Quantum mechanics
Particle in the box

Rati Kaewkam

7 November 2025

Problem Setup

Suppose the potential $V(x)$ is given by:

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

Time-independent Schrödinger equation

The equation for the spatial part $\psi(x)$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

Inside the box, $V = 0$ (for $0 \leq x \leq L$):

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} &= E\psi \\ \frac{d^2\psi}{dx^2} &= -\frac{2mE}{\hbar^2}\psi \\ \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \end{aligned}$$

To simplify, we define a constant k^2:

$$k^2 = \frac{2mE}{\hbar^2}$$

This transforms the equation into the second-order ODE:

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

The general solution to this equation is:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Applying Boundary Conditions

The wave function $\psi(x)$ must be zero at the boundaries (where $V = \infty$).

At $x = 0$:

$$\begin{aligned} \psi(0) &= 0 \\ A\sin(0) + B\cos(0) &= 0 \\ A(0) + B(1) &= 0 \\ \therefore B &= 0 \end{aligned}$$

At $x = L$:

$$\psi(L) = 0$$
$$A\sin(kL) = 0$$

Since $A = 0$ would mean that there would be no particle, we must have:

$$kL = n\pi, \quad \text{where } n = 1, 2, 3, \ldots$$

This quantizes the possible values of k:

$$k_n = \frac{n\pi}{L}$$

Find A (Normalization)

We normalize the wave function $\psi(x)$ so that the total probability of finding the particle in the box is 1.

$$\int_0^L |\psi(x)|^2 dx = \int_0^L (A\sin(kx))^2 dx = 1$$

$$A^2 \int_0^L \sin^2(kx) dx = 1$$

To solve the integral, use the identity:

$$\cos(2\theta) = 1 - 2\sin^2(\theta) \implies \sin^2(\theta) = \frac{1 - \cos(2\theta)}{2}$$

So, $\sin^2(kx) = \frac{1-\cos(2kx)}{2}$.

$$A^2 \int_0^L \left(\frac{1 - \cos(2kx)}{2}\right) dx = 1$$
$$\frac{A^2}{2}\left[\int_0^L 1 dx - \int_0^L \cos(2kx) dx\right] = 1$$
$$\frac{A^2}{2}\left[[x]_0^L - \left[\frac{1}{2k}\sin(2kx)\right]_0^L\right] = 1$$
$$\frac{A^2}{2}\left[(L - 0) - \left(\frac{1}{2k}\sin(2kL) - \frac{1}{2k}\sin(0)\right)\right] = 1$$
$$\frac{A^2}{2}\left[L - \frac{1}{2k}\sin(2kL)\right] = 1$$

Substitute our condition $kL = n\pi$:

$$\frac{A^2}{2}\left[L - \frac{1}{2k}\sin(2n\pi)\right] = 1$$
$$\frac{A^2}{2}[L - 0] = 1$$
$$\frac{A^2 L}{2} = 1$$
$$A^2 = \frac{2}{L}$$
$$\therefore A = \sqrt{\frac{2}{L}}$$

Energy eigenstates

From our definitions $k^2 = \frac{2mE}{\hbar^2}$ and $k_n = \frac{n\pi}{L}$:

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE_n}{\hbar^2}$$

Solving for energy E_n gives the quantized energy levels:

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

Stationary State Wave function

These are the normalized energy eigenfunctions (or stationary states):

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

General Wave function (Linear Combination)

The most general solution for the *initial state* $\Psi(x, t = 0)$ is a superposition:

$$\Psi(x, 0) = \sum_{n=1}^{\infty} C_n \psi_n(x) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Time-Dependent Schrödinger Equation

We use the separation of variables: $\Psi(x, t) = \psi(x)\varphi(t)$. The time-dependent part of the Schrödinger equation is the following.

$$\begin{aligned}
i\hbar \frac{d\varphi}{dt} &= E\varphi \\
\frac{d\varphi}{\varphi} &= -\frac{iE}{\hbar} dt \\
\int \frac{d\varphi}{\varphi} &= \int -\frac{iE}{\hbar} dt \\
\ln \varphi &= -\frac{iEt}{\hbar} \\
\varphi(t) &= e^{-\frac{iEt}{\hbar}}
\end{aligned}$$

We combine the parts $\Psi(x, t) = \sum C_n \psi_n(x)\varphi_n(t)$, using the specific energy E_n for each state ψ_n:

$$\Psi(x, t) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{iE_n t}{\hbar}}$$

Substituting the formula for E_n:

$$\Psi(x, t) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{i}{\hbar}\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)t}$$