QUANTUM MECHANICS

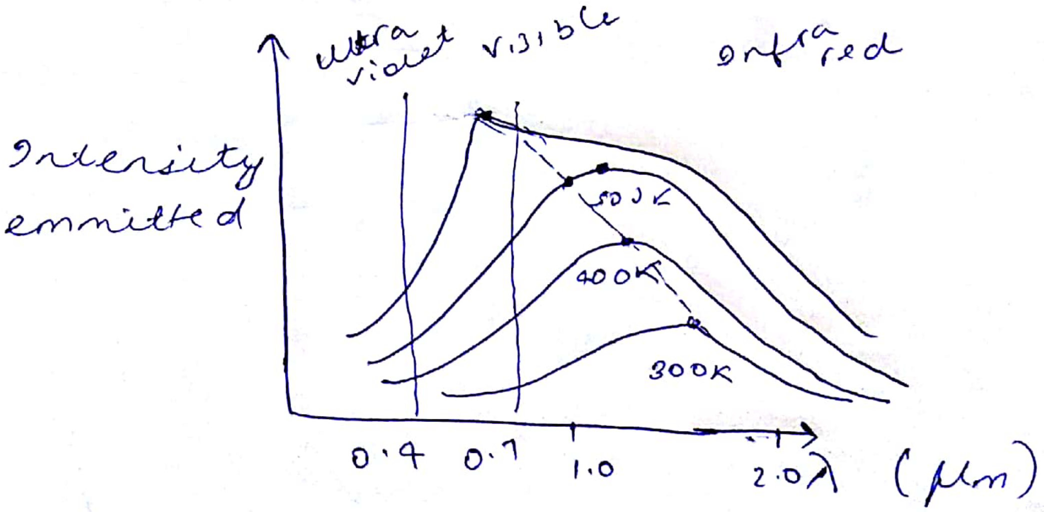
1895 : X ray discovery
1896 : Radioactivity discovery

} unknown rays, penetrate opaque bodies and made it possible to see what had been invisible

1897 : Electron discovery
(existence of bodies smaller than the atoms)

Black body radiation

Theoretical notion : A black body can absorb 100% radiation and emit max. amount of energy possible at a given temperature.



→ Black body radiation curve changes with temp.
→ At a given tempr, a black body

radiates energy at all wavelength

→ As temp. increases, peak wavelength emitted by the black body decreases

→ Total energy emitted (the total area under the curve) increases with temp.

i) Double slit expt.
ii) Photoelectric ~~expt~~. effect
iii) Atomic spectra
iv) Stern - Gerlach expt. (response of atoms to magnetic fields)
v) Heat capacity of solids
vi) scattering of X-rays by solids (compton effect)
vii) Diffraction of electrons by crystals

Ψ ⇒ wave function
defines a state of a quantum system

$\Psi(x, t)$ for one dimension
All the physical properties of a system can be expressed as operators.

$$\hat{P}_x \equiv -i\hbar \frac{\partial}{\partial x}$$

where $\hat{P}_x$ is momentum operator

and $\hbar = \frac{h}{2\pi}$

$$\hat{P}_x \psi(x,t) = p\,\psi(x,t)$$

$\hookrightarrow$ momentum

IIIly $\hat{H} \equiv i\hbar \frac{\partial}{\partial t}$

$$\hat{H}\psi(x,t) = E\,\psi(x,t) \longrightarrow (1)$$

energy

$$\hat{H} = \hat{kE} + \hat{PE}$$

$$= \frac{\hat{P}_x(\hat{P}_x)}{2m} + \hat{u}(x)$$

$2m \rightarrow$ mass

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{u}(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \hat{u}(x)\,\Psi(x,t)$$

$$= i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \hat{u}(x)\psi(x,t) = E\psi(x,t)$$

[Schrodinger's eqn.]

kinetic energy

$$= \frac{\hat{P}_x \hat{P}_x}{2m}$$

$$= \frac{-i\hbar}{2m} \frac{\partial}{\partial x} \left[-i\hbar \frac{\partial}{\partial x} \right]$$

$$= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

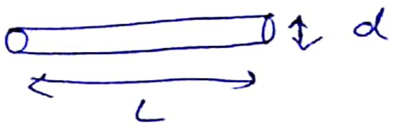
$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + \hat{U}(x)\psi(x,t)$$

{ From 1 }

$$= E\,\psi(x,t)$$

[schrodinger equation]

model : Particle in a one-dimensional box.

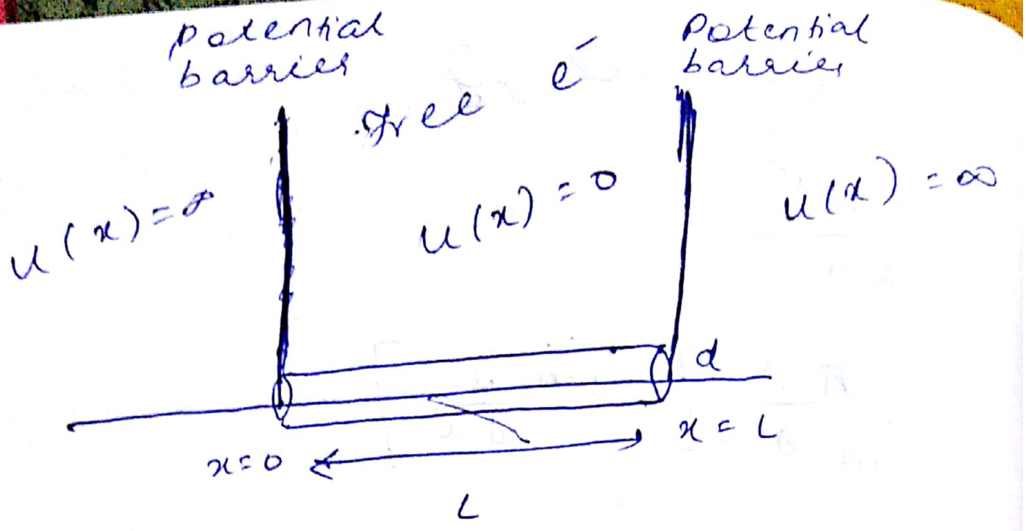


where $d << L$

$\approx$ 1D system

Place the wire on x axis with one end at $x = 0$ and other at $x = L$. The electron cannot go out of the wire

$\Rightarrow$ potential is ∞ at ends and beyond



$u(x) = \infty$ at $x = 0$
$u(x) = \infty$ at $x = L$
$u(x) = 0$ at $0 < x < L$

Inside the wire,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \underbrace{u(x)}_{\text{equal to zero}}\psi(x) = E\psi(x)$$

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

$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0 \quad \left(\text{where } k = \sqrt{\frac{2mE}{\hbar^2}}\right)$$

The solution of this differential eqn. is

$$\psi(x) = A\cos kx + B\sin kx \longrightarrow (1)$$

(general solution)

where A and B are arbitrary constants.

The boundary conditions are:

At $x=0$, ~~$\psi(x)$~~ $\psi(x=0)=0$

$\Rightarrow A=0$ [from ①]

At $x=L$, $\psi(x=L)=0$

$\Rightarrow B\sin kL=0$

$\Rightarrow kL=n\pi$

n is an integer

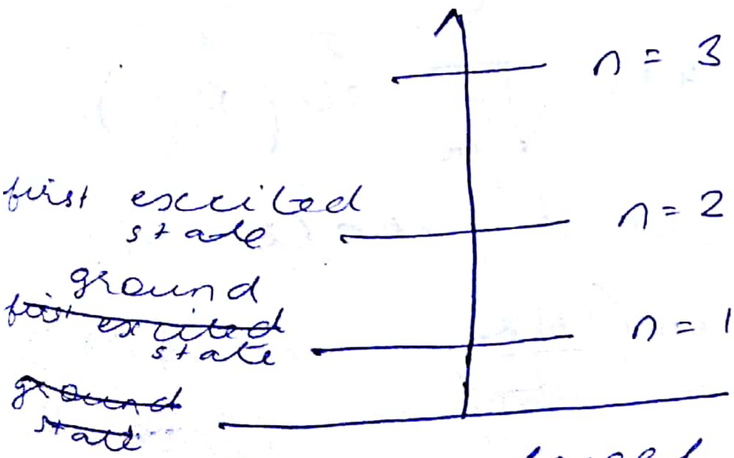
$$k=\frac{n\pi}{L}$$

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

$$\Rightarrow E=\frac{n^2h^2}{8mL^2} = n^2\left(\frac{h^2}{8mL^2}\right)$$

Energy is quantized

Fundamental unit of energy



$n=3$; $E_3=\frac{9h^2}{8mL^2}$

$n=2$; $E_2=\frac{4h^2}{8mL^2}$

$n=1$; $E_1=\frac{h^2}{8mL^2}$

Energy level diagram

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

$\psi^*(x)\psi(x)\,dx$ gives probability of finding the e^- between x and $x+dx$, where $\psi^*(x)$ is the complex conjugate
(Born's)

$$\int_{x=0}^{L} \psi^*(x)\psi(x)\,dx = 1$$

[since total probability = 1]

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

$$\Rightarrow B = \sqrt{\frac{2}{L}}$$

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

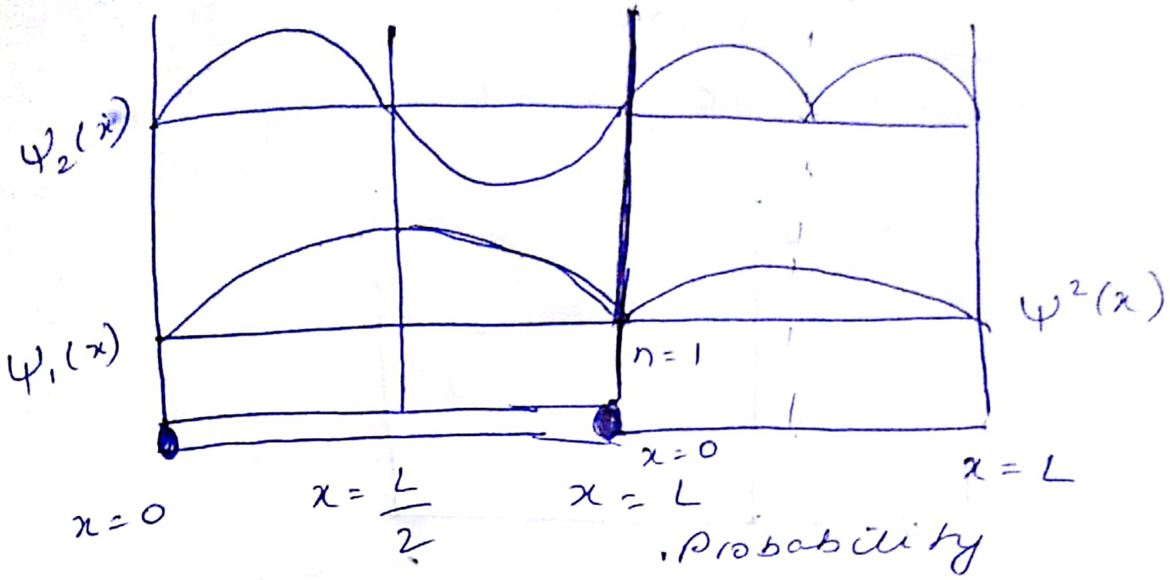
$\psi_n(x)$ denotes n^{th} state of system

For $n=1$, $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$

For first excited state,
$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$

and so on.

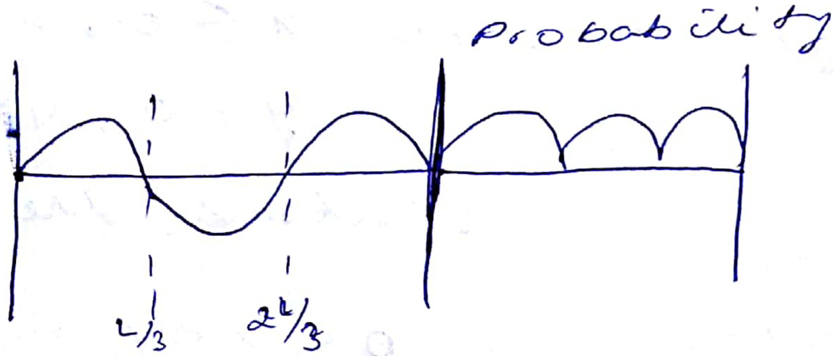
(n is quantum number)



probability of finding e^- is max at centre is ground state.

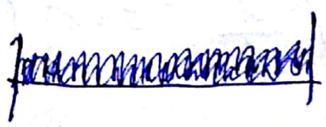
In first excited state, probability of finding e^- at centre is 0

For second state, graph is



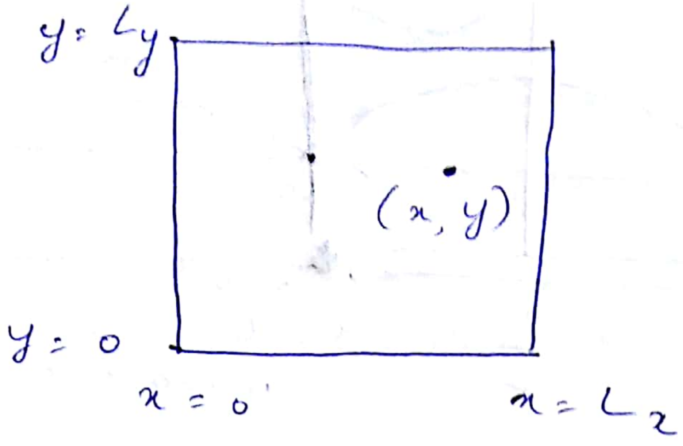
and so on

Therefore when $n \to \infty$, probability becomes



continuous spectrum (classical physics).

Model : Particle in a two dimensional box



~~$\psi(x, y)$~~

Schrodinger equation for 2D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) = E \longrightarrow (A)$$

Inside the box $U(x,y) = 0$

$U(x,y) = \infty$, for $x \leq 0$, $x \geq L_x$
$y \leq 0$, $y \geq L_y$
[outside the box]

$U(x,y) = 0$ for $0 < x < L$
$0 < y < L$
[inside the box]

$$\psi_{n_1, n_2}(x,y) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_1 \pi x}{L_x}\right) \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_2 \pi y}{L_y}\right)$$

is the general solution

$$\Rightarrow \psi_{n_1, n_2} = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{n_1 \pi x}{L_x}\right) \sin\left(\frac{n_2 \pi y}{L_y}\right)$$

(where $n_1, n_2 = 1, 2, 3, \ldots$).

$$E_{n_1, n_2} = \frac{n_1^2 h^2}{8 m L_x^2} + \frac{n_2^2 h^2}{8 m L_y^2}$$

If $L_x = L_y = L$

$$\Rightarrow E_{n_1, n_2} = \frac{(n_1^2 + n_2^2) h^2}{8 m L^2}$$

ground state :

$\Rightarrow n_1 = 1, \; n_2 = 1$

~~$\Rightarrow E_{n_1, n_2}$~~

$$\Rightarrow E_{11} = \frac{h^2}{4 m L^2}$$

In first excited state,

$n_1 = 1, \; n_2 = 2 \longrightarrow$ a

$$\Rightarrow E_{1,2} = \frac{5 h^2}{8 m L^2}$$

$n_1 = 2, \; n_2 = 1 \Rightarrow E_{1,2} = \frac{5 h^2}{8 m L^2} \longrightarrow$ b

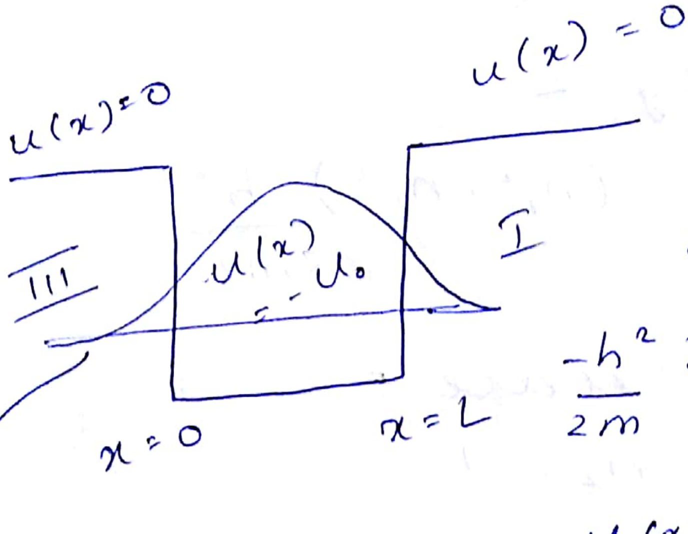
This is a degenerate state, since both ~~ca~~ are first excited states (a and b)

They are distinct states since wave function and probability will differ.

Probability density

$$= \int_{y=0}^{L_y} \int_{x=0}^{L_x} \psi^*(x,y)\, \psi(x,y)\, dx\, dy$$

$$= 1$$



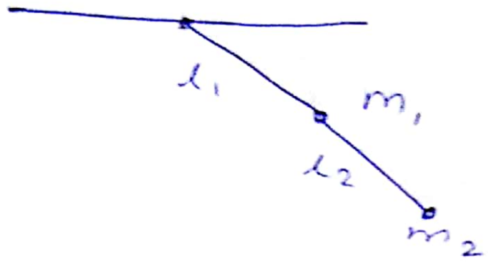
Quantum Tunnelling

$E << U_0$

$$\frac{-h^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\,\psi(x) = E\,\psi(x)$$

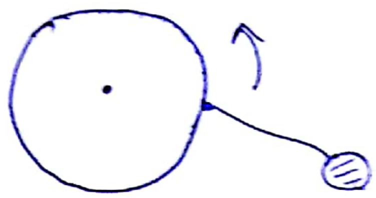
Classical mechanics

→ A coplanar pendulum



(Mechanics by Landau
→ four solved problems)

→ sliding pendulum
→ circular pendulum



(some frequency given)

Quantum

Expectation value

$$\text{Probability} = \int_{x_1}^{x_2} \psi_n^*(x)\, \psi_n(h)\, dx$$

mean or expectation $\Big\}$ $\hat{A} \Rightarrow \langle A \rangle$

$$= \int_0^L \psi^*(x)\, \hat{A}\, \psi(x)\, dx$$

$$\Rightarrow \langle x \rangle = \int_0^L x\, \psi^*(x)\, \psi(x) \cdot dx$$

$\langle x^2 \rangle$; $\langle P \rangle$; $\langle P^2 \rangle$

Error / uncertainty in x

$= \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$

$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2$