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, $\tau$, 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

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

To calculate the time evolution of $\Psi$ 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

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

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{initial_conditions_particle_half_box.png}
\caption{Initial conditions for particle in half a box}
\end{figure}
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 $\Psi$ for the time-evolving state and small $\psi_n$ 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

$$a_n = -\sqrt{2} \left[ \frac{(-1)^{n+1}}{(n + 2)\pi} + \frac{(-1)^{n-1}}{(n - 2)\pi} \right]$$

$$= \frac{4\sqrt{2}(-1)^{n+1}}{(n + 2)(n - 2)\pi},$$

where we have used the fact that

$$\sin \left( \pi + \frac{n\pi}{2} \right) = (-1)^{n+1}; \quad \sin \left( \pi - \frac{n\pi}{2} \right) = (-1)^{n-1}. $$
The numerical values for the first few overlap integrals are

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

\[ a_2 = \frac{1}{\sqrt{2}} = .707 \quad a_7 = \frac{4\sqrt{2}}{(9)(5)\pi} = .040 \]

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

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

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

\[ = \sum_n a_n \sqrt{\frac{1}{L}} \sin \left( \frac{n\pi x}{2L} \right) e^{-i n^2 \omega_1 t}, \]

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 \( 2\pi. \) 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 \( \Psi \left( x, \frac{1}{2} \right), \) 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](image_url)  

**Figure 1.3** The component of \( \psi_0, \) (left panel) must be equal to that of all the \( \psi_n, n \text{ odd}, \) 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 $\psi_2$ is back to its original value (left), while the phase of all the $\psi_n$, $n$ odd, has changed by $(-1)$ (middle). This leads to complete cancellation of $\Psi(x, \frac{L}{2})$ 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 $t = \frac{L}{2}$,

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

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 $\psi_n$ change sign and $\psi_2$ remains unchanged, $\Psi(x, t = \frac{L}{2})$ 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).