SCIENCE - 1

1. Random walk
2. diffusion
3. Langevin dynamics (microscopic)

⋮

Quantum Mechanics

End of 19th century

1895: the discovery of x-ray
1896: the discovery of radioactivity
1897: the discovery of electrons

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

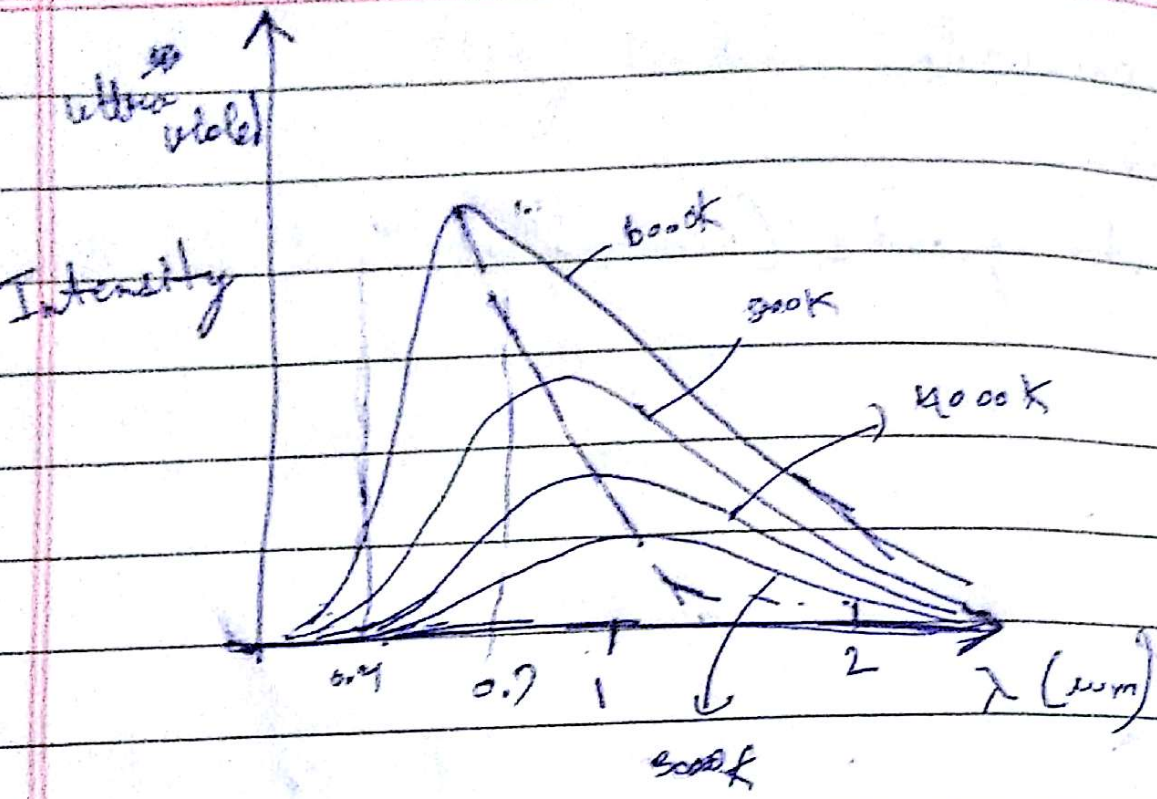
existence of bodies smaller than atom

↓

understand the internal structure of atom

Black body Radiation

Theoretical notion : black body ⇒ Absorbs 100% radiation
⇒ emits the maximum amount of energy possible at a given temp.



→ Black body radiation curve changes with temp.

→ At a given temp. a black body radiates energy at all wavelength

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

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

→ Double slit experiment
→ Photoelectric effect
→ Atomic spectra
→ stern – Gerlach experiment (Response of atoms to magnetic field)
→ Heat capacity of solids
→ Scattering of X-rays by solids (Compton effect)
→ Diffraction of electrons by Crystals.

$\Psi \Rightarrow$ wave func^n
↳ defines a state of a quantum system

for one dimension ← $\Psi(x,t)$ ⇒ all physical properties of the system can be expressed as operators

its an operator ⇐ $\hat{P}_x = -i\hbar \frac{\partial}{\partial x}$, $\hbar = \frac{h}{2\pi}$ → planks constant , $i = \sqrt{-1}$

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

$\hat{H} \equiv i\hbar \frac{\partial}{\partial t}$; $\hat{H}\Psi(x,t) = E\,\Psi(x,t)$
energy

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

$$= \underbrace{\frac{\hat{p}_x(\hat{p}_x)}{2m}}_{\hat{K}} + \hat{U}(x)$$

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

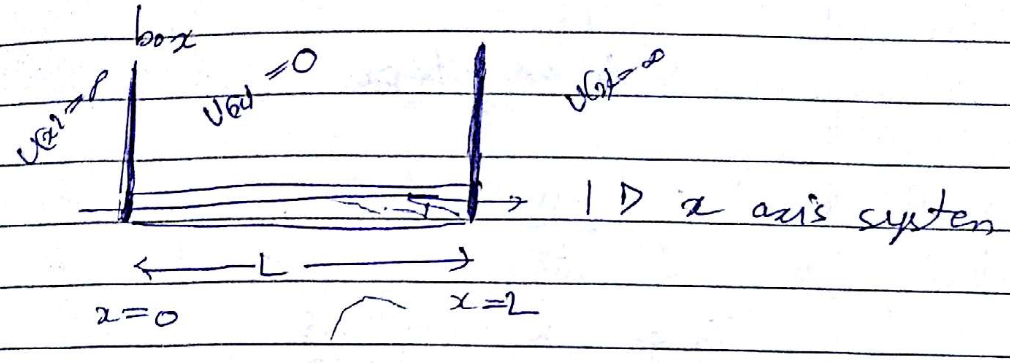
$$\hat{H}\Psi(x,t) = E\,\cancel{\ell}\,\Psi(x,t)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + \hat{U}(x)\,\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$$\boxed{\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + \hat{U}(x)\,\Psi(x,t) = E\,\Psi(x,t)}$$

↳ Schrodinger eqn.

model: ~~Electron~~ Particle in a ~~3D~~ one ~~3D~~ dimensional box



$U(x) = \infty$ at $x = 0$

$U(x) = \infty$ at $x = L$

$U(x) = 0$ for $x < 0 < L$

Inside the wire

$$-\frac{h^2}{2m}\frac{\partial^2 \psi_x}{\partial x^2} + \cancel{U_x \psi(x)} = E\psi(x)$$

$$\frac{\partial^2 \psi}{\partial x^2} + K^2\psi = 0$$

General sol^n

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

here A & B are arbitrary constants

boundary cond^n at

$x = 0$ -

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

$$A = 0$$

$x = L$

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

$$B\sin kL = 0$$

Scanned by CamScanner

$$KL = n\pi$$

n is an Integer

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

Since $K = \sqrt{\frac{2mE}{\hbar^2}}$

$$\cancel{E = \frac{n^2 h^2}{\quad}}$$

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

Energy is quantized

fundamental unit of energy.

Inside the wire

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

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

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

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

complex conjugate Ψ^*

$\Psi^*(x)\,\Psi(x)\,dx \Rightarrow$ Prob. of finding the sys b/w x & $x + dx$

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

$$\int_0^L \Psi^*(x)\,\Psi(x)\,dx = 1$$

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

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

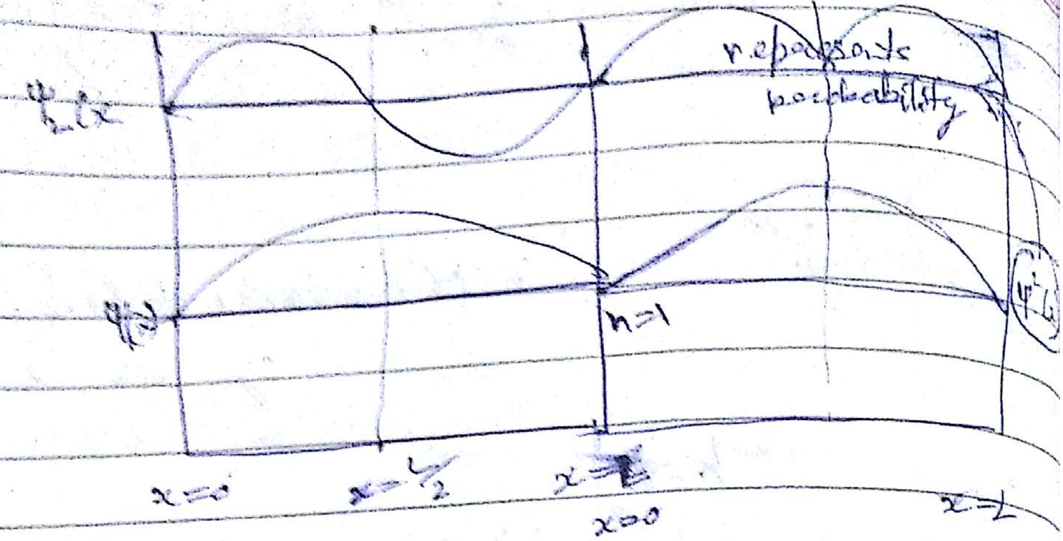
$$\Psi_n(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right)$$

quantum numbers

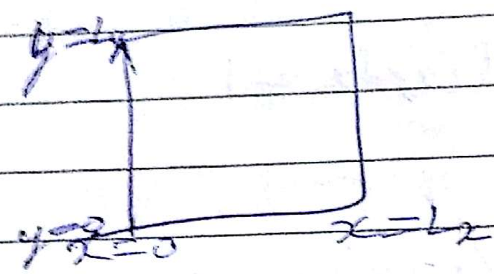
$$\Psi_1(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{\pi x}{L}\right)$$ ground state

$$\Psi_2(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{2\pi x}{L}\right)$$ 1st excited state

$$\Psi_3(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{3\pi x}{L}\right)$$ 2nd excited state



Particle in a 2D box



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

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

$$U(x,y) = \infty$$

$$x \leq 0 \qquad x \geq L$$

$$y \leq 0 \qquad y \geq L$$

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

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

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

If $L_x = L_y = L$

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

$n_1 = 1 \; n_2 = 1$; $E_{1,1} = \frac{h^2}{4 m L^2}$

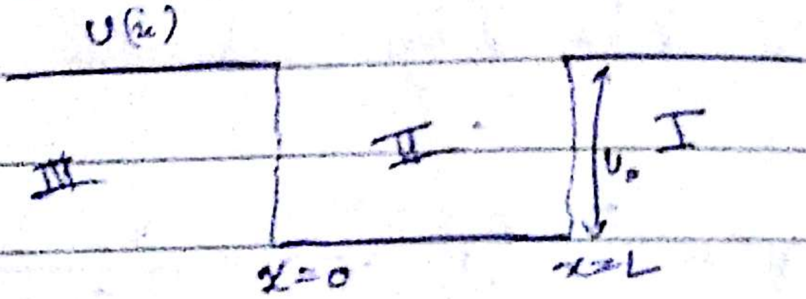
$n_1 = 1 \; n_2 = 2$; $E_{1,2} = \frac{5 h^2}{8 m L^2}$

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

ground state $E_{1,1}$

First excited stat $\underbrace{E_{2,1} \; E_{1,2}}_{\text{degenerate state}}$

Model with 3 wire

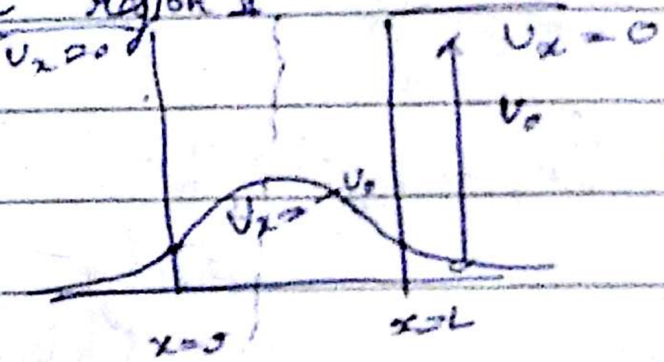


$U_0 \Rightarrow$ barrier height

(energy to get out of w

For region II

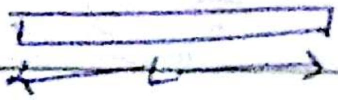
quantum tunnelling

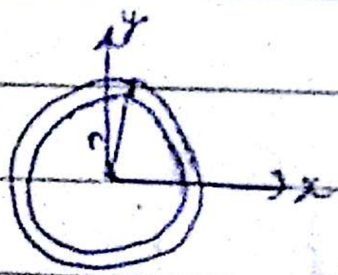


Assuming $E << U_0$

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

wire with no ends

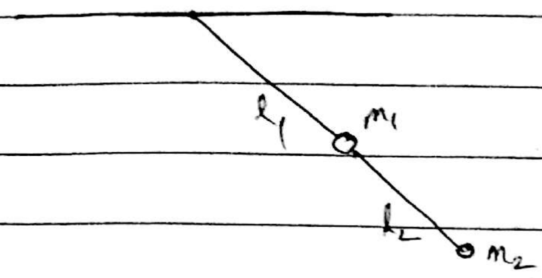




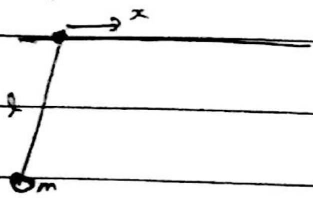
$2\pi r = L$

Classical Mechanics

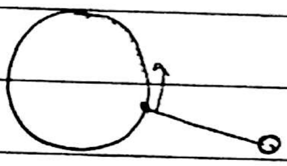
→ A coplanar pendulum



→ sliding pendulum



→ Circular pendulum



Quantum mechanic

- particle in a box problem ~~&~~ calculate prob

Expectation value (or) mean value =

~~Prob~~ $\underbrace{\hat{A}}_{\text{'A' parameters}} = \langle A \rangle = \int_0^L \psi^*(x)\,\hat{A}\,\psi(x)\,dx$

'A' parameters operator $\langle x \rangle = \int_0^L \psi^2(x)\, x\, \psi(x)\,dx$; $\langle x^2 \rangle$; $\langle p \rangle$; $\langle p^2 \rangle$

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