ABESIT Ghaziabad (290)

Course: Engg. Physics (KAS201T)

Unit-III

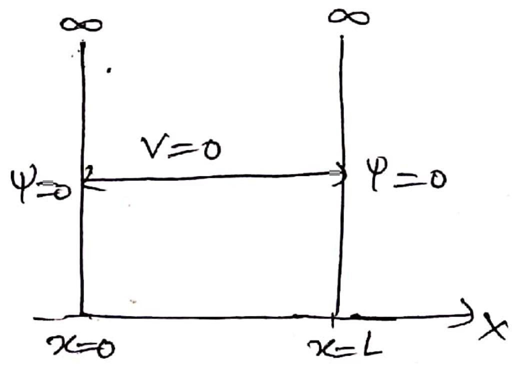
Quantum Mechanics

Lecture 33: Solution to stationary state Schrodinger wave equation for one-dimensional particle in a box

Outcome: Apply Schrodinger wave equation to solve one dimensional particle in a box.

Particle in one dimensional Potential well (Particle in a Box):-

Consider a particle moving inside a box along the x-direction. The particle is moving back and forth between $x=0$ to $x=L$. L is the width of the box.



Suppose the walls of the box are infinitely hard so that the particle does not lose energy when bounces back from the walls.

Suppose that the potential energy V of the particle is zero inside the box, but becomes infinite at the walls and outside that is

$V=0$ for $0<x<L$

$V=\infty$ for $x\leq 0$ and for $x\geq L$

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The boundary conditions for wave function is

$\psi = 0$ for $x = 0$

and $\psi = 0$ for $x = L$

The time independent schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

Since inside the box $V=0$, then

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad \text{——} \quad (1)$$

Let $k^2 = \dfrac{2mE}{\hbar^2}$ —— (2)

then

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{——} \quad (3)$$

The general solution of this equation is

$$\psi = A\sin kx + B\cos kx \quad \text{——} \quad (4)$$

where A and B are constant

Using boundary conditions of wave function

$\psi = 0$ at $x = 0$ then equ (4) becomes

$$0 = A\sin 0 + B\cos 0$$

$$B = 0 \quad \text{——} \quad (5)$$

Then equation (4) reduces to

$$\psi = A\sin kx \quad \text{——} \quad (6)$$

Now using the boundary condition

$\psi = 0$ at $x = L$

then $0 = A\sin kL$

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i.e either $A=0$ or $\sin KL=0$

But A cannot zero because in this condition ψ will be zero for the region $0<x<a$, which shows the absence of the particle in the box.

But $A\neq 0$ Hence

$$\sin KL = 0$$

$$\sin KL = \sin n\pi$$

$$KL = n\pi$$

$$k = \frac{n\pi}{L} \quad \text{--- (7)} \quad \text{where } n = 1,2,3\ldots \quad n\neq 0$$

To find the eigen function

using equ (7) in equ. (6) then

$$\psi_n(x) = A\sin\frac{n\pi x}{L}$$

For the calculation of A, using the normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1$$

$$\int_{-\infty}^{\infty} \left|A\sin\left(\frac{n\pi x}{L}\right)\right|^2 dx = 1$$

or

$$A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx = 1$$

$$\frac{A^2}{2}\int_0^L 1-\cos\left(\frac{2n\pi x}{L}\right)dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{L}{2n\pi}\sin\frac{2n\pi x}{L}\right]_0^L = 1$$

$$\frac{A^2}{2}(L) = 1$$

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

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then the eigen function (wavefunction)

$$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

The Corresponding energy eigen values
Substituting the value of k from equ.(7) in equ.(2)

$$\frac{n^2\pi^2}{L^2} = \frac{2m}{\hbar^2} E$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \left(\hbar = \frac{h}{2\pi}\right)$$

$$\boxed{E = \frac{n^2 h^2}{8mL^2}} \quad \text{--- (8)}$$

This is eigen energy value in particle in one dimensional box.

if $n = 1$

$$E_1 = \frac{h^2}{8mL^2}$$

This is the lowest possible energy of the particle.

Eigen values and Eigen functions :- When the schrodinger time independent wave equation is solved for any particle with its wave function subject to certain boundary conditions, the solutions exist only for particular values of energy E_n which are known as the eigen values. The wave functions ψ_n corresponding to the eigen values are know as eigen functions.

Ques. A particle is in motion along a line $x=0$ and $x=L$ with zero potential energy. A points for which $x<0$ and $x>L$, the potential energy is infinite. Solving Schrodinger equation, obtain energy eigen values and Normalized wave function for the particle.