Problem 2.36

Solve the time-independent Schrödinger equation with appropriate boundary conditions for the "centered" infinite square well: $V(x) = 0$ (for $-a < x < +a$), $V(x) = \infty$ (otherwise). Check that your allowed energies are consistent with mine (Equation 2.30), and confirm that your ψs can be obtained from mine (Equation 2.31) by the substitution $x \to (x + a)/2$ (and appropriate renormalization). Sketch your first three solutions, and compare Figure 2.2. Note that the width of the well is now $2a$.

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 a centered infinite square well,

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

Split up the PDE over the intervals that the potential energy is defined on.

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + (\infty)\Psi(x,t), \quad |x| \ge a \qquad\qquad i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}, \quad |x| < a$$

On the interval $|x| \ge a$, only $\Psi(x, t) = 0$ can satisfy the equation. Requiring the wave function to be continuous leads to two boundary conditions, $\Psi(-a, t) = 0$ and $\Psi(a, t) = 0$, for the remaining PDE on $-a < x < a$. Because this PDE and its associated boundary conditions are linear and hoomgeneous, the method of separation of variables can be applied successfully. Assume a product solution of the form $\Psi(x, t) = \psi(x)\phi(t)$ and plug it into the PDE

$$i\hbar\frac{\partial}{\partial t}[\psi(x)\phi(t)] = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\psi(x)\phi(t)] \quad \to \quad i\hbar\psi(x)\phi'(t) = -\frac{\hbar^2}{2m}\psi''(x)\phi(t)$$

and the boundary conditions.

$$\begin{aligned} \Psi(-a,t) = 0 \quad &\to \quad \psi(-a)\phi(t) = 0 \quad \to \quad \psi(-a) = 0 \\ \Psi(a,t) = 0 \quad &\to \quad \psi(a)\phi(t) = 0 \quad \to \quad \psi(a) = 0 \end{aligned}$$

Divide both sides of the PDE by $\psi(x)\phi(t)$ in order to separate variables.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)}$$

The only way a function of t can be equal to a function of x is if both are equal to a constant E.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} = E$$

As a result of using the method of separation of variables, the Schrödinger equation has reduced to two ODEs, one in x and one in t.

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

Values of E for which the boundary conditions are satisfied are called the eigenvalues (or eigenenergies in this context), and the nontrivial solutions associated with them are called the eigenfunctions (or eigenstates in this context). The ODE in x is known as the time-independent Schrödinger equation (TISE) and can be written as

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi.$$

Check to see if there are positive eigenvalues: $E = \mu^2$.

$$\frac{d^2\psi}{dx^2} = -\frac{2m\mu^2}{\hbar^2}\psi$$

The general solution can be written in terms of sine and cosine.

$$\psi(x) = C_1\cos\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) + C_2\sin\left(\frac{\sqrt{2m}\mu}{\hbar}x\right)$$

Apply the two boundary conditions here.

$$\psi(-a) = C_1\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) - C_2\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) = 0$$

$$\psi(a) = C_1\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) + C_2\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) = 0$$

Solve this first equation for C_2

$$C_2 = C_1\frac{\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}{\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}$$

and substitute it into the second one.

$$C_1\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) + \left[C_1\frac{\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}{\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}\right]\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) = 0$$

Multiply both sides by $\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)$.

$$2C_1\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right) = 0$$

Assume that $C_1 \neq 0$, divide both sides by C_1, and use the fact that $\sin 2x = 2\sin x \cos x$.

$$\sin\left(2\frac{\sqrt{2m}\mu}{\hbar}a\right) = 0$$

This implies that the sine's argument is an integer multiple of π.

$$2\frac{\sqrt{2m}\mu}{\hbar}a = n\pi, \quad n = 0, \pm1, \pm2, \ldots$$

Solve for μ.

$$\mu = \frac{\hbar n\pi}{\sqrt{2m}(2a)}$$

There are positive eigenvalues,

$$\boxed{E_n = \mu^2 = \frac{\hbar^2 n^2 \pi^2}{2m(2a)^2}, \quad n = 1, 2, \ldots,}$$

and the eigenfunctions associated with them are

$$\begin{aligned}
\psi(x) &= C_1 \cos\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) + C_2 \sin\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) \\
&= C_1 \cos\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) + \left[C_1 \frac{\cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}{\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)}\right] \sin\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) \\
&= \frac{C_1}{\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)} \left[\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)\cos\left(\frac{\sqrt{2m}\mu}{\hbar}x\right) + \cos\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)\sin\left(\frac{\sqrt{2m}\mu}{\hbar}x\right)\right] \\
&= \frac{C_1}{\sin\left(\frac{\sqrt{2m}\mu}{\hbar}a\right)} \sin\left[\frac{\sqrt{2m}\mu}{\hbar}(a+x)\right] \quad \rightarrow \quad \psi_n(x) = A\sin\left[\frac{n\pi}{2a}(a+x)\right].
\end{aligned}$$

Since there are positive eigenvalues, solve the ODE in t with this value of E.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = E_n \quad \rightarrow \quad \frac{\phi'(t)}{\phi(t)} = -\frac{iE_n}{\hbar} \quad \rightarrow \quad \frac{d}{dt}\ln\phi(t) = -\frac{iE_n}{\hbar} \quad \rightarrow \quad \phi(t) = e^{-iE_n t/\hbar}$$

Note that n is a natural number in the formula for E_n because $n = 0$ leads to the zero eigenvalue, and negative integers lead to redundant values of E. A is arbitrary, but in order to make the usual probabilistic interpretation, it's chosen so that the integral of $[\psi(x)]^2$ over $-a < x < a$ is 1.

$$\begin{aligned}
1 &= \int_{-a}^{a} [\psi(x)]^2\,dx \\
&= \int_{-a}^{a} A^2 \sin^2\left[\frac{n\pi}{2a}(a+x)\right] dx \\
&= A^2 \int_{-a}^{a} \frac{1}{2}\left\{1 - \cos\left[\frac{n\pi}{a}(a+x)\right]\right\} dx
\end{aligned}$$

Make the following substitution.

$$u = \frac{n\pi}{a}(a + x)$$
$$du = \frac{n\pi}{a}\,dx \quad \rightarrow \quad dx = \frac{a}{n\pi}\,du$$

As a result,

$$\begin{aligned} 1 &= A^2 \int_0^{2n\pi} \frac{1}{2}(1 - \cos u)\left(\frac{a}{n\pi}\,du\right) \\ &= A^2 \frac{a}{2n\pi}(u - \sin u)\Big|_0^{2n\pi} \\ &= A^2 \frac{a}{2n\pi}(2n\pi) \\ &= A^2 a. \end{aligned}$$

Solve for A.

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

Therefore, the eigenstates for the positive eigenvalues are

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{a}} \sin\left[\frac{n\pi}{2a}(a + x)\right].}$$

Check to see if zero is an eigenvalue: $E = 0$.

$$\frac{d^2\psi}{dx^2} = 0$$

The general solution is a straight line.

$$\psi(x) = C_3 x + C_4$$

Apply the two boundary conditions to determine C_3 and C_4.

$$\psi(-a) = -C_3 a + C_4 = 0$$
$$\psi(a) = C_3 a + C_4 = 0$$

Solving this system of equations yields $C_3 = 0$ and $C_4 = 0$, resulting in the trivial solution $\psi(x) = 0$. Therefore, zero is not an eigenvalue. Finally, check to see if there are negative eigenvalues: $E = -\gamma^2$.

$$\frac{d^2\psi}{dx^2} = \frac{2m\gamma^2}{\hbar^2}\psi$$

The general solution can be written in terms of hyperbolic sine and hyperbolic cosine.

$$\psi(x) = C_5 \cosh\left(\frac{\sqrt{2m}\gamma}{\hbar}x\right) + C_6 \sinh\left(\frac{\sqrt{2m}\gamma}{\hbar}x\right)$$

Apply the two boundary conditions here.

$$\psi(-a) = C_5 \cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) - C_6 \sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) = 0$$
$$\psi(a) = C_5 \cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) + C_6 \sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) = 0$$

Solve this first equation for C_6

$$C_6 = C_5 \frac{\cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right)}{\sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right)}$$

and substitute it into the second one.

$$C_5 \cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) + \left[C_5 \frac{\cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right)}{\sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right)}\right] \sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) = 0$$

Multiply both sides by $\sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right)$.

$$2C_5 \sinh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) \cosh\left(\frac{\sqrt{2m\gamma}}{\hbar}a\right) = 0$$

Use the fact that $\sinh 2x = 2 \sinh x \cosh x$.

$$C_5 \sinh\left(2\frac{\sqrt{2m\gamma}}{\hbar}a\right) = 0$$

Unfortunately, there are no nonzero values of γ that make the hyperbolic sine zero. In order for the equation to be satisfied, then, it's necessary that $C_5 = 0$, which then means that $C_6 = 0$. The trivial solution results, and that means there are no negative eigenvalues. Mr. Griffiths analyzed the infinite square well modelled by

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

on pages 31-32 of the textbook and came up with

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

In order to obtain the centered infinite square well, replace a with $2a$ to double its width

$$V(x,t) = V(x) = \begin{cases} \infty & \text{if } x \leq 0 \\ 0 & \text{if } 0 < x < 2a \\ \infty & \text{if } x \geq 2a \end{cases}$$

and then replace x with $a + x$ to center the well about the origin.

$$V(x,t) = V(x) = \begin{cases} \infty & \text{if } a + x \leq 0 \\ 0 & \text{if } 0 < a + x < 2a \\ \infty & \text{if } a + x \geq 2a \end{cases} \quad \rightarrow \quad V(x,t) = V(x) = \begin{cases} \infty & \text{if } x \leq -a \\ 0 & \text{if } -a < x < a \\ \infty & \text{if } x \geq a \end{cases}$$

Make these same changes in Mr. Griffiths's formulas to get the boxed results here.

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \rightarrow \quad E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad \rightarrow \quad \psi_n(x) = \sqrt{\frac{2}{2a}}\sin\left(\frac{n\pi}{2a}x\right) \quad \rightarrow \quad \psi_n(x) = \frac{1}{\sqrt{a}}\sin\left[\frac{n\pi}{2a}(a+x)\right]$$

No renormalization is necessary. Below is a side-by-side comparison of the first three eigenstates for the infinite square well (in red) and the centered infinite square well (in blue).