Problem 2.7

A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = \begin{cases} Ax, & 0 \le x \le a/2, \\ A(a-x), & a/2 \le x \le a. \end{cases}$$

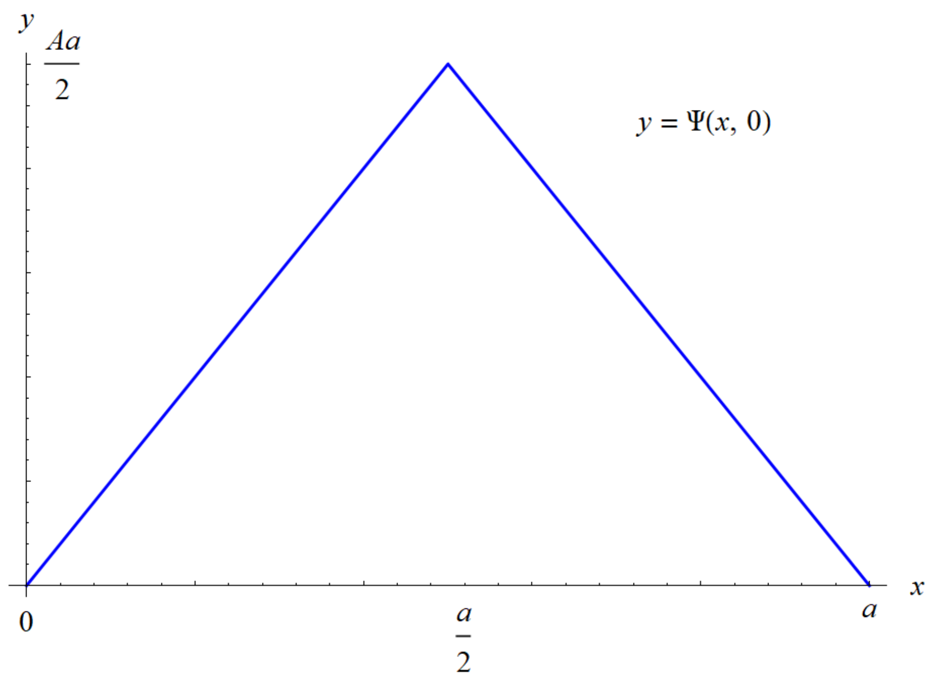
(a) Sketch $\Psi(x,0)$, and determine the constant A.

(b) Find $\Psi(x,t)$.

(c) What is the probability that a measurement of the energy would yield the value E_1?

(d) Find the expectation value of the energy, using Equation 2.21.[21]

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

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

[21]Remember, there is no restriction in principle on the *shape* of the starting wave function, as long as it is normalizable. In particular, $\Psi(x,0)$ need not have a continuous derivative. However, if you try to calculate $\langle H \rangle$ using $\int \Psi(x,0)^* \hat{H} \Psi(x,0)\,dx$ in such a case, you may encounter technical difficulties, because the second derivative of $\Psi(x,0)$ is ill defined. It works in Problem 2.9 because the discontinuities occur at the end points, where the wave function is zero anyway. In Problem 2.39 you'll see how to manage cases like Problem 2.7.

and zero elsewhere. The coefficients B_n are determined by using the provided initial condition. Before doing so, though, first normalize the initial wave function by finding A.

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx \\
&= \int_{-\infty}^{\infty} \Psi(x,0)\Psi^*(x,0)\,dx \\
&= \int_0^{a/2} (Ax)(Ax)^*\,dx + \int_{a/2}^{a} [A(a-x)][A(a-x)]^*\,dx \\
&= A^2 \int_0^{a/2} x^2\,dx + A^2 \int_{a/2}^{a} (a-x)^2\,dx \\
&= A^2\left(\frac{a^3}{24}\right) + A^2\left(\frac{a^3}{24}\right) \\
&= A^2\left(\frac{a^3}{12}\right)
\end{aligned}$$

Solve for A.

$$A = 2\sqrt{\frac{3}{a^3}}$$

As a result, the initial wave function becomes

$$\Psi(x,0) = \begin{cases} 2\sqrt{\dfrac{3}{a^3}}x & 0 \le x \le a/2 \\ 2\sqrt{\dfrac{3}{a^3}}(a-x) & a/2 \le x \le a \end{cases}.$$

Set $t = 0$ in the general solution.

$$\Psi(x,0) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{a}$$

To solve for B_n, multiply both sides by $\sin\frac{p\pi x}{a}$, where p is an integer,

$$\Psi(x,0)\sin\frac{p\pi x}{a} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{a}\sin\frac{p\pi x}{a}$$

and then integrate both sides with respect to x from 0 to a.

$$\begin{aligned}
\int_0^a \Psi(x,0)\sin\frac{p\pi x}{a}\,dx &= \int_0^a \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{a}\sin\frac{p\pi x}{a}\,dx \\
&= \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} B_n \int_0^a \sin\frac{n\pi x}{a}\sin\frac{p\pi x}{a}\,dx
\end{aligned}$$

Because the sine functions are orthogonal, this integral on the right is zero if $n \neq p$. Every term in this infinite series vanishes, then, except for the one corresponding to $n = p$.

$$\begin{aligned}\int_0^a \Psi(x,0)\sin\frac{n\pi x}{a}\,dx &= \sqrt{\frac{2}{a}}B_n\int_0^a \sin^2\frac{n\pi x}{a}\,dx \\ &= \sqrt{\frac{2}{a}}B_n\left(\frac{a}{2}\right) \\ &= \sqrt{\frac{a}{2}}B_n\end{aligned}$$

Solve for B_n.

$$\begin{aligned}B_n &= \sqrt{\frac{2}{a}}\int_0^a \Psi(x,0)\sin\frac{n\pi x}{a}\,dx \\
&= \sqrt{\frac{2}{a}}\left[\int_0^{a/2} 2\sqrt{\frac{3}{a^3}}x\sin\frac{n\pi x}{a}\,dx + \int_{a/2}^a 2\sqrt{\frac{3}{a^3}}(a-x)\sin\frac{n\pi x}{a}\,dx\right] \\
&= \frac{2\sqrt{6}}{a^2}\left[\int_0^{a/2} x\sin\frac{n\pi x}{a}\,dx + \int_{a/2}^a (a-x)\sin\frac{n\pi x}{a}\,dx\right] \\
&= \frac{2\sqrt{6}}{a^2}\left(\int_0^{a/2} x\sin\frac{n\pi x}{a}\,dx + a\int_{a/2}^a \sin\frac{n\pi x}{a}\,dx - \int_{a/2}^a x\sin\frac{n\pi x}{a}\,dx\right) \\
&= \frac{2\sqrt{6}}{a^2}\left[\int_0^{a/2}\left(-\frac{a}{\pi}\frac{\partial}{\partial n}\cos\frac{n\pi x}{a}\right)dx + a\int_{a/2}^a \sin\frac{n\pi x}{a}\,dx - \int_{a/2}^a\left(-\frac{a}{\pi}\frac{\partial}{\partial n}\cos\frac{n\pi x}{a}\right)dx\right] \\
&= \frac{2\sqrt{6}}{a}\left(-\frac{1}{\pi}\frac{d}{dn}\int_0^{a/2}\cos\frac{n\pi x}{a}\,dx + \int_{a/2}^a \sin\frac{n\pi x}{a}\,dx + \frac{1}{\pi}\frac{d}{dn}\int_{a/2}^a \cos\frac{n\pi x}{a}\,dx\right) \\
&= \frac{2\sqrt{6}}{a}\left[-\frac{1}{\pi}\frac{d}{dn}\left(\frac{a}{n\pi}\sin\frac{n\pi}{2}\right) + \frac{a}{n\pi}\left(\cos\frac{n\pi}{2} - \cos n\pi\right) + \frac{1}{\pi}\frac{d}{dn}\left(-\frac{a}{n\pi}\sin\frac{n\pi}{2} + \frac{a}{n\pi}\sin n\pi\right)\right] \\
&= \frac{2\sqrt{6}}{a}\left[-\frac{1}{\pi}\left(-\frac{a}{n^2\pi}\sin\frac{n\pi}{2} + \frac{a}{2n}\cos\frac{n\pi}{2}\right) + \frac{a}{n\pi}\left(\cos\frac{n\pi}{2} - \cos n\pi\right)\right. \\
&\qquad \left. + \frac{1}{\pi}\left(\frac{a}{n^2\pi}\sin\frac{n\pi}{2} - \frac{a}{2n}\cos\frac{n\pi}{2} - \frac{a}{n^2\pi}\sin n\pi + \frac{a}{n}\cos n\pi\right)\right] \\
&= \frac{2\sqrt{6}}{a}\left(\frac{2a}{n^2\pi^2}\sin\frac{n\pi}{2} - \frac{a}{n^2\pi^2}\underbrace{\sin n\pi}_{=0}\right) \\
&= \frac{4\sqrt{6}}{n^2\pi^2}\sin\frac{n\pi}{2}\end{aligned}$$

With these coefficients, the general solution becomes

$$\begin{aligned}\Psi(x,t) &= \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} B_n \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a} \\
&= \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty}\frac{4\sqrt{6}}{n^2\pi^2}\sin\frac{n\pi}{2}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a} \\
&= \frac{8}{\pi^2}\sqrt{\frac{3}{a}}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\frac{n\pi}{2}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}, \quad 0 \le x \le a.\end{aligned}$$

Notice that the summand is zero for even values of n; consequently, this infinite series can be simplified (that is, made to converge faster) by summing over the odd integers only. Make the substitution $n = 2k - 1$.

$$\Psi(x,t) = \frac{8}{\pi^2}\sqrt{\frac{3}{a}} \sum_{2k-1=1}^{\infty} \frac{1}{(2k-1)^2} \sin\frac{(2k-1)\pi}{2} \exp\left[-i\frac{\hbar\pi^2(2k-1)^2}{2ma^2}t\right] \sin\frac{(2k-1)\pi x}{a}$$

Therefore,

$$\boxed{\Psi(x,t) = \frac{8}{\pi^2}\sqrt{\frac{3}{a}} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{(2k-1)^2} \exp\left[-i\frac{\hbar\pi^2(2k-1)^2}{2ma^2}t\right] \sin\frac{(2k-1)\pi x}{a}, \quad 0 \le x \le a.}$$

Writing the general solution in terms of the eigenstates,

$$\begin{aligned}
\Psi(x,t) &= \frac{8}{\pi^2}\sqrt{\frac{3}{a}} \sum_{n=1}^{\infty} \frac{1}{n^2} \sin\frac{n\pi}{2} \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \sin\frac{n\pi x}{a} \\
&= \frac{8}{\pi^2}\sqrt{\frac{3}{2}} \sum_{n=1}^{\infty} \frac{1}{n^2} \sin\frac{n\pi}{2} \left(\sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}\right) \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \\
&= \sum_{n=1}^{\infty} \frac{8}{\pi^2}\sqrt{\frac{3}{2}} \frac{1}{n^2} \sin\frac{n\pi}{2} \psi_n(x) \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right),
\end{aligned}$$

we can see that the probability of measuring energy,

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

is

$$P(E_n) = \left|\frac{8}{\pi^2}\sqrt{\frac{3}{2}} \frac{1}{n^2} \sin\frac{n\pi}{2}\right|^2 = \frac{96}{n^4\pi^4} \sin^2\frac{n\pi}{2}.$$

For $E_1 = \hbar^2\pi^2/(2ma^2)$ in particular,

$$P(E_1) = \frac{96}{\pi^4} \approx 0.986.$$

The expectation value of the energy is

$$\langle H \rangle = \sum_{n=1}^{\infty} P(E_n)E_n = \sum_{n=1}^{\infty} \frac{96}{n^4\pi^4} \sin^2\frac{n\pi}{2} \left(\frac{\hbar^2\pi^2 n^2}{2ma^2}\right) = \frac{48\hbar^2}{\pi^2 ma^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \sin^2\frac{n\pi}{2}.$$

As before, sum over the odd integers only by making the substitution $n = 2k - 1$.

$$\begin{aligned}
\langle H \rangle = \frac{48\hbar^2}{\pi^2 ma^2} \sum_{2k-1=1}^{\infty} \frac{1}{(2k-1)^2} \sin^2\frac{(2k-1)\pi}{2} = \frac{48\hbar^2}{\pi^2 ma^2} \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} [(-1)^{k-1}]^2 &= \frac{48\hbar^2}{\pi^2 ma^2} \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} \\
&= \frac{48\hbar^2}{\pi^2 ma^2} \left(\frac{\pi^2}{8}\right) \\
&= \frac{6\hbar^2}{ma^2}
\end{aligned}$$