As in the calculation of the probability density above, all the time dependence of $\langle \hat{x} \rangle_t$ is contained in the interference term. Quite generally, to obtain time dependence in *any* experimental observable it is necessary to have a superposition of states with different energies.

1.3 A Worked Example: Particle in Half a Box

As an example of an analytically solvable model, consider a particle in a box that extends from 0 to L. Assume the particle is in the lowest level of the box. At $t = 0$ the size of the box is suddenly expanded, so that the box extends from 0 to $2L$ as in Fig. 1.1. The object is to calculate the smallest period of time, τ, at which $\Psi(x, \tau) = \Psi(x, 0)$, and to draw a picture of $\Psi(x, t)$ at $t = \tau/2$.

At $t = 0$, $\Psi(x, 0)$ is a normalized eigenstate of the old box $[0, L]$:

$$\Psi(x, 0) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right).$$

Note that the eigenfunctions $\psi_n(x)$ and eigenvalues E_n of the new box $[0, 2L]$ are

$$\psi_n(x) = \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right) \qquad E_n = \frac{n^2\pi^2\hbar^2}{8mL^2} \qquad n = 1, 2, \ldots$$

To calculate the time evolution of Ψ we expand $\Psi(x, 0)$ in a complete set of the *new* eigenfunctions, $\psi_n(x)$, since the time dependence of each of the new eigenfunctions is just a simple phase factor under the new Hamiltonian. The expansion takes the form

$$\Psi(x, 0) = \sum_n a_n \, \psi_n(x),$$

where

$$a_n = \int_0^L \Psi(x, 0) \, \psi_n^*(x) \, dx = \int_0^L \left\{\sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)\right\} \left\{\sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right)\right\} dx.$$

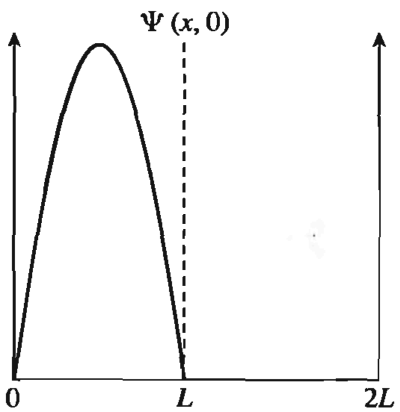

Figure 1.1 Initial conditions for particle in half a box

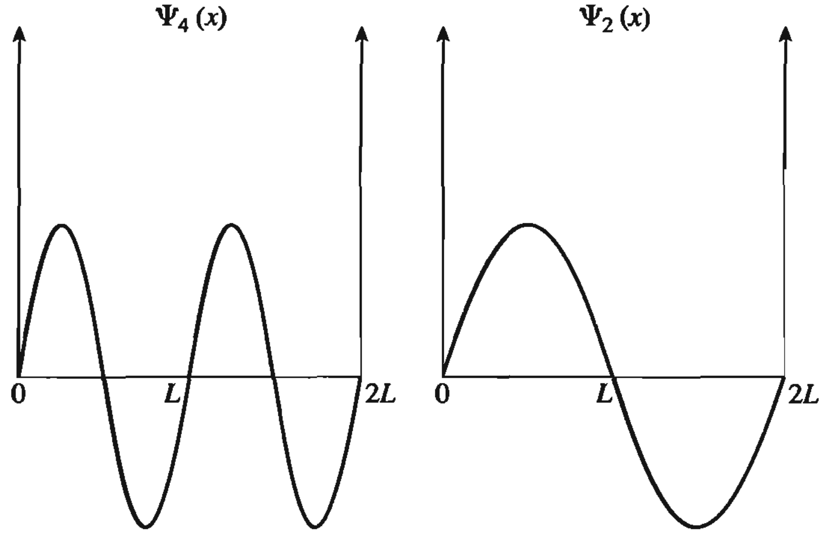

Figure 1.2 $\Psi(x, 0)$ is orthogonal to all $\psi_n(x)$ if n is even. This is because $\Psi(x, 0)$ vanishes outside of the range $[0, L]$, and in that range all the even eigenstates of the full box correspond, within a normalization factor, to excited eigenstates of the half box. This is shown in the left panel for $n = 4$. The one exception is the $n = 2$ state, shown in the right panel, which is essentially a replica of $\Psi(x, 0)$ in the range $[0, L]$. Note that we use capital Ψ for the time-evolving state and small ψ_n for the eigenstates.

Before doing this integral, notice that $a_n = 0$ for all even n, except $n = 2$, by symmetry (see Figure 1.2). Since $n = 2$ is the only state of its symmetry with nonvanishing coefficient, we calculate this overlap integral first:

$$a_2 = \int_0^L \left\{\sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)\right\} \left\{\sqrt{\frac{1}{L}} \sin\left(\frac{\pi x}{L}\right)\right\} dx = \frac{1}{\sqrt{2}}.$$

To find a_n, n odd, we use the formula

$$\int_0^a \sin(bx)\sin(cx)\,dx = -\frac{1}{2}\left[\frac{\sin[(b+c)a]}{b+c} - \frac{\sin[(b-c)a]}{b-c}\right].$$

Setting $a = L,\ b = \frac{\pi}{L},\ c = \frac{n\pi}{2L}$, we find

$$\begin{aligned} a_n &= -\sqrt{2}\left[\frac{(-1)^{\frac{n+1}{2}}}{(n+2)\pi} + \frac{(-1)^{\frac{n-1}{2}}}{(n-2)\pi}\right] \\ &= \frac{4\sqrt{2}(-1)^{\frac{n+1}{2}}}{(n+2)(n-2)\pi}, \end{aligned}$$

where we have used the fact that

$$\sin\left(\pi + \frac{n\pi}{2}\right) = (-1)^{\frac{n+1}{2}}; \qquad \sin\left(\pi - \frac{n\pi}{2}\right) = (-1)^{\frac{n-1}{2}}.$$

The numerical values for the first few overlap integrals are

$$a_1 = \frac{-4\sqrt{2}}{(3)(-1)\pi} = .600 \qquad a_5 = \frac{-4\sqrt{2}}{(7)(3)\pi} = -.086$$

$$a_2 = \frac{1}{\sqrt{2}} = .707 \qquad a_7 = \frac{4\sqrt{2}}{(9)(5)\pi} = .040$$

$$a_3 = \frac{4\sqrt{2}}{(5)\pi} = .360 \qquad a_9 = \frac{-4\sqrt{2}}{(11)(7)\pi} = -.023.$$

As a check, note that $\sum_{n=1}^{9} |a_n|^2 = .999 \cong 1$.

We now combine the eigenstates with their phase factors and their coefficients to analyze the time dependence of the wavepacket. Recall that

$$\Psi(x,t) = \sum_n a_n \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right) e^{-i\frac{n^2\pi^2\hbar}{8mL^2}t}$$
$$= \sum_n a_n \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right) e^{-in^2\omega_1 t},$$

where we have defined $\omega_1 = \frac{\pi^2\hbar}{8mL^2}$. To find the fundamental period, note that when $\omega_1 t = 2\pi$, then $n^2\omega_1 t$ is also an integer multiple of 2π. Therefore, at $t = \tau = \frac{2\pi}{\omega_1}$ the phase factor for *all* n is equal to 1, and so $\Psi(x,\tau) = \Psi(x,0)$. Thus, $\tau = \frac{2\pi}{\omega_1} = \frac{16mL^2}{\hbar\pi}$ is the fundamental period.

Before drawing $\Psi\left(x, \frac{\tau}{2}\right)$, we ask: what makes $\Psi(x,0)$ cancel on the right and not on the left? We know that $\sum_{n \text{ odd}} a_n\psi_n(x)$ must be symmetric (since it is the sum of symmetric functions); hence, we may infer that it must look as shown in Figure 1.3 to give cancellation on the right-hand side at $t = 0$.

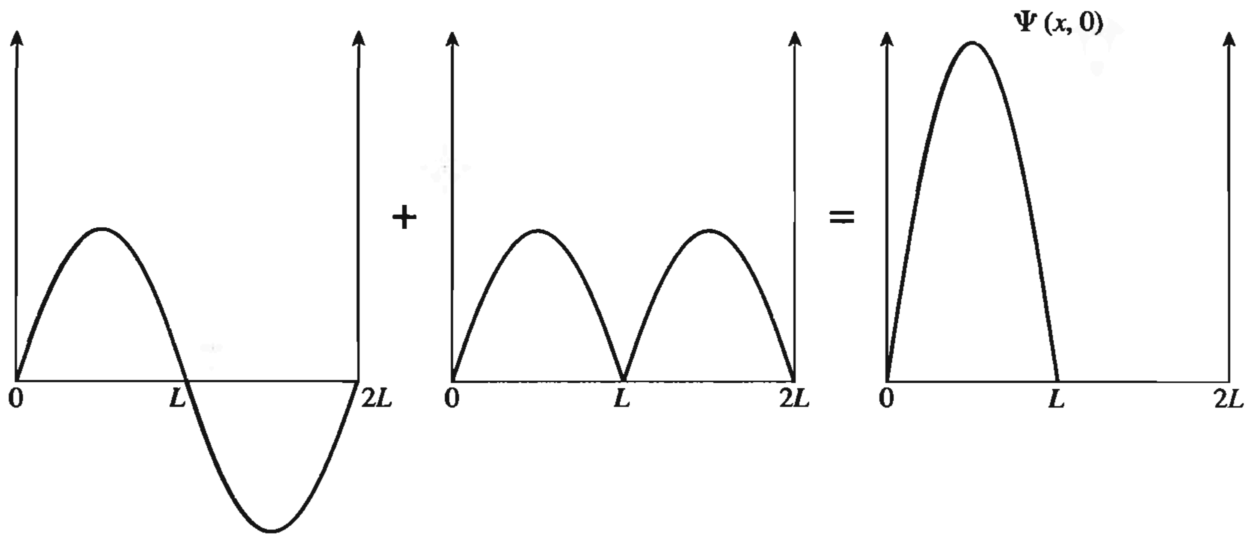

Figure 1.3 The component of ψ_2 (left panel) must be equal to that of all the ψ_n, n odd, put together (middle panel), to give precise cancellation in the amplitude of $\Psi(x,0)$ on the right-hand side of the box at $t = 0$ (right panel). Note that the amplitude in the box on the right is twice that of the boxes on the left.

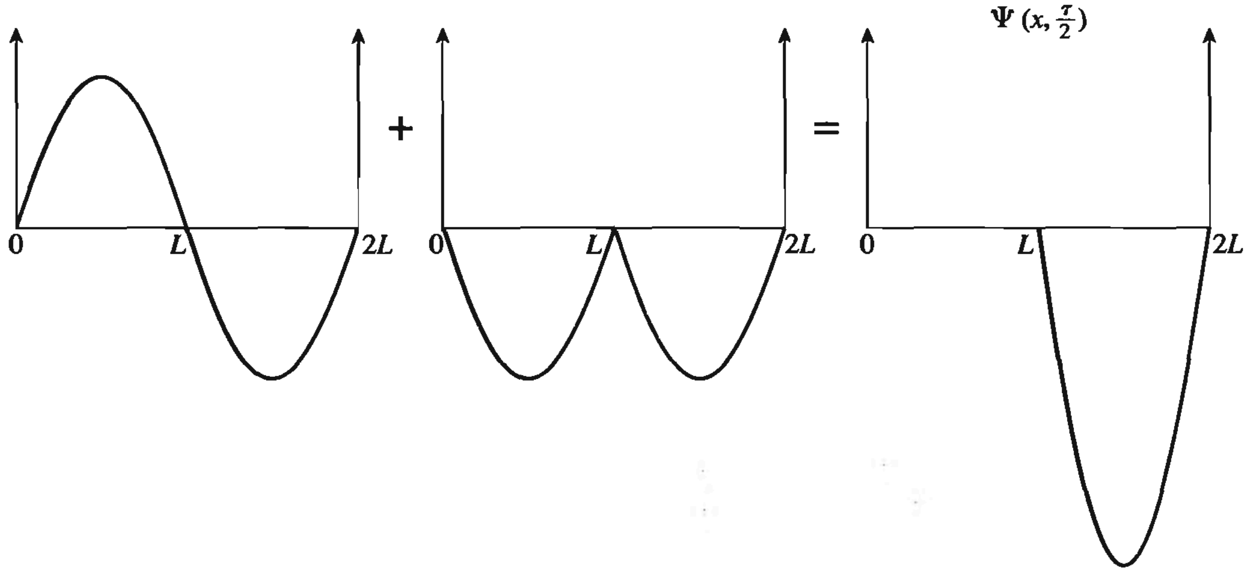

Figure 1.4 After half a period, the phase of ψ_2 is back to its original value (left), while the phase of all the ψ_n, n odd, has changed by (-1) (middle). This leads to complete cancellation of $\Psi(x, \frac{\tau}{2})$ on the *left-hand side of the box* (right panel). Note that the negative sign of the amplitude has no consequence for the probability density, which is proportional to $|\Psi|^2$. As in Figure 1.3, the amplitude in the box on the right is twice that of the boxes on the left.

We now ask what happens after half a period. When $t = \frac{\tau}{2}$,

$$\Psi(x, t) = \sum_n a_n \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi x}{2L}\right) e^{-in^2\pi}.$$

For all odd n, $a_n e^{-in^2\pi} = -a_n$, while for $n = 2$, $a_n e^{-in^2\pi} = a_n$. Since all the odd ψ_n change sign and ψ_2 remains unchanged, $\Psi(x, t = \frac{\tau}{2})$ must look as shown in Figure 1.4, that is, the wavepacket is localized on the right-hand side of the box and cancels completely on the left-hand side.

Further Reading and Historical Notes

Schrödinger's original papers have been translated into English and collected (Schrödinger, 1928). It is interesting to note that Schrödinger started with the time-*independent* Schrödinger equation, and obtained the time-dependent Schrödinger equation only in the fourth paper in his series (Schrödinger, 1926a, Part IV). In (Schrödinger, 1926b), Schrödinger explores the time dependence of a displaced Gaussian in a harmonic potential—what would be called a "coherent state" in modern terminology, which we will discuss at length in Chapter 3. For a discussion of the introduction of time in Schrödinger's original papers and a provocative analysis, see Briggs (2000, 2001).