UNIT IV

Quantum Physics

4.6.Particle in a three dimensional box

Application of Schrodinger Wave Equation to a Particle (Electron) Enclosed in a OneDimensional Potential Box

Consider a particle of mass m moving back and forth between the walls of a 1D box. Since the walls are of infinite potential the particle does not penetrate out from the box. Also, the particle has elastic collisions with the walls. Therefore, the potential energy of the electron inside the box is constant and it is taken as zero for simplicity. The potential energy V of the particle is on the wall of the box is infinity.

Thus the potential function is

$$V(x) = 0 \quad 0<x<a$$

$$V(x) = \infty \quad 0 \geq x \geq a$$

This function is known as square well potential

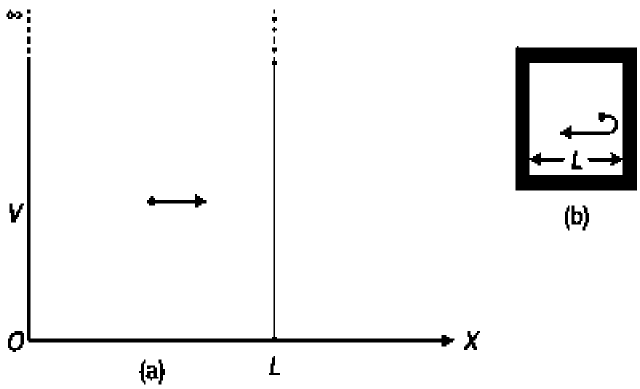

Fig 4.6.1 Particle in 1D box

(Source: "Advanced Engineering Physics" by Sujay Kumar Bhattacharya, Saumen Pal)

Here the particle cannot move outside and the boundary conditions can be written as

$$\Psi = 0 \qquad \text{at } x=0 \text{ and } a$$

$$\Psi \neq 0 \qquad at \;\; 0 \leq x \leq 0$$

The Schrodinger's equation in 1D is

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\Psi = 0 \text{------------------------}(1)$$

But V= 0 inside the potential well

(1) Becomes

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

Put

$$\frac{2mE}{\hbar^2} = k^2 \text{----------------------}(3)$$

(2) Becomes

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

Solution for this equation is

Ψ(x) = A sinkx + Bcos Kx--------------------(4)

A and B are constants.

To find A and B

Apply boundary conditions

At x=0 $\Psi = 0$

Sub in (4)

$$0 = B$$

$$\therefore \Psi = A\sin kx \text{----------------------}(5)$$

At x =a $\Psi = 0$

0=A sin ka

A sinka=0

A cannot be zero

∴ Sinka =0

Ka=nπ

$$\therefore k = \frac{n\pi}{a}$$

Sub this in (3)

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \text{---------}(6)$$

And we know that

$$\hbar^2 = \frac{h^2}{4\pi^2}$$

Sub this in (6)

$$E = \frac{n^2h^2}{8ma^2} \text{-------------}(7)$$

This is the expression for energy Eigen value for a particle moving in 1D box.

To find energy Eigen functionΨ

$$\Psi = \mathrm{A}\sin kx$$

$$\Psi = \mathrm{A}\sin\frac{n\pi}{a}x \text{-------------}(8) \qquad (\because K = \frac{n\pi}{a})$$

Normalisation of wave function

We know that

Within the potential well the particle is present

Then the probability of finding the particle is

$$\int \Psi\Psi^* d\tau = 1$$

Here it is 1D

$$\int_0^a \Psi\Psi^* dx = 1$$

$$\therefore \int_0^a \mathrm{A}\sin\frac{n\pi}{a}x\,\mathrm{A}\sin\frac{n\pi}{a}x\,dx = 1$$

$$\int_0^a \mathrm{A}^2\sin^2\frac{n\pi}{a}x\,dx = 1$$

$$\mathrm{A}^2\int_0^a \sin^2\frac{n\pi}{a}x\,dx = 1$$

$$\mathrm{A}^2\int_0^a \frac{1-\cos 2\frac{n\pi}{a}x}{2}\ dx = 1$$

$$\mathrm{A}^2\int_0^a\ dx - \cos 2\frac{n\pi}{a}xdx = 1$$

$$\frac{\mathrm{A}^2}{2}\left(\mathrm{x} - \frac{sin\frac{2n\pi}{a}x}{\frac{2n\pi}{a}}\right)_0^a = 1$$

Substituting the upper & lower limit

We get

$$\frac{A^2}{2}\left(a-\frac{\sin\frac{2n\pi}{a}a}{\frac{2n\pi}{a}}\right)-0=1$$

$$\frac{A^2 a}{2}=1$$

$$A^2 = 2/a$$

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

Sub this in (8)

$$\Psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$$

This is the expression for Eigen function or wave function of a particle moving in a 1D potential well.

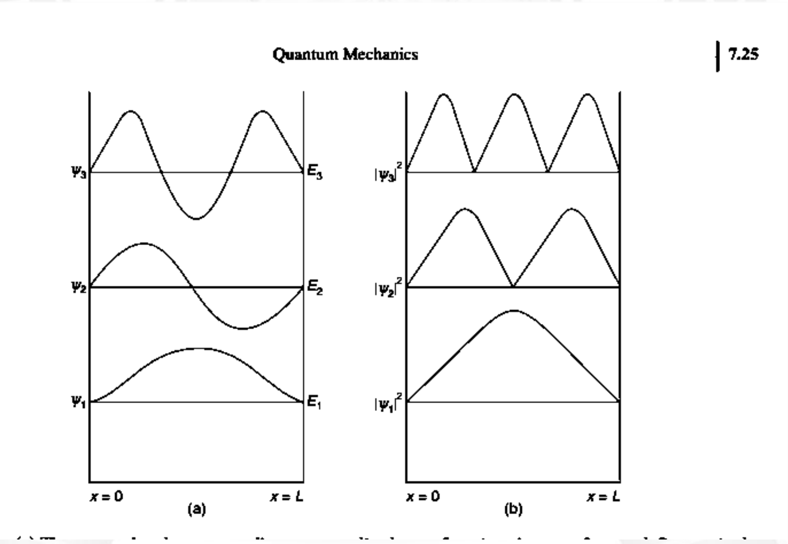

Fig 4.4.2 Particle in a box

Source: "Advanced Engineering Physics" by Sujay Kumar Bhattacharya, Saumen Pal

Result:

1. Energy Eigen value is inversely proportional to the square of width of the potential well.
2. Energy Eigen value is inversely proportional to the mass of the particle.
3. From the figure it is shown that the probability of finding the particle is maximum at the centre for the first energy value.

From the figure it is shown that the probability of finding the particle is minimum at the centre for the second energy value.

Particle in a Three dimension box:

The solution of one dimension potential well is extended for a three dimensional potential box.

In a three dimensional potential box the particle can move in any direction .so we use three quantum numbers $n_{x,}n_y$ *and* n_z *to the* three coordinate axes namely x,y and z respectively.

If a,b,c are the lengths of the box along x,y and z axes then,

$$E_{n_{x,}n_y,n_z} = \frac{n_x^2}{8m}\frac{h^2}{a^2}$$

If a= b = c as for a cubical box then

$$E_{n_{x,}n_y,n_z} = \frac{h^2}{8ma^2}\left[\, n_x^2 + n_y^2 + n_z^2 \,\right] \text{------------(1)}$$

The corresponding normalized wave function is

$$\boldsymbol{\psi}_{n_{x,}n_y,n_z} = \sqrt{\left(\frac{2}{a}\right)}\sqrt{\left(\frac{2}{a}\right)}\sqrt{\left(\frac{2}{a}\right)}\,\boldsymbol{sin}\,\frac{n_{x,}\pi x}{a}\,\mathbf{sin}\frac{n_y\pi y}{a}\,\mathbf{sin}\frac{n_z\pi z}{a}$$

$$= \sqrt{\left(\frac{8}{a^3}\right)}\,\boldsymbol{sin}\,\frac{n_{x,}\pi x}{a}\,\mathbf{sin}\frac{n_y\pi y}{a}\,\mathbf{sin}\frac{n_z\pi z}{a} \text{-----------------}\mathbf{(2)}$$

From the equations (1), (2)we understand that several combinations of the three quantum numbers($n_{x,}n_y$,nz) lead to different energy eigen values and eigen function.

2.3.2.Degenerate states:

For several combinations of quantum numbers,we have the same energy eigen value but different eigen function.Such a state of energy levels is called degenerate state.

The three combinations of quantum numbers (1,1,2),(1,2,1) and (2,1,1) which give the same Eigen value but different Eigen functions are called 3- fold degenerate state.

Example:

If ($n_{x,}n_y$, n_z) is (1,1,2) ,(1,2,1) and (2,1,1)

Then

$$E_{112} = \frac{h^2}{8ma^2}\left(1^2 + 1^2 + 2^2 \right) = \frac{6h^2}{8ma^2}$$

$$E_{121} = \frac{6h^2}{8ma^2}$$

$$E_{211} = \frac{6h^2}{8ma^2}$$

The corresponding wave functions are

$$\boldsymbol{\psi_{112}} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{2\pi z}{a} \text{---}$$

$$\boldsymbol{\psi_{121}} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a} \text{---}$$

$$\boldsymbol{\psi_{211}} = \sqrt{\left(\frac{8}{a^3}\right)} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a} \text{---}$$