

## Lec 19

Wave  
Function

$\psi(x, t) \Rightarrow$  1D ; single particle

$\psi(x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_N, y_N, z_N, t)$

$\hookrightarrow$  N particle system

$\rightarrow$  All physical observables can be expressed as operators.  
Ex: linear momentum  $\left\{ \hat{p}_x = -i \hbar \frac{\partial}{\partial x} \right.$

$$i = \sqrt{-1}$$

$$\hbar = \frac{h}{2\pi} \rightarrow \text{Planck's constant} \quad 6.62 \times 10^{-34} \text{ Js}$$

$$\text{Kinetic Energy } \hat{K} = \frac{\hat{p} \cdot \hat{p}}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\hat{p}_x \psi(x, t) = -i \hbar \frac{\partial}{\partial x} \psi(x, t)$$

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

$\rightarrow$  scalar measure of linear momentum

• Schrodinger equation:

$$\hat{H} = \hat{K} + \hat{U} \text{ - Hamiltonian}$$

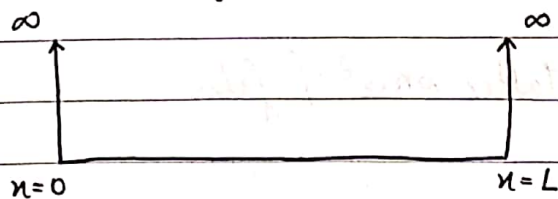
$$\hat{H} \psi(x, t) = E \psi(x, t) \rightarrow \text{scalar (total energy)}$$

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

• time independent schrodinger  
 $\downarrow$

At a given  $t$ , how  $\psi$  varies with  $x$ .

Particle confined in a one-dimensional box.



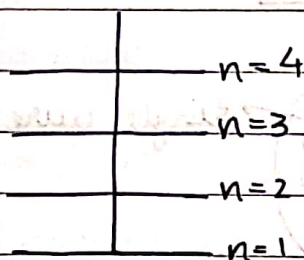
$$U(x) = 0, \quad 0 < x < L$$

$$U(x) = \infty \quad \text{if } x=0 \text{ or } x=L$$

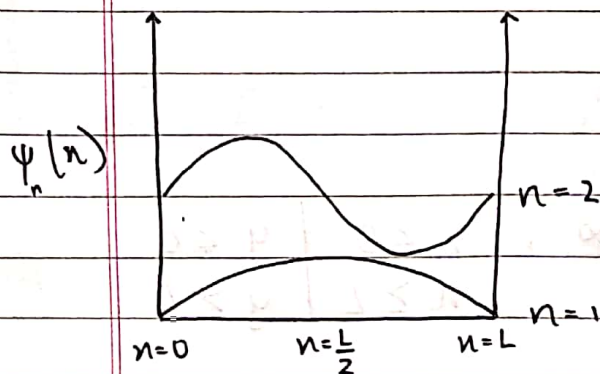
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$$

$$\psi_n^*(x) \psi(x) \Rightarrow \text{Probability Density}$$

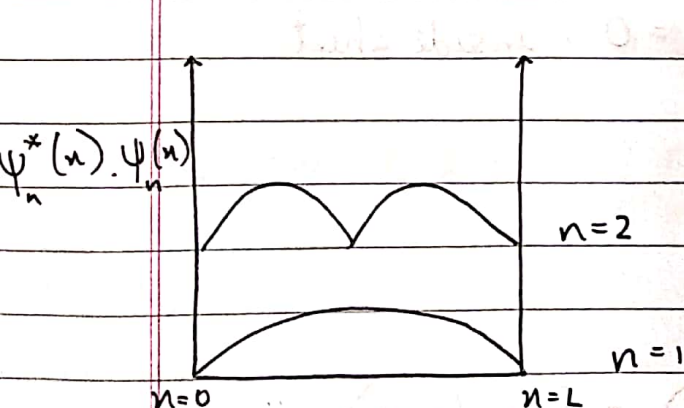
$$E_n = n^2 \frac{h^2}{8mL^2}$$



ground state.



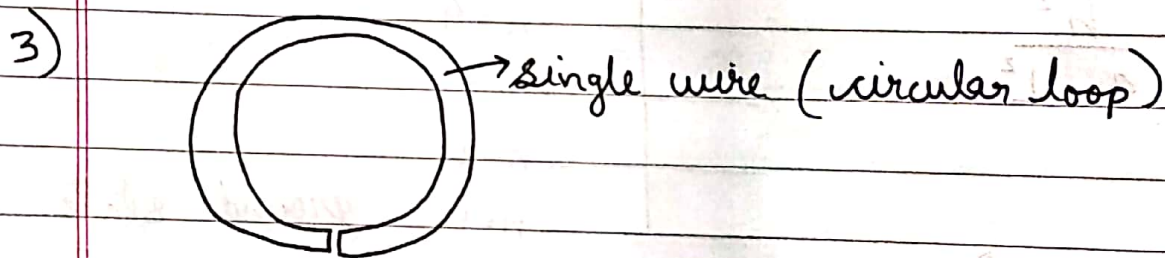
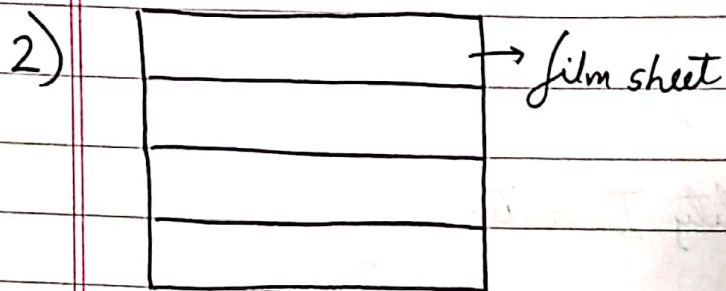
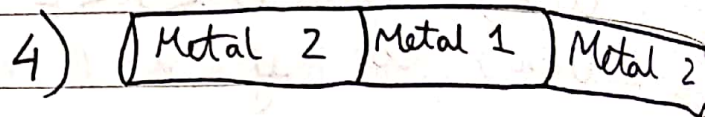
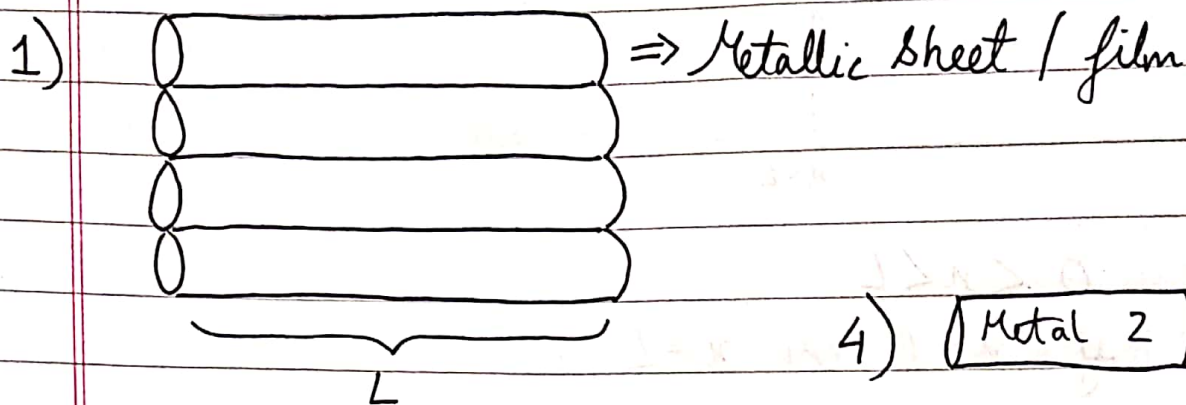
$\psi$  varies with  $x$



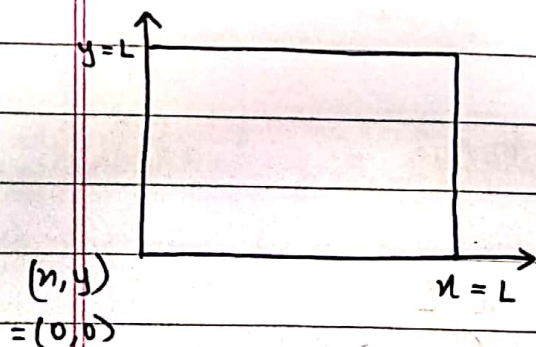
$$\begin{aligned} \langle x \rangle &= \int_{x=0}^{x=L} x P(x) dx \\ &= \int_{x=0}^{x=L} x \psi_n^*(x) \psi_n(x) dx \end{aligned}$$



# # Extension of 1D Model



• Particle in a 2D box.



$$U(n,y) = \infty ; \quad \begin{array}{l|l} n \leq 0 & y \leq 0 \\ n \geq L & y \geq L \end{array}$$

$$U(n,y) = 0 ; \text{ inside sheet}$$

Wave Function  $\psi(n,y)$

• Inside the sheet :  $U(n,y) = 0$

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

$$\psi(x, y) = X(x) Y(y)$$

$$\rightarrow Y(y) \cdot \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} X(x) \right) + X(x) \cdot \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} Y(y) \right) = E \cdot X(x) \cdot Y(y)$$

$\hookrightarrow E_1 + E_2$

divide by  $X(x) Y(y)$  on both sides.

$$\frac{1}{X(x)} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} X(x) \right) = E_1$$

$$\frac{1}{Y(y)} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} Y(y) \right) = E_2$$

$$E_1 = \frac{n_1^2 h^2}{8mL^2} ; E_2 = \frac{n_2^2 h^2}{8mL^2}$$

$$E = E_1 + E_2 = (n_1^2 + n_2^2) \frac{h^2}{8mL^2}$$

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

Ground State :  $n_1 = n_2 = 1$  :  $E_{1,1} = \frac{2h^2}{8mL^2}$

1st excited State :  $n_1 = 1, n_2 = 2$  ;  $E_{1,2} = E_{2,1} = \frac{5h^2}{8mL^2}$   
 $n_1 = 2, n_2 = 1$