Particle in a 1-Dimensional box

A particle in a 1-dimensional box is a fundamental quantum mechanical approximation describing the translational motion of a single particle confined inside an infinitely deep well from which it *cannot* escape.

Consider a box where the potential energy is *0 inside the box* (V=0 for 0<x<L) and *goes to infinity at the walls of the box* (V=∞ for x<0 or x>L). We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box.

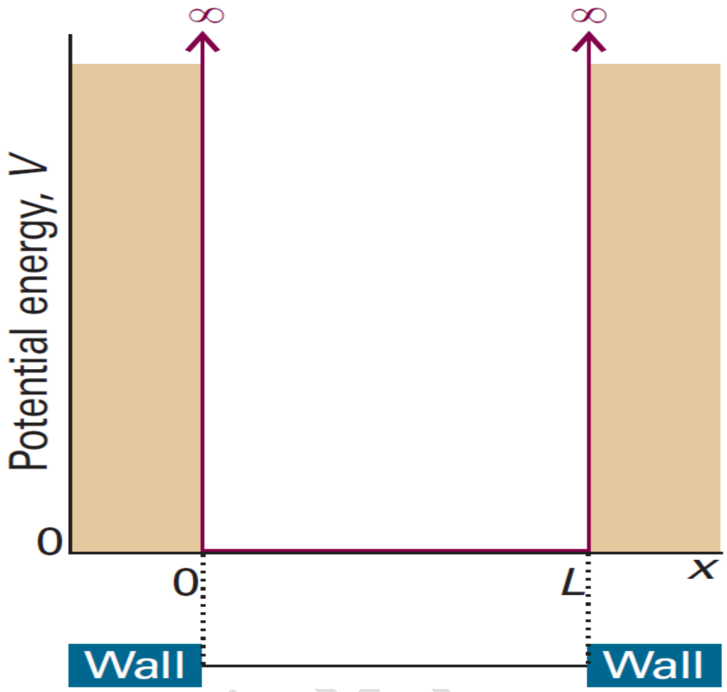


Figure: A particle in a one-dimensional region with impenetrable walls. Its potential energy is zero between x = 0 and x = L, and rises abruptly to infinity as soon as it touches the walls.

The time-independent Schrödinger equation for a particle of mass *m* moving in one direction with energy *E* is

$$\frac{-h^2}{8\pi^2 m}\frac{d^2}{dx^2} + V]\psi_{(x)} = E\psi_{(x)} \qquad \text{---(1)}$$

Where,

- m is the mass of the particle
- ψ(x) is the stationary time-independent wavefunction
- V(x) is the potential energy as a function of position
- E is the energy, a real number

Inside the box, the potential energy is zero. So the equation become

$$\frac{-h^2}{8\pi^2 m}\frac{d^2}{dx^2}\Psi_{(x)} = E\Psi_{(x)} \qquad \text{---(2)}$$

This equation has been well studied and gives a general solution of:

$\psi_{(x)}$=A sin(kx) + B cos(kx) ---(3)

where A, B, and k are constants.

The solution to the Schrödinger equation we found above is the general solution for a 1-dimensional system. We now need to apply our **boundary conditions** to find the solution to our particular system. According to our boundary conditions, the probability of finding the particle at x=0 or x=L is zero. When x=0, sin(0)=0sin(0)=0, and cos(0)=1cos(0)=1; therefore, *B must equal 0* to fulfill this boundary condition.

$\psi_{(x)}$= A sin(k.0) + B cos(k.0) = 0 ---(4)

⇒B cos0 = 0

⇒ B = 0

The wave function thus become

$\psi_{(x)}$=A sin(kx) ---(5)

Value of k:

Differentiate the wavefunction with respect to x,

$$\frac{dy}{dx}\Psi_{(x)} = kA\cos(kx)$$

$$\Rightarrow \frac{d^2}{dx^2}\Psi_{(x)} = -k^2 A\sin(kx)$$

$$\Rightarrow \frac{d^2}{dx^2}\Psi_{(x)} = -k^2\Psi_{(x)}$$

Rearranging equation (2), we can get the value of $\frac{d^2}{dx^2}\Psi_{(x)}$ as $\frac{8\pi^2 m}{-h^2} E\Psi_{(x)}$. So,

$$\frac{8\pi^2 m}{-h^2} E\Psi_{(x)} = -k^2\Psi_{(x)}$$

$$k = \sqrt{\frac{8\pi^2 mE}{h^2}}$$

Now we plug k into our wavefunction (5):

$\psi_{(x)}$=A sin($\sqrt{\frac{8\pi^2 mE}{h^2}}$.x)

Value of A:

To determine A, we have to apply the boundary conditions again. Recall that the *probability of finding a particle at x = 0 or x = L is zero.*

$$\psi_{(x)} = A \sin\left(\sqrt{\frac{8\pi^2 mE}{h^2}} \,.\, L\right) = 0$$

This is only true when

$$\sqrt{\frac{8\pi^2 mE}{h^2}} \,.\, L = n\pi$$

where n = 1,2,3…

$$\psi_{(x)} = A \sin\left(\frac{n\pi}{L} x\right)$$

To determine A, recall that the total probability of finding the particle inside the box is 1, meaning there is no probability of it being outside the box. When we find the probability and set it equal to 1, we are *normalizing* the wavefunction.

$$\int_0^L \psi^2{}_{(x)} dx = 1$$

$$\int_0^L A \sin\left(\frac{n\pi x}{L}\right) dx = 1$$

Using the solution for this integral from an integral table, we find our normalization constant, A:

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

Which results in the normalized wavefunction for a particle in a 1-dimensional box:

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

Determine the Allowed Energies

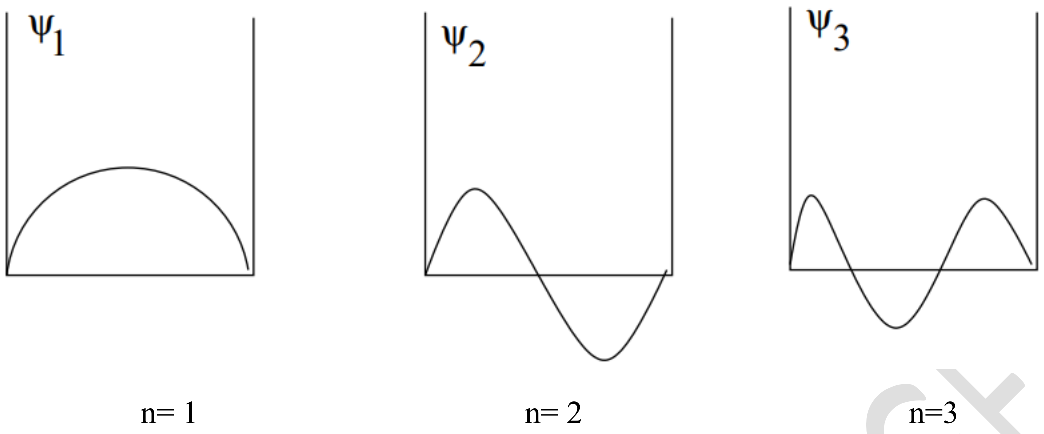
Solving for E results in the allowed energies for a particle in a box:

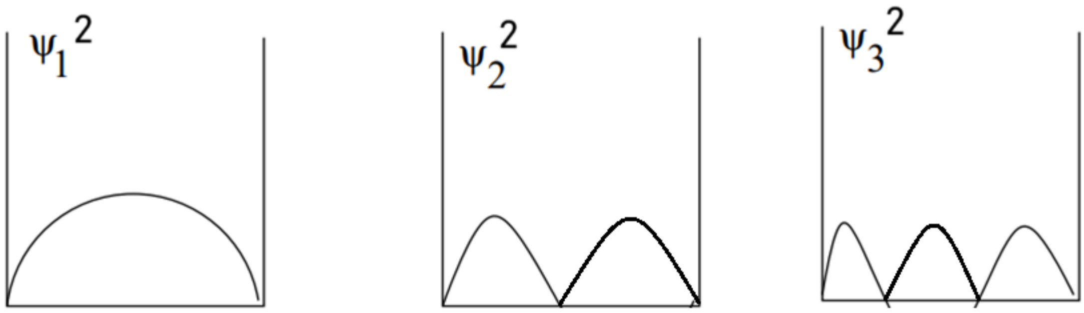
$$E = \frac{n^2 h^2}{8mL^2}$$

This is an important result that tells us:

1. The energy of a particle is quantized and
2. The lowest possible energy of a particle is NOT zero. This is called the zero-point energy and means the particle can never be at rest because it always has some kinetic energy.

The wavefunction for a particle in a box at the n=1, n=2 and n=3 energy levels look like this:





Questions:

Find the eigenvalue of the operator $\frac{d^2}{dx^2}$ if the eigenfunction is $\cos 2x$.

Show whether the operator $\hat{O}$ in the equation $\hat{O}\psi = \psi^2$ is linear or not.

The one-particle wave function $\psi(x, y, z, t)$ has the dimensions ________ . *(Fill in the blank)*

(a) Normalise the H-like function $\psi = e^{-n}$.

(b) Show that the wave function for a particle in one-dimensional box of length *a*, where the potential energy is zero, is not an eigenfunction of the linear momentum operator in one dimension.

(d) Show that the functions $\sin\frac{\pi x}{a}$ and $\cos\frac{\pi x}{a}$ are orthogonal within the limit $0 \le x \le a$.

(ii) For a particle in a one-dimensional box of length *a*, find the probability of finding the particle in the region $0 \le x \le a/4$ in the ground state.

What is a Hermitian operator? Show that the eigenvalue of a Hermitian operator is real.

(ii) The functions $\psi_1 = \left(\frac{1}{\pi}\right)^{1/2} \cos x$ and $\psi_2 = \left(\frac{1}{\pi}\right)^{1/2} \sin x$ are defined in the interval $x = 0$ to $x = 2\pi$. Examine if the functions are orthogonal to each other. 2

Derive expression for the total energy of a particle in a three-dimensional box. Explain the concept of degeneracy. 5+2=7

One dimensional box.

For a particle in a one-dimensional box of length a, find the probability of finding the particle in the region $0 \le x \le a/4$ in the ground state.

One dimensional box.

What is a Hermitian operator? Show that the eigenvalue of a Hermitian operator is real.

A particle in a box cannot have zero energy quantum mechanically. Explain. 3

Find the values of momentum and energy for an electron in a box of length $1A^\circ$ for $n = 1, 2$. 4

Prove that $\psi(x) = e^{iCx}$ is acceptable eigenfunction where C is finite constant. 3