The Free Particle: Continuous States:-

This is the simplest one-dimensional problem, it corresponds to $V(x)=0$ for any value of x.

In this case the Schrödinger eqn is given by

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

$$\Rightarrow \left(\frac{d^2}{dx^2}+k^2\right)\psi(x) = 0 \quad -- \text{①}$$

where $k^2 = \frac{2mE}{\hbar^2}$, k being the wave number.

$k=\frac{p}{\hbar}$

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

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

The most general solution to ① is a combination of two linearly independent waves

$$\psi_+(x) = e^{ikx} \text{ and } \psi_-(x) = e^{-ikx}$$

$$\psi_k(x) = A_+e^{ikx} + A_-e^{ikx}$$

where A_+ & A_- are two arbitrary constants.

The complete wave function is given by stationary states

multiply by $e^{\frac{-iEt}{\hbar}}$

$$\psi_k(x,t) = A_+e^{i(kx-\omega t)} + A_-e^{-i(kx+\omega t)}$$

since $\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}$,

wave travelling to the right

wave travelling to the left.

The intensities of these waves are given by $|A_+|^2$ and $|A_-|^2$, respectively.

We should note that the waves $\psi_+(x,t)$ and $\psi_-(x,t)$ are associated, respectively, with a free particle ~~moving~~ travelling to the right and to the left with well defined momenta and energy

$$p_\pm = \pm\hbar k, \quad E_\pm = \frac{\hbar^2k^2}{2m}.$$

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Three problems :--

1. The probabilities densities corresponding to either solutions

$$\rho_{\pm}(x,t) = |\psi_{\pm}(x,t)|^2 = |A_{\pm}|^2$$

are constant, for they depend neither on x nor on t.

$\downarrow$

This is a consequence ~~of~~ due to complete loss of information about the position and time for a state with definite values of momentum $p_{\pm} = \pm\hbar k$, and energy $E_{\pm} = \frac{\hbar^2 k^2}{2m}$.

2. An apparent discrepancy between the speed of the wave and the speed of the particle.

$$v_{wave} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{\hbar^2 k^2/2m}{\hbar k} = \frac{\hbar k}{2m}$$

On the other hand classical speed of the particle

$$v_{classical} = \frac{p}{m} = \frac{\hbar k}{m} = 2 v_{wave}$$

3. The wave function is not normalized.

$$\int_{-\infty}^{\infty} \psi_{\pm}^*(x,t)\, \psi_{\pm}(x,t)\, dx = |A_{\pm}|^2 \int_{-\infty}^{+\infty} dx \to \infty$$

The soln $\psi_{\pm}(x,t)$ are thus unphysical, physical wave functions must be square integrable

$\Downarrow$

Thus soln. of Schrödinger eqn that are physically acceptable cannot be plane waves.

$\Downarrow$

Instead, we can construct physical solutions by means of a linear superposition of plane waves.

$\downarrow$

Answer is provided by wave packets.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk,$$

A free particle can not be represented by plane wave it should be represented by a wave packet. $\Leftarrow$ where $\phi(k)$, the amplitude of the wave packets, is given by Fourier transform of $\psi(x,0)$ as

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0)\, e^{-ikx}\, dx$$

$\Rightarrow$ This solve all problems

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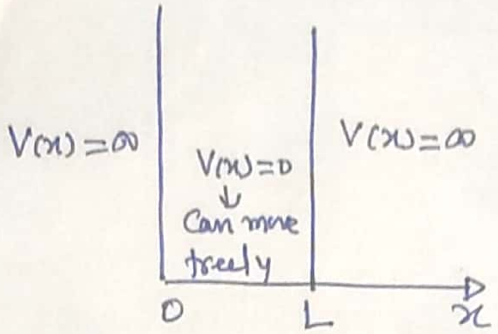
Ex 1:.

The Particle in a box:-

(The infinite Square well potential)



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

or

$$V(x) = \begin{cases} +\infty & x < 0 \\ 0 & 0 \le x \le a \\ +\infty & x > a \end{cases}$$

$\psi = 0$ for $x \le 0$ & $x \ge L$

Within the Box, Schrödinger eqⁿ becomes

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

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

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

The soln. of eqⁿ① is

$$\psi = A\sin kx + B\cos kx \quad \text{--②}$$

• Classically:— Particle remains confined inside the box, moving at constant momentum $p = \pm\sqrt{2mE}$ back and forth as a result of repeated reflection from the walls of the well

QM ⇒ Particle to have only bound state solns and a discrete nondegenerate energy spectrum

The solns are $\psi(x) = A'e^{ikx} + B'e^{-ikx}$

Boundary conditions for evaluating A & B

(i) $\psi = 0$ for $x = 0$

$$\Downarrow$$

$B = 0$ $\quad (\because \cos 0 = 1)$

The second term can not describe the particle because it does not vanish at $x = 0$.

(ii) $\psi = 0$ for $x = L$

$$0 = A\sin\sqrt{\frac{2mE}{\hbar^2}}\,L + 0$$

$$\left(\sqrt{\frac{2mE}{\hbar^2}}\right)L = n\pi \qquad \text{where } n = 1, 2, 3 \ldots$$

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

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Wave functions:-

$$\psi_n = A \sin\sqrt{\frac{2mE_n}{\hbar^2}}\, x$$

Putting value of E_n

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

$A \to ?$

$$\int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx$$

$$\int_{-\infty}^{+\infty} |\psi_n|^2 dx$$

$$\int_0^L |\psi_n|^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \qquad \because \sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$$

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

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

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

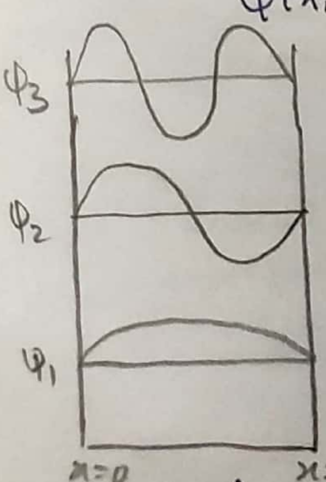
$$\int_{-\infty}^{+\infty} |\psi_n|^2 dx = 1 = \frac{A^2}{2}(L)$$

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

$$\boxed{\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)} \qquad n = 1, 2, 3, \ldots$$

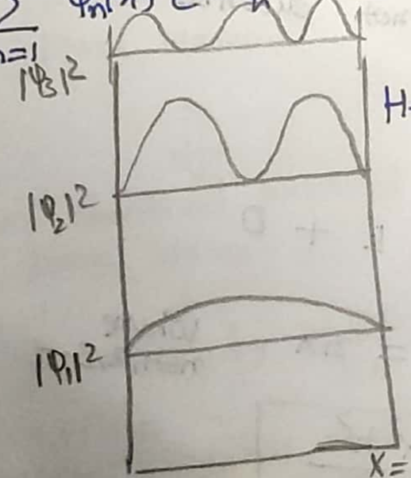
The time-dependent Schrödinger eqn is given by

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



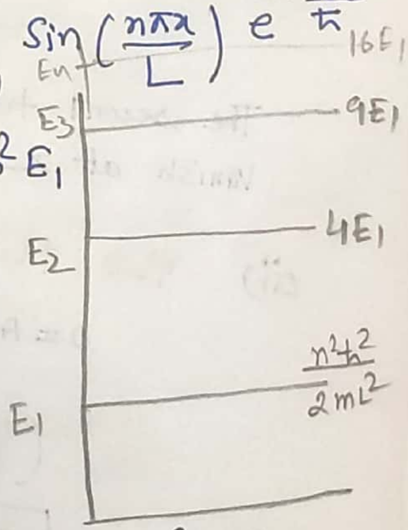
Wave-function

(First three stationary states)



Probability density

Here $E_n = n^2 E_1$

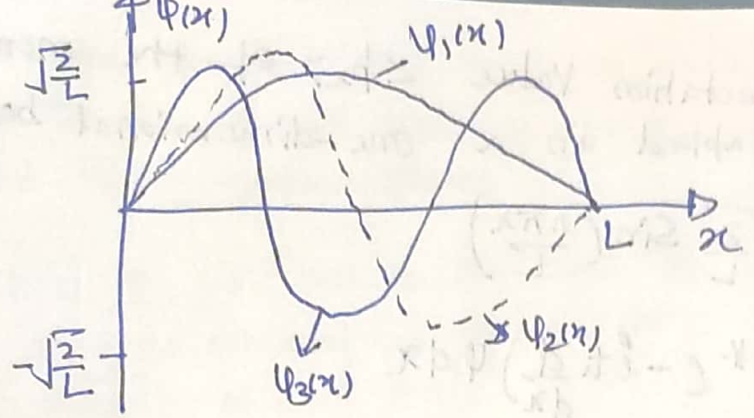


Energy

↓ They are alternately even and odd, with respect to

... $\psi_2 \to$ odd, $\psi_3 \to$ even

②



Q:- Find the expectation value $\langle x \rangle$ of the position of a particle trapped in a box of L side.

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\psi|^2 dx \qquad \langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi \, dx$$

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

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

$$= \frac{2}{L}\left[\frac{x^2}{4} - \frac{x \sin\left(\frac{2n\pi x}{L}\right)}{\frac{4n\pi}{L}} - \frac{\cos\left(\frac{2n\pi x}{L}\right)}{8\left(\frac{n\pi}{L}\right)^2}\right]_0^L$$

$$\langle x \rangle = \frac{2}{L}\left(\frac{L^2}{4}\right) = \frac{L}{2}$$

The average position of the particle in the middle of the box in all quantum states.

$\langle x \rangle \Rightarrow$ average not probability.

Q:- Calculate the expectation value $\langle p_x \rangle$ of the momentum of a particle trapped in a one-dimensional box.

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

$$\langle p_x \rangle = \int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{d}{dx}\right) \psi \, dx$$

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

$$= 0$$

The expectation value $\langle p_x \rangle$ of the particle's momentum is zero $\rightleftarrows$

$$\left[\int \sin ax \cos ax \, dx = \frac{1}{2a} \sin^2(ax) \right.$$

$$\left. \langle p \rangle = -i\hbar \frac{2}{L}\left(\frac{n\pi}{L}\right) \left[\sin^2 \frac{n\pi x}{L} \right]_0^L = 0 \right]$$

$$\sin^2 0 = \sin^2 n\pi = 0$$

$n = 1, 2, 3 \ldots$

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