that go to make it up. For waves on a string, the group velocity is the same as the phase velocity. For water waves it is one-half the phase velocity, as you may have noticed when you toss a rock into a pond (if you concentrate on a particular ripple, you will see it build up from the rear, move forward through the group, and fade away at the front, while the group as a whole propagates out at half the speed). What I need to show is that for the wave function of a free particle in quantum mechanics

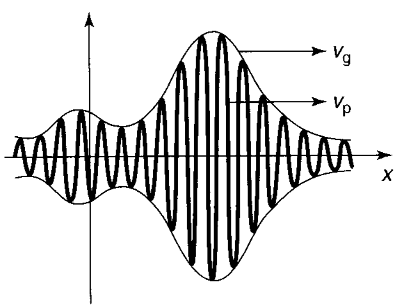

FIGURE 2.11: A wave packet. The "envelope" travels at the group velocity; the "ripples" travel at the phase velocity.

the group velocity is *twice* the phase velocity—just right to represent the classical particle speed.

The problem, then, is to determine the group velocity of a wave packet with the general form

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

(In our case $\omega = (\hbar k^2/2m)$, but what I have to say now applies to *any* kind of wave packet, regardless of its **dispersion relation**—the formula for ω as a function of k.) Let us assume that $\phi(k)$ is narrowly peaked about some particular value k_0. (There is nothing *illegal* about a broad spread in k, but such wave packets change shape rapidly—since different components travel at different speeds—so the whole notion of a "group," with a well-defined velocity, loses its meaning.) Since the integrand is negligible except in the vicinity of k_0, we may as well Taylor-expand the function $\omega(k)$ about that point, and keep only the leading terms:

$$\omega(k) \cong \omega_0 + \omega_0'(k - k_0),$$

where ω_0' is the derivative of ω with respect to k, at the point k_0.

Changing variables from k to $s \equiv k - k_0$ (to center the integral at k_0), we have

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0 + s) e^{i[(k_0+s)x - (\omega_0 + \omega_0' s)t]}\, ds.$$

At $t = 0$,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0 + s) e^{i(k_0+s)x}\, ds,$$

and at later times

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} e^{i(-\omega_0 t + k_0 \omega_0' t)} \int_{-\infty}^{+\infty} \phi(k_0 + s) e^{i(k_0+s)(x - \omega_0' t)}\, ds.$$

Except for the shift from x to $(x - \omega_0' t)$, the integral is the same as the one in $\Psi(x, 0)$. Thus

$$\Psi(x,t) \cong e^{-i(\omega_0 - k_0\omega_0')t}\, \Psi(x - \omega_0' t, 0). \qquad [2.105]$$

Apart from the phase factor in front (which won't affect $|\Psi|^2$ in any event) the wave packet evidently moves along at a speed ω_0':

$$v_{\text{group}} = \frac{d\omega}{dk} \qquad [2.106]$$

(evaluated at $k = k_0$). This is to be contrasted with the ordinary phase velocity

$$v_{\text{phase}} = \frac{\omega}{k}. \qquad [2.107]$$

In our case, $\omega = (\hbar k^2/2m)$, so $\omega/k = (\hbar k/2m)$, whereas $d\omega/dk = (\hbar k/m)$, which is twice as great. This confirms that it is the group velocity of the wave packet, not the phase velocity of the stationary states, that matches the classical particle velocity:

$$v_{\text{classical}} = v_{\text{group}} = 2v_{\text{phase}}. \tag{2.108}$$

Problem 2.18 Show that $[Ae^{ikx} + Be^{-ikx}]$ and $[C\cos kx + D\sin kx]$ are equivalent ways of writing the same function of x, and determine the constants C and D in terms of A and B, and vice versa. *Comment:* In quantum mechanics, when $V = 0$, the exponentials represent *traveling* waves, and are most convenient in discussing the free particle, whereas sines and cosines correspond to *standing* waves, which arise naturally in the case of the infinite square well.

Problem 2.19 Find the probability current, J (Problem 1.14) for the free particle wave function Equation 2.94. Which direction does the probability current flow?

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* ***Problem 2.20** This problem is designed to guide you through a "proof" of Plancherel's theorem, by starting with the theory of ordinary Fourier series on a *finite* interval, and allowing that interval to expand to infinity.

(a) Dirichlet's theorem says that "any" function $f(x)$ on the interval $[-a, +a]$ can be expanded as a Fourier series:

$$f(x) = \sum_{n=0}^{\infty}[a_n \sin(n\pi x/a) + b_n \cos(n\pi x/a)].$$

Show that this can be written equivalently as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a}.$$

What is c_n, in terms of a_n and b_n?

(b) Show (by appropriate modification of Fourier's trick) that

$$c_n = \frac{1}{2a}\int_{-a}^{+a} f(x)e^{-in\pi x/a}\,dx.$$

(c) Eliminate n and c_n in favor of the new variables $k = (n\pi/a)$ and $F(k) = \sqrt{2/\pi}\,ac_n$. Show that (a) and (b) now become

$$f(x) = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} F(k)e^{ikx}\,\Delta k; \quad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-a}^{+a} f(x)e^{-ikx}\,dx,$$

where Δk is the increment in k from one n to the next.

(d) Take the limit $a \to \infty$ to obtain Plancherel's theorem. *Comment:* In view of their quite different origins, it is surprising (and delightful) that the two formulas—one for $F(k)$ in terms of $f(x)$, the other for $f(x)$ in terms of $F(k)$—have such a similar structure in the limit $a \to \infty$.

Problem 2.21 A free particle has the initial wave function

$$\Psi(x, 0) = Ae^{-a|x|},$$

where A and a are positive real constants.

(a) Normalize $\Psi(x, 0)$.

(b) Find $\phi(k)$.

(c) Construct $\Psi(x, t)$, in the form of an integral.

(d) Discuss the limiting cases (a very large, and a very small).

***Problem 2.22 The gaussian wave packet.** A free particle has the initial wave function

$$\Psi(x, 0) = Ae^{-ax^2},$$

where A and a are constants (a is real and positive).

(a) Normalize $\Psi(x, 0)$.

(b) Find $\Psi(x, t)$. *Hint:* Integrals of the form

$$\int_{-\infty}^{+\infty} e^{-(ax^2+bx)}\, dx$$

can be handled by "completing the square": Let $y \equiv \sqrt{a}\,[x + (b/2a)]$, and note that $(ax^2 + bx) = y^2 - (b^2/4a)$. *Answer:*

$$\Psi(x, t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/[1+(2i\hbar at/m)]}}{\sqrt{1 + (2i\hbar at/m)}}.$$

(c) Find $|\Psi(x, t)|^2$. Express your answer in terms of the quantity

$$w \equiv \sqrt{\frac{a}{1 + (2\hbar at/m)^2}}.$$

Sketch $|\Psi|^2$ (as a function of x) at $t = 0$, and again for some very large t. Qualitatively, what happens to $|\Psi|^2$, as time goes on?

(d) Find $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$, σ_x, and σ_p. *Partial answer:* $\langle p^2\rangle = a\hbar^2$, but it may take some algebra to reduce it to this simple form.

(e) Does the uncertainty principle hold? At what time t does the system come closest to the uncertainty limit?
