Problem 2.37

A particle in the infinite square well (Equation 2.22) has the initial wave function

$$\Psi(x,0) = A\sin^3(\pi x/a) \quad (0 \leq x \leq a).$$

Determine A, find $\Psi(x,t)$, and calculate $\langle x \rangle$, as a function of time. What is the expectation value of the energy? *Hint:* $\sin^n\theta$ and $\cos^n\theta$ can be reduced, by repeated application of the trigonometric sum formulas, to linear combinations of $\sin(m\theta)$ and $\cos(m\theta)$, with $m = 0, 1, 2, \ldots, n$.

Solution

Schrödinger's equation describes the time evolution of the wave function $\Psi(x,t)$.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0$$

For an infinite square well,

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

Applying the method of separation of variables reduces the PDE to two ODEs, one in x and one in t.

$$\left.\begin{aligned} i\hbar\frac{\phi'(t)}{\phi(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} &= E \end{aligned}\right\}$$

Subject to the boundary conditions, $\psi(0) = 0$ and $\psi(a) = 0$, the TISE yields normalized solutions of the form,

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a},$$

with corresponding energies,

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},$$

where $n = 1, 2, \ldots$. With this formula for E, the solution to the ODE in t is $\phi_n(t) = e^{-iE_nt/\hbar}$. According to the principle of superposition, the general solution for $\Psi(x,t)$ is a linear combination of the product solutions $\phi_n(t)\psi_n(x)$ for all n.

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

Set $t = 0$ and apply the provided initial condition to determine c_n.

$$\begin{aligned}
\Psi(x,0) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} &= A \sin^3 \frac{\pi x}{a} \\
&= A \left(\frac{e^{i\pi x/a} - e^{-i\pi x/a}}{2i} \right)^3 \\
&= A \left(\frac{e^{3i\pi x/a} - 3e^{2i\pi x/a} e^{-i\pi x/a} + 3e^{i\pi x/a} e^{-2i\pi x/a} - e^{-3i\pi x/a}}{8i^3} \right) \\
&= A \left(\frac{e^{3i\pi x/a} - 3e^{i\pi x/a} + 3e^{-i\pi x/a} - e^{-3i\pi x/a}}{-8i} \right) \\
&= A \left[\frac{3}{4} \left(\frac{e^{i\pi x/a} - e^{-i\pi x/a}}{2i} \right) - \frac{1}{4} \left(\frac{e^{3i\pi x/a} - e^{-3i\pi x/a}}{2i} \right) \right] \\
&= A \left(\frac{3}{4} \sin \frac{\pi x}{a} - \frac{1}{4} \sin \frac{3\pi x}{a} \right) \\
&= \frac{3A}{4} \sin \frac{\pi x}{a} - \frac{A}{4} \sin \frac{3\pi x}{a} \\
&= \frac{3A}{4} \sqrt{\frac{a}{2}} \left(\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \right) - \frac{A}{4} \sqrt{\frac{a}{2}} \left(\sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a} \right) \\
&= \frac{3A}{4} \sqrt{\frac{a}{2}} \psi_1(x) - \frac{A}{4} \sqrt{\frac{a}{2}} \psi_3(x)
\end{aligned}$$

Comparing the coefficients, we see that

$$\begin{cases} c_1 \sqrt{\frac{2}{a}} = \frac{3A}{4} & \text{if } n = 1 \\ c_3 \sqrt{\frac{2}{a}} = -\frac{A}{4} & \text{if } n = 3 \\ c_n \sqrt{\frac{2}{a}} = 0 & \text{if } n \neq 1 \text{ and } n \neq 3 \end{cases},$$

which means

$$\Psi(x,t) = \frac{3A}{4} \exp\left(-i \frac{\pi^2 \hbar}{2ma^2} t \right) \sin \frac{\pi x}{a} - \frac{A}{4} \exp\left(-i \frac{9\pi^2 \hbar}{2ma^2} t \right) \sin \frac{3\pi x}{a}.$$

Normalize the initial wave function to determine A.

$$\begin{aligned}
1 &= \int_0^a |\Psi(x,0)|^2 \, dx \\
&= \int_0^a \left(A \sin^3 \frac{\pi x}{a} \right)^2 dx \\
&= \int_0^a \left[\frac{3A}{4} \sqrt{\frac{a}{2}} \psi_1(x) - \frac{A}{4} \sqrt{\frac{a}{2}} \psi_3(x) \right]^2 dx \\
&= \int_0^a \left\{ \frac{9A^2}{16} \frac{a}{2} [\psi_1(x)]^2 - 2 \frac{3A}{4} \frac{A}{4} \frac{a}{2} \psi_1(x) \psi_3(x) + \frac{A^2}{16} \frac{a}{2} [\psi_3(x)]^2 \right\} dx
\end{aligned}$$

Use the orthonormality of the eigenstates to evaluate the integral.

$$\begin{aligned}1 &= \frac{9A^2}{16}\frac{a}{2}\underbrace{\int_0^a [\psi_1(x)]^2\,dx}_{=1} - 2\frac{3A}{4}\frac{A}{4}\frac{a}{2}\underbrace{\int_0^a \psi_1(x)\psi_3(x)\,dx}_{=0} + \frac{A^2}{16}\frac{a}{2}\underbrace{\int_0^a [\psi_3(x)]^2\,dx}_{=1} \\ &= \frac{5aA^2}{16}\end{aligned}$$

Solve for A.

$$A = \frac{4}{\sqrt{5a}}$$

Therefore, the wave function is

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{5a}}\left[3\exp\left(-i\frac{\pi^2\hbar}{2ma^2}t\right)\sin\frac{\pi x}{a} - \exp\left(-i\frac{9\pi^2\hbar}{2ma^2}t\right)\sin\frac{3\pi x}{a}\right].}$$

Alternatively, it can be written in terms of the eigenstates.

$$\begin{aligned}\Psi(x,t) &= \frac{3A}{4}\sqrt{\frac{a}{2}}\psi_1(x)e^{-iE_1t/\hbar} - \frac{A}{4}\sqrt{\frac{a}{2}}\psi_3(x)e^{-iE_3t/\hbar} \\ &= \frac{3}{\sqrt{10}}\psi_1(x)e^{-iE_1t/\hbar} - \frac{1}{\sqrt{10}}\psi_3(x)e^{-iE_3t/\hbar}\end{aligned}$$

Writing the solution this way allows us to determine the expectation value of energy.

$$\langle E\rangle = \sum_n E_nP(E_n) = E_1P(E_1) + E_3P(E_3) = E_1\left|\frac{3}{\sqrt{10}}\right|^2 + E_3\left|-\frac{1}{\sqrt{10}}\right|^2 = \frac{9}{10}E_1 + \frac{1}{10}E_3$$

Therefore,

$$\boxed{\langle E\rangle = \frac{9\pi^2\hbar^2}{10ma^2}.}$$

Now calculate the expectation value of x at time t.

$$\begin{aligned}\langle x\rangle &= \int_0^a \Psi^*(x,t)x\Psi(x,t)\,dx \\ &= \int_0^a \left\{\frac{1}{\sqrt{5a}}\left[3\exp\left(i\frac{\pi^2\hbar}{2ma^2}t\right)\sin\frac{\pi x}{a} - \exp\left(i\frac{9\pi^2\hbar}{2ma^2}t\right)\sin\frac{3\pi x}{a}\right]\right\}x \\ &\qquad \times\left\{\frac{1}{\sqrt{5a}}\left[3\exp\left(-i\frac{\pi^2\hbar}{2ma^2}t\right)\sin\frac{\pi x}{a} - \exp\left(-i\frac{9\pi^2\hbar}{2ma^2}t\right)\sin\frac{3\pi x}{a}\right]\right\}dx \\ &= \frac{1}{5a}\int_0^a x\left[9\sin^2\frac{\pi x}{a} + \sin^2\frac{3\pi x}{a} - 3\exp\left(-i\frac{4\pi^2\hbar}{ma^2}t\right)\sin\frac{\pi x}{a}\sin\frac{3\pi x}{a} - 3\exp\left(i\frac{4\pi^2\hbar}{ma^2}t\right)\sin\frac{\pi x}{a}\sin\frac{3\pi x}{a}\right]dx \\ &= \frac{1}{5a}\int_0^a x\left\{9\sin^2\frac{\pi x}{a} + \sin^2\frac{3\pi x}{a} - 3\left[\exp\left(-i\frac{4\pi^2\hbar}{ma^2}t\right) + \exp\left(i\frac{4\pi^2\hbar}{ma^2}t\right)\right]\sin\frac{\pi x}{a}\sin\frac{3\pi x}{a}\right\}dx \\ &= \frac{1}{5a}\int_0^a x\left[9\sin^2\frac{\pi x}{a} + \sin^2\frac{3\pi x}{a} - 6\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\sin\frac{\pi x}{a}\sin\frac{3\pi x}{a}\right]dx\end{aligned}$$

Split up the integral and proceed to evaluate it.

$$\begin{aligned}
\langle x\rangle &= \frac{9}{5a}\int_0^a x\sin^2\frac{\pi x}{a}\,dx \\
&\quad + \frac{1}{5a}\int_0^a x\sin^2\frac{3\pi x}{a}\,dx \\
&\qquad - \frac{6}{5a}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\int_0^a x\sin\frac{\pi x}{a}\sin\frac{3\pi x}{a}\,dx \\
&= \frac{9}{5a}\int_0^a \frac{x}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx \\
&\quad + \frac{1}{5a}\int_0^a \frac{x}{2}\left(1-\cos\frac{6\pi x}{a}\right)dx \\
&\qquad - \frac{6}{5a}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\int_0^a \frac{x}{2}\left[\cos\left(\frac{\pi x}{a}-\frac{3\pi x}{a}\right)-\cos\left(\frac{\pi x}{a}+\frac{3\pi x}{a}\right)\right]dx \\
&= \frac{9}{10a}\left(\int_0^a x\,dx - \int_0^a x\cos\frac{2\pi x}{a}\,dx\right) \\
&\quad + \frac{1}{10a}\left(\int_0^a x\,dx - \int_0^a x\cos\frac{6\pi x}{a}\,dx\right) \\
&\qquad - \frac{3}{5a}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\left(\int_0^a x\cos\frac{2\pi x}{a}\,dx - \int_0^a x\cos\frac{4\pi x}{a}\,dx\right) \\
&= \frac{9}{10a}\left[\frac{a^2}{2} - \int_0^a \frac{\partial}{\partial X}\left(\frac{a}{\pi}\sin\frac{X\pi x}{a}\right)\bigg|_{X=2}dx\right] \\
&\quad + \frac{1}{10a}\left[\frac{a^2}{2} - \int_0^a \frac{\partial}{\partial X}\left(\frac{a}{\pi}\sin\frac{X\pi x}{a}\right)\bigg|_{X=6}dx\right] \\
&\qquad - \frac{3}{5a}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\left[\int_0^a \frac{\partial}{\partial X}\left(\frac{a}{\pi}\sin\frac{X\pi x}{a}\right)\bigg|_{X=2}dx - \int_0^a \frac{\partial}{\partial X}\left(\frac{a}{\pi}\sin\frac{X\pi x}{a}\right)\bigg|_{X=4}dx\right] \\
&= \frac{a}{2} - \frac{9}{10\pi}\frac{d}{dX}\left(\int_0^a \sin\frac{X\pi x}{a}\,dx\right)\bigg|_{X=2} - \frac{1}{10\pi}\frac{d}{dX}\left(\int_0^a \sin\frac{X\pi x}{a}\,dx\right)\bigg|_{X=6} \\
&\quad - \frac{3}{5\pi}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\left[\frac{d}{dX}\left(\int_0^a \sin\frac{X\pi x}{a}\,dx\right)\bigg|_{X=2} - \frac{d}{dX}\left(\int_0^a \sin\frac{X\pi x}{a}\,dx\right)\bigg|_{X=4}\right] \\
&= \frac{a}{2} - \frac{9}{10\pi}\frac{d}{dX}\left(\frac{a-a\cos\pi X}{\pi X}\right)\bigg|_{X=2} - \frac{1}{10\pi}\frac{d}{dX}\left(\frac{a-a\cos\pi X}{\pi X}\right)\bigg|_{X=6} \\
&\quad - \frac{3}{5\pi}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\left[\frac{d}{dX}\left(\frac{a-a\cos\pi X}{\pi X}\right)\bigg|_{X=2} - \frac{d}{dX}\left(\frac{a-a\cos\pi X}{\pi X}\right)\bigg|_{X=4}\right] \\
&= \frac{a}{2} - \frac{9}{10\pi}\left[\frac{a(-1+\cos\pi X+\pi X\sin\pi X)}{\pi X^2}\right]\bigg|_{X=2} - \frac{1}{10\pi}\left[\frac{a(-1+\cos\pi X+\pi X\sin\pi X)}{\pi X^2}\right]\bigg|_{X=6} \\
&\quad - \frac{3}{5\pi}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)\left\{\left[\frac{a(-1+\cos\pi X+\pi X\sin\pi X)}{\pi X^2}\right]\bigg|_{X=2} - \left[\frac{a(-1+\cos\pi X+\pi X\sin\pi X)}{\pi X^2}\right]\bigg|_{X=4}\right\} \\
&= \frac{a}{2} - \frac{9}{10\pi}(0) - \frac{1}{10\pi}(0) - \frac{3}{5\pi}\cos\left(\frac{4\pi^2\hbar}{ma^2}t\right)[(0)-(0)] \quad\to\quad \boxed{\langle x\rangle = \frac{a}{2}}
\end{aligned}$$