Problem 2.6

Although the *overall* phase constant of the wave function is of no physical significance (it cancels out whenever you calculate a measurable quantity), the *relative* phase of the coefficients in Equation 2.17 *does* matter. For example, suppose we change the relative phase of ψ_1 and ψ_2 in Problem 2.5:

$$\Psi(x,0) = A\left[\psi_1(x) + e^{i\phi}\psi_2(x)\right],$$

where ϕ is some constant. Find $\Psi(x,t)$, $|\Psi(x,t)|^2$, and $\langle x\rangle$, and compare your results with what you got before. Study the special cases $\phi = \pi/2$ and $\phi = \pi$. (For a graphical exploration of this problem see the applet in footnote 9 of this chapter.)

Solution

In Problem 2.3 the general solution to the Schrödinger equation for the infinite square well potential,

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases},$$

was found to be

$$\Psi(x,t) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} B_n \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}, \quad 0 \le x \le a$$

and zero elsewhere. The coefficients B_n are determined by using the provided initial condition,

$$\begin{aligned}\Psi(x,0) &= A\left[\psi_1(x) + e^{i\phi}\psi_2(x)\right] \\ &= A\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}e^{i\phi}\sin\frac{2\pi x}{a}\right) \\ &= A\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a} + e^{i\phi}\sin\frac{2\pi x}{a}\right).\end{aligned}$$

Before doing so, though, first normalize the initial wave function to find A.

$$\begin{aligned}1 &= \int_{-\infty}^{\infty}|\Psi(x,0)|^2\,dx \\ &= \int_{-\infty}^{\infty}\Psi(x,0)\Psi^*(x,0)\,dx \\ &= \int_0^a\left[A\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a} + e^{i\phi}\sin\frac{2\pi x}{a}\right)\right]\left[A\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a} + e^{i\phi}\sin\frac{2\pi x}{a}\right)\right]^* dx \\ &= \int_0^a\left[A\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a} + e^{i\phi}\sin\frac{2\pi x}{a}\right)\right]\left[A\sqrt{\frac{2}{a}}\left(\sin\frac{\pi x}{a} + e^{-i\phi}\sin\frac{2\pi x}{a}\right)\right] dx \\ &= \frac{2A^2}{a}\int_0^a\left(\sin^2\frac{\pi x}{a} + e^{-i\phi}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + e^{i\phi}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right)dx\end{aligned}$$

Continue simplifying the right side.

$$\begin{aligned}
1 &= \frac{2A^2}{a}\int_0^a \left[\sin^2\frac{\pi x}{a} + (e^{-i\phi}+e^{i\phi})\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right]dx \\
&= \frac{2A^2}{a}\left[\int_0^a \sin^2\frac{\pi x}{a}\,dx + (2\cos\phi)\int_0^a \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx + \int_0^a \sin^2\frac{2\pi x}{a}\,dx\right] \\
&= \frac{2A^2}{a}\left\{\int_0^a \frac{1}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx + 2\cos\phi\int_0^a \frac{1}{2}\left[\cos\left(\frac{\pi x}{a}-\frac{2\pi x}{a}\right) - \cos\left(\frac{\pi x}{a}+\frac{2\pi x}{a}\right)\right]dx \right. \\
&\qquad \left. + \int_0^a \frac{1}{2}\left(1-\cos\frac{4\pi x}{a}\right)dx\right\} \\
&= \frac{A^2}{a}\left[\int_0^a \left(1-\cos\frac{2\pi x}{a}\right)dx + 2\cos\phi\int_0^a \left(\cos\frac{\pi x}{a} - \cos\frac{3\pi x}{a}\right)dx + \int_0^a \left(1-\cos\frac{4\pi x}{a}\right)dx\right] \\
&= \frac{A^2}{a}\left[\left(x-\frac{a}{2\pi}\sin\frac{2\pi x}{a}\right)\Bigg|_0^a + 2\cos\phi\left(\frac{a}{\pi}\sin\frac{\pi x}{a} - \frac{a}{3\pi}\sin\frac{3\pi x}{a}\right)\Bigg|_0^a + \left(x-\frac{a}{4\pi}\sin\frac{4\pi x}{a}\right)\Bigg|_0^a\right] \\
&= \frac{A^2}{a}\left[(a) + (2\cos\phi)(0) + (a)\right] \\
&= 2A^2
\end{aligned}$$

Solve for A.

$$A = \frac{1}{\sqrt{2}}$$

With it, the initial condition becomes

$$\Psi(x,0) = \frac{1}{\sqrt{a}}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i\phi}\sin\frac{2\pi x}{a}.$$

Now set $t = 0$ in the general solution.

$$\Psi(x,0) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{a} = \sqrt{\frac{2}{a}}B_1\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}B_2\sin\frac{2\pi x}{a} + \sqrt{\frac{2}{a}}B_3\sin\frac{3\pi x}{a} + \cdots$$

Comparing the coefficients, we see that

$$\begin{aligned}
\sqrt{\frac{2}{a}}B_1 &= \frac{1}{\sqrt{a}} &&\rightarrow && B_1 = \frac{1}{\sqrt{2}} \\
\sqrt{\frac{2}{a}}B_2 &= \frac{1}{\sqrt{a}}e^{i\phi} &&\rightarrow && B_2 = \frac{1}{\sqrt{2}}e^{i\phi} \\
\sqrt{\frac{2}{a}}B_n &= 0, \quad n \geq 3 &&\rightarrow && B_n = 0, \quad n \geq 3.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\Psi(x,t) &= \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} B_n \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a} \\
&= \sqrt{\frac{2}{a}}B_1\exp\left(-i\frac{\hbar\pi^2 1^2}{2ma^2}t\right)\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}B_2\exp\left(-i\frac{\hbar\pi^2 2^2}{2ma^2}t\right)\sin\frac{2\pi x}{a} \\
&= \frac{1}{\sqrt{a}}\exp\left(-i\frac{\hbar\pi^2}{2ma^2}t\right)\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i\phi}\exp\left(-i\frac{2\hbar\pi^2}{ma^2}t\right)\sin\frac{2\pi x}{a},
\end{aligned}$$

or using $\omega = \pi^2\hbar/2ma^2$ to simplify the result,

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i\phi}e^{-4i\omega t}\sin\frac{2\pi x}{a}, \quad 0 \le x \le a.}$$

Writing the solution in terms of the eigenstates,

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right)e^{-i\omega t} + \frac{e^{i\phi}}{\sqrt{2}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)e^{-4i\omega t} \\ &= \frac{1}{\sqrt{2}}\psi_1(x)e^{-i\omega t} + \frac{e^{i\phi}}{\sqrt{2}}\psi_2(x)e^{-4i\omega t},\end{aligned}$$

we can see that the probabilities of measuring

$$\begin{aligned}E_1 &= \frac{\pi^2\hbar^2}{2ma^2} \\ E_2 &= \frac{4\pi^2\hbar^2}{2ma^2} = \frac{2\pi^2\hbar^2}{ma^2}\end{aligned}$$

are

$$\begin{aligned}P(E_1) &= \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2} \\ P(E_2) &= \left|\frac{e^{i\phi}}{\sqrt{2}}\right|^2 = \frac{1}{2},\end{aligned}$$

respectively. The expectation value of the energy is

$$\langle H\rangle = P(E_1)E_1 + P(E_2)E_2 = \left(\frac{1}{2}\right)\frac{\pi^2\hbar^2}{2ma^2} + \left(\frac{1}{2}\right)\frac{2\pi^2\hbar^2}{ma^2} = \frac{\pi^2\hbar^2}{4ma^2} + \frac{\pi^2\hbar^2}{ma^2} = \frac{5\pi^2\hbar^2}{4ma^2}.$$

The probability distribution for the particle's position at time t is

$$\begin{aligned}|\Psi(x,t)|^2 &= \Psi(x,t)\Psi^*(x,t) \\ &= \left[\frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right]\left[\frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right]^* \\ &= \left[\frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right]\left[\frac{1}{\sqrt{a}}e^{i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{-i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right] \\ &= \frac{1}{a}\sin^2\frac{\pi x}{a} + \frac{1}{a}e^{i(3\omega t-\phi)}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \frac{1}{a}e^{-i(3\omega t-\phi)}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \frac{1}{a}\sin^2\frac{2\pi x}{a} \\ &= \frac{1}{a}\left\{\sin^2\frac{\pi x}{a} + \left[e^{i(3\omega t-\phi)} + e^{-i(3\omega t-\phi)}\right]\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right\} \\ &= \frac{1}{a}\left[\sin^2\frac{\pi x}{a} + 2\cos(3\omega t-\phi)\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right], \quad 0 \le x \le a.\end{aligned}$$

Observe that the wave function remains normalized for all t.

$$\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,dx = \frac{1}{a}\Bigg(\underbrace{\int_0^a \sin^2\frac{\pi x}{a}\,dx}_{=a/2} + 2\cos(3\omega t-\phi)\underbrace{\int_0^a \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx}_{=0} + \underbrace{\int_0^a \sin^2\frac{2\pi x}{a}\,dx}_{=a/2}\Bigg) = 1$$

Now calculate the expectation value of x at time t.

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \Psi^*(x,t)(x)\Psi(x,t)\,dx \\
&= \int_0^a \left[\frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right]^* (x)\left[\frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i(\phi-4\omega t)}\sin\frac{2\pi x}{a}\right] dx \\
&= \frac{1}{a}\int_0^a x\left[\sin^2\frac{\pi x}{a} + 2\cos(3\omega t-\phi)\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right] dx \\
&= \frac{1}{a}\left[\int_0^a x\sin^2\frac{\pi x}{a}\,dx + 2\cos(3\omega t-\phi)\int_0^a x\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx + \int_0^a x\sin^2\frac{2\pi x}{a}\,dx\right] \\
&= \frac{1}{a}\left\{\int_0^a \frac{x}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx + 2\cos(3\omega t-\phi)\int_0^a \frac{x}{2}\left[\cos\left(\frac{\pi x}{a}-\frac{2\pi x}{a}\right) - \cos\left(\frac{\pi x}{a}+\frac{2\pi x}{a}\right)\right]dx \right.\\
&\qquad \left. + \int_0^a \frac{x}{2}\left(1-\cos\frac{4\pi x}{a}\right)dx\right\} \\
&= \frac{1}{2a}\left[\int_0^a x\,dx - \int_0^a x\cos\frac{2\pi x}{a}\,dx + 2\cos(3\omega t-\phi)\left(\int_0^a x\cos\frac{\pi x}{a}\,dx - \int_0^a x\cos\frac{3\pi x}{a}\,dx\right)\right.\\
&\qquad \left. + \int_0^a x\,dx - \int_0^a x\cos\frac{4\pi x}{a}\,dx\right] \\
&= \frac{1}{2a}\left[\frac{a^2}{2} - 0 + 2\cos(3\omega t-\phi)\left(-\frac{2a^2}{\pi^2}+\frac{2a^2}{9\pi^2}\right) + \frac{a^2}{2} - 0\right] \\
&= \frac{1}{2a}\left[a^2 - \frac{32a^2}{9\pi^2}\cos(3\omega t-\phi)\right] \\
&= \frac{a}{2} - \frac{16a}{9\pi^2}\cos(3\omega t-\phi)
\end{aligned}$$

The expectation value of x oscillates in time with an amplitude and angular frequency of

$$\frac{16a}{9\pi^2} \approx 0.180a \quad \text{and} \quad 3\omega = \frac{3\hbar\pi^2}{2ma^2},$$

respectively. Finally, use Ehrenfest's theorem to calculate $\langle p\rangle$.

$$\begin{aligned}
\langle p\rangle &= m\frac{d\langle x\rangle}{dt} \\
&= m\frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,t)(x)\Psi(x,t)\,dx \\
&= m\frac{d}{dt}\left[\frac{a}{2} - \frac{16a}{9\pi^2}\cos(3\omega t-\phi)\right] \\
&= \frac{16ma\omega}{3\pi^2}\sin(3\omega t-\phi) \\
&= \frac{16ma}{3\pi^2}\left(\frac{\hbar\pi^2}{2ma^2}\right)\sin\left(\frac{3\hbar\pi^2}{2ma^2}t-\phi\right) \\
&= \frac{8\hbar}{3a}\sin\left(\frac{3\hbar\pi^2}{2ma^2}t-\phi\right)
\end{aligned}$$

If $\phi = \pi/2$, then

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i\pi/2}e^{-4i\omega t}\sin\frac{2\pi x}{a} \\ &= \frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}ie^{-4i\omega t}\sin\frac{2\pi x}{a}, \quad 0 \le x \le a\end{aligned}$$

$$\begin{aligned}|\Psi(x,t)|^2 &= \frac{1}{a}\left[\sin^2\frac{\pi x}{a} + 2\cos\left(3\omega t - \frac{\pi}{2}\right)\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right] \\ &= \frac{1}{a}\left(\sin^2\frac{\pi x}{a} + 2\sin 3\omega t\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right), \quad 0 \le x \le a\end{aligned}$$

$$\begin{aligned}\langle x\rangle &= \frac{a}{2} - \frac{16a}{9\pi^2}\cos\left(3\omega t - \frac{\pi}{2}\right) \\ &= \frac{a}{2} - \frac{16a}{9\pi^2}\sin 3\omega t\end{aligned}$$

$$\begin{aligned}\langle p\rangle &= \frac{8\hbar}{3a}\sin\left(\frac{3\hbar\pi^2}{2ma^2}t - \frac{\pi}{2}\right) \\ &= -\frac{8\hbar}{3a}\cos\left(\frac{3\hbar\pi^2}{2ma^2}t\right).\end{aligned}$$

If $\phi = \pi$, then

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} + \frac{1}{\sqrt{a}}e^{i\pi}e^{-4i\omega t}\sin\frac{2\pi x}{a} \\ &= \frac{1}{\sqrt{a}}e^{-i\omega t}\sin\frac{\pi x}{a} - \frac{1}{\sqrt{a}}e^{-4i\omega t}\sin\frac{2\pi x}{a}, \quad 0 \le x \le a\end{aligned}$$

$$\begin{aligned}|\Psi(x,t)|^2 &= \frac{1}{a}\left[\sin^2\frac{\pi x}{a} + 2\cos(3\omega t - \pi)\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right] \\ &= \frac{1}{a}\left(\sin^2\frac{\pi x}{a} - 2\cos 3\omega t\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \sin^2\frac{2\pi x}{a}\right), \quad 0 \le x \le a\end{aligned}$$

$$\begin{aligned}\langle x\rangle &= \frac{a}{2} - \frac{16a}{9\pi^2}\cos(3\omega t - \pi) \\ &= \frac{a}{2} + \frac{16a}{9\pi^2}\cos 3\omega t\end{aligned}$$

$$\begin{aligned}\langle p\rangle &= \frac{8\hbar}{3a}\sin\left(\frac{3\hbar\pi^2}{2ma^2}t - \pi\right) \\ &= -\frac{8\hbar}{3a}\sin\left(\frac{3\hbar\pi^2}{2ma^2}t\right).\end{aligned}$$