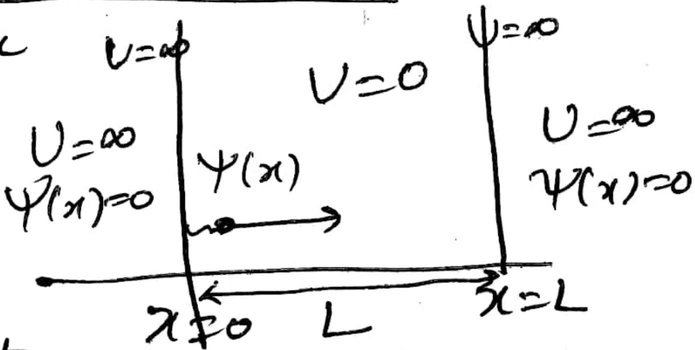
Application of Time Independent Sch. Eqn.

Motion of a particle in box (1-D case)

Consider a microscopic particle of rest mass m be moving in a box having width 'L' along X-axis. Let the motion of the particle be non relativistic.



As particle is in motion, then according to de-Broglie hypothesis, a wave is associated with it. Let us assume the pot. energy of particle be zero inside the box and infinite elsewhere. or in other words, value of potential on the walls of box is infinite, so that the particle by itself cannot climb the walls & thus cannot go outside the box. So wavefn. $\psi(x)=0$ on the walls and outside the walls and hence there will be finite probability to locate the particle within the box and zero prob. on the walls & outside the walls. Also consider the walls of the box to be infinitely hard so that collision between the walls & particle is elastic and as such no transfer of energy of momentum takes places between walls & particles. Provided the physical conditions remain to be same, the motion of the particle will be time independent. ∴ to discuss the motion of particle in a box, we can apply Schrodinger eqn.

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

within box, $U = 0$ $\quad 0 < x < L$

$$\therefore \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0.$$

Put $\frac{2mE}{\hbar^2} = k^2$ —— (1)

which gives $\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0$

The solution of this differential eqn. is given by $\psi(x) = A\sin kx + B\cos kx$

when $x = 0$, $\psi(x) = 0 \Rightarrow 0 = A\cdot 0 + B\cdot 1$

$\Rightarrow B = 0$

$\therefore \psi(x) = A\sin kx$ —— (2)

when $x = L$, $\psi(x) = 0 \Rightarrow 0 = A\sin kL$

i.e $A \sin kL = 0$

but $A \neq 0$

$\Rightarrow \sin kL = 0$

$\Rightarrow kL = n\pi, \quad n = 0, 1, 2 \ldots$

but $n \neq 0$

as it will make either

$k = 0$ or $L = 0$

which is not ~~po~~ssible

$\therefore n = 1, 2, 3, \ldots$

$n = 1 \rightarrow$ ground state

$n = 2 \rightarrow$ first excited state

~~&~~ so on.

$\therefore kL = n\pi, \quad n = 1, 2 \ldots$

$\Rightarrow k = \frac{n\pi}{L} \Rightarrow k^2 = \frac{n^2\pi^2}{L^2}$

from (1) $\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$

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

These are energy eigen values for a particle moving in a box (1-D motion).

Substituting the values of k in eqn. no. (2), we get

$$\psi_n(x) = A \sin \frac{n\pi}{L} x \ , \ n = 1, 2 \ldots$$

These are the eigen wave fns. for the 1-D motion of particle in a box.

We will find the value of A by using normalization condition.

i.e $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

$$\Rightarrow \underbrace{\int_{-\infty}^{0} |\psi|^2 dx}_{0} + \int_{0}^{L} |\psi|^2 dx + \underbrace{\int_{L}^{\infty} |\psi|^2 dx}_{0} = 1$$

as particle can't go beyond walls, ∴ first & third integrals = 0 &

we have $\int_{0}^{L} |\psi|^2 dx = 1$

$$\Rightarrow A^2 \int_{0}^{L} \sin^2 \frac{n\pi}{L} x \, dx = 1$$

$$\Rightarrow A^2 \int_{0}^{L} \frac{1 - \cos 2 \frac{n\pi}{L} x}{2} dx = 1$$

$$\Rightarrow A^2 \cdot \frac{1}{2} \int_{0}^{L} dx = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

(retaining +ve sign)

∴ Eigen wavefns. for motion of particle in a box are

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

∴ energy eigen values are

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

Clearly energy values are discrete as $E_n \propto n^2$ and $n = 1, 2, 3$ —

i.e. energy values can't be continuous.

Clearly velocity & momentum values will also be discrete. So when we give boundary to motion of particle, it can't have all possible values of energy & momentum except for certain discrete values. This is known as quantum confinement.