Problem 2.5

A particle in the infinite square well has as its initial wave function an even mixture of the first two stationary states:

$$\Psi(x,0) = A[\psi_1(x) + \psi_2(x)].$$

(a) Normalize $\Psi(x,0)$. (That is, find A. This is very easy, if you exploit the orthonormality of ψ_1 and ψ_2. Recall that, having normalized Ψ at $t = 0$, you can rest assured that it *stays* normalized—if you doubt this, check it explicitly after doing part (b).)

(b) Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time, as in Example 2.1. To simplify the result, let $\omega \equiv \pi^2\hbar/2ma^2$.

(c) Compute $\langle x \rangle$. Notice that it oscillates in time. What is the angular frequency of the oscillation? What is the amplitude of the oscillation? (If your amplitude is greater than $a/2$, go directly to jail.)

(d) Compute $\langle p \rangle$. (As Peter Lorre would say, "Do it ze *kveek* vay, Johnny!")

(e) If you measured the energy of the particle, what values might you get, and what is the probability of getting each of them? Find the expectation value of H. How does it compare with E_1 and E_2?

Solution

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

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

was found to be

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

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

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

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

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx \\ &= \int_{-\infty}^{\infty} \Psi(x,0)\Psi^*(x,0)\,dx \end{aligned}$$

Substitute $\Psi(x,0)$ and evaluate the integral.

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

Solve for A.

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

With it, the initial condition becomes

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

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

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

Therefore,

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

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

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

Writing the solution in terms of the eigenstates,

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

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

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

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

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

Observe that the wave function remains normalized for all t.

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

Now calculate the expectation value of x at time t.

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

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 $\langle p\rangle$.

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