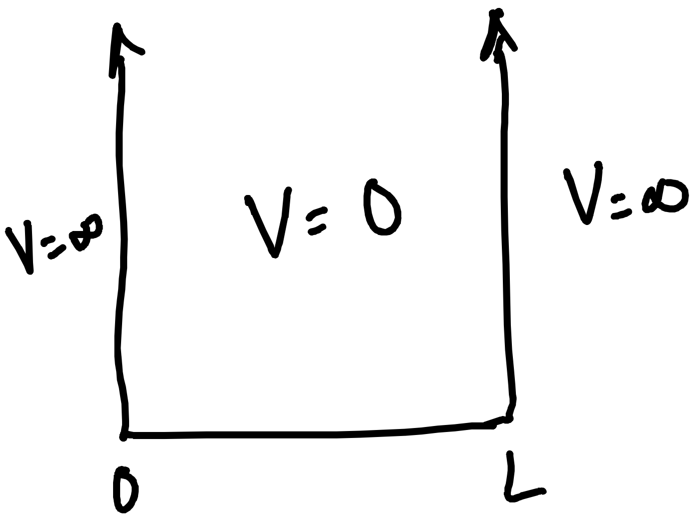
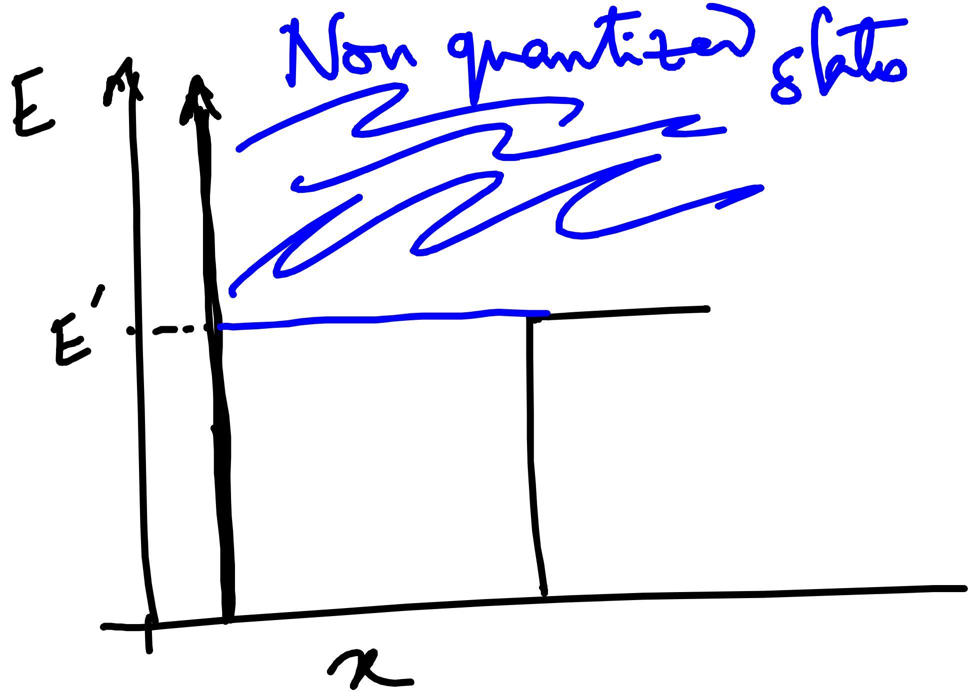
Particle in 2D & 3D box

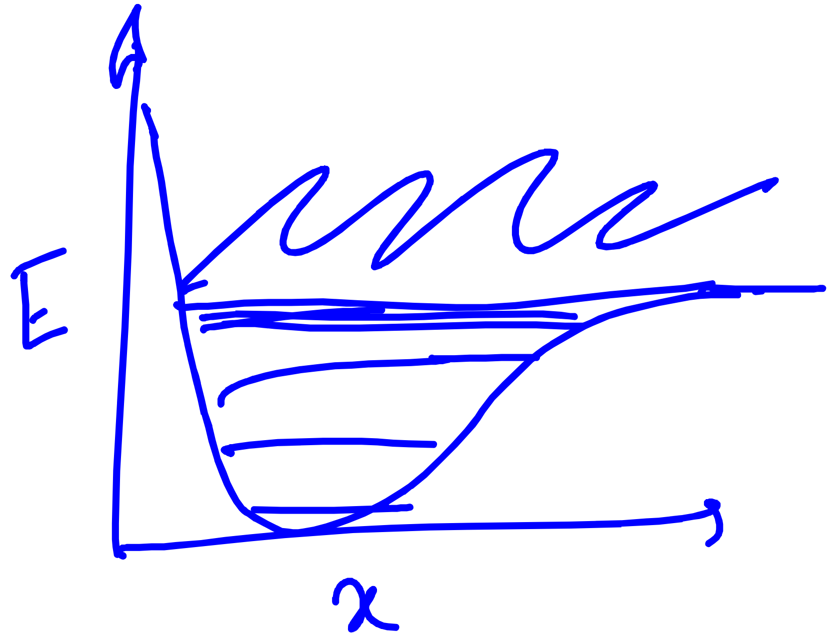
Particle in "1D" box



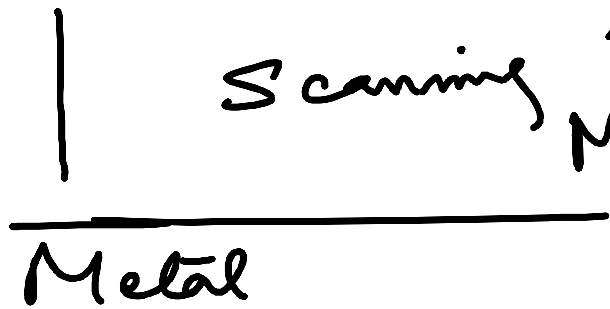
QM Recepie

- Solve Schrödinger Eqn. as follows:
- Define V (system dependent)
- Define boundary Condition
- $\hat{H}$ operator
- Find particular soln.





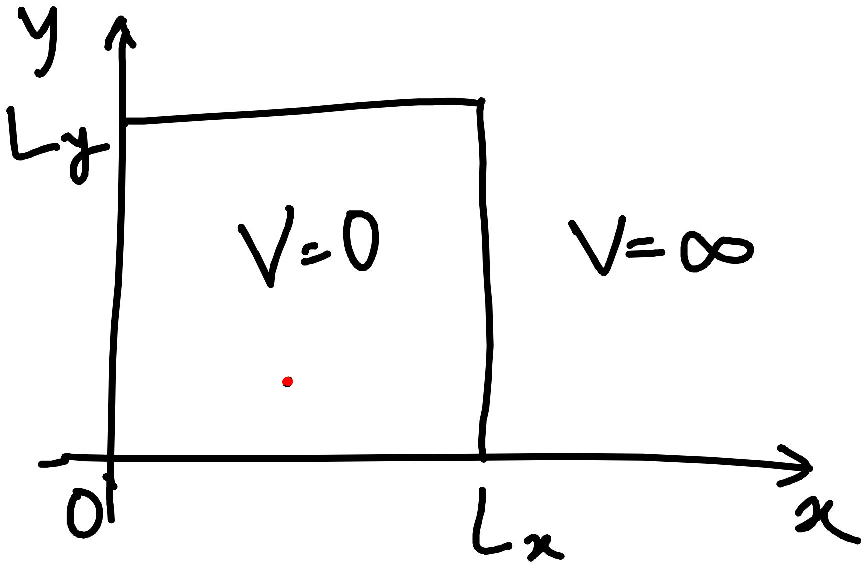
"Tunnelling"



Scanning Tunnelling Microscopy

2D box.

$$V(x,y) = \begin{cases} 0 & \text{if } 0<x<L_x \\ & \text{\& } 0<y<L_y \\ \infty & \end{cases}$$



$$\Psi \equiv \Psi(x,y)$$

$V(x,y)$

Hamiltonian $\quad \hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}} + \cancel{V} \to 0$

$$\hat{H}\Psi(x,y) = E\Psi(x,y)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = E\Psi(x,y)$$

Boundary condn's

for all $y \rightarrow \Psi(0,y) = \Psi(L_x, y) = 0$

for all $x \rightarrow \Psi(x,0) = \Psi(x, L_y) = 0$

Seperation of variables $\Psi(x,y) = X(x)\cdot Y(y)$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{d^2X}{dx^2}}_{E_x}\underbrace{-\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{d^2Y}{dy^2}}_{E_y}=E$$

$$E_x + E_y = E$$

$$-\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{d^2X}{dx^2} = E_x \quad \& \quad -\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{d^2Y}{dy^2} = E_y$$

$$X(0) = X(L_x) = 0 \qquad Y(0) = Y(L_y) = 0$$

$$X(x) = A_x \sin \frac{n_x \pi x}{L_x} \quad , \quad n_x = 1, 2, 3 \ldots$$

$$Y(y) = A_y \sin \frac{n_y \pi y}{L_y} \quad , \quad n_y = 1, 2, 3, \ldots$$

$$E_x = \frac{n_x^2 h^2}{8 m L_x^2} \quad \& \quad E_y = \frac{n_y^2 h^2}{8 m L_y^2}$$

$$E = E_x + E_y$$

$$= \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) \frac{h^2}{8m} \quad , \quad n_x = 1, 2, 3 \ldots \quad n_y = 1, 2, 3 \ldots$$

$$\psi(x,y) = \underbrace{A_x A_y}_{A} \cdot \sin\frac{n_x \pi x}{L_x} \cdot \sin\frac{n_y \pi y}{L_y}$$

$$\int_0^{L_x}\int_0^{L_y} dx\, dy\, A^2 \sin^2\frac{n_x \pi x}{L_x} \cdot \sin^2\frac{n_y \pi y}{L_y} = 1$$

$$A = \sqrt{\frac{2}{L_x}}\sqrt{\frac{2}{L_y}}$$

$$\psi(x,y) = \sqrt{\frac{2}{L_x}} \sin\frac{n_x \pi x}{L_x} \cdot \sqrt{\frac{2}{L_y}} \sin\frac{n_y \pi y}{L_y}$$

$$P\left(x \in (a_1, a_2),\ y \in (b_1, b_2)\right) = \frac{2}{L_x}\frac{2}{L_y}\int_{a_1}^{a_2} dx \cdot \sin^2 \frac{n_x \pi x}{L_x} \cdot \int_{b_1}^{b_2} dy\ \sin^2 \frac{n_y \pi y}{L_y}$$

$E_{11} \longrightarrow$ Lowest energy (Ground state)

$\underbrace{\qquad\qquad}$

$(n_x, n_y) \longrightarrow$ wave f^n or state of the system

square box

$$\underline{L_x = L_y = L}$$

Ψ_{12} & Ψ_{21}

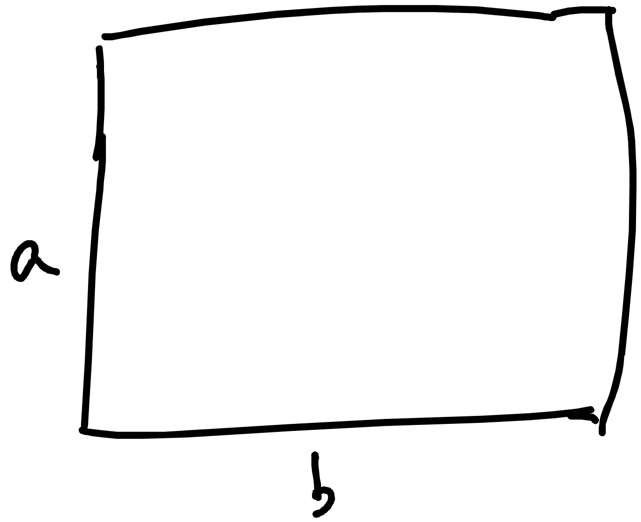
$$E_{12} = E_{21} = \frac{5h^2}{8mL^2}$$

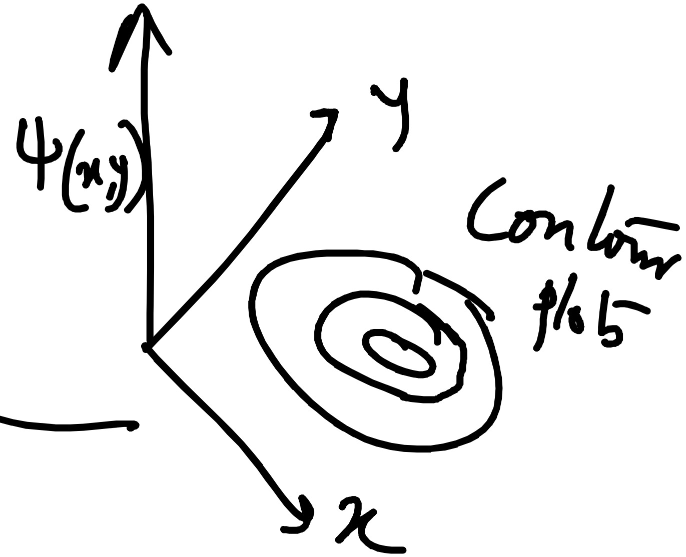
"Degenerate States" $\longleftrightarrow$ "non-degenerate"

$$\downarrow$$

$$E \longleftrightarrow \Psi$$

$$\left.\begin{matrix}\Psi\\ \vdots\end{matrix}\right\} E$$

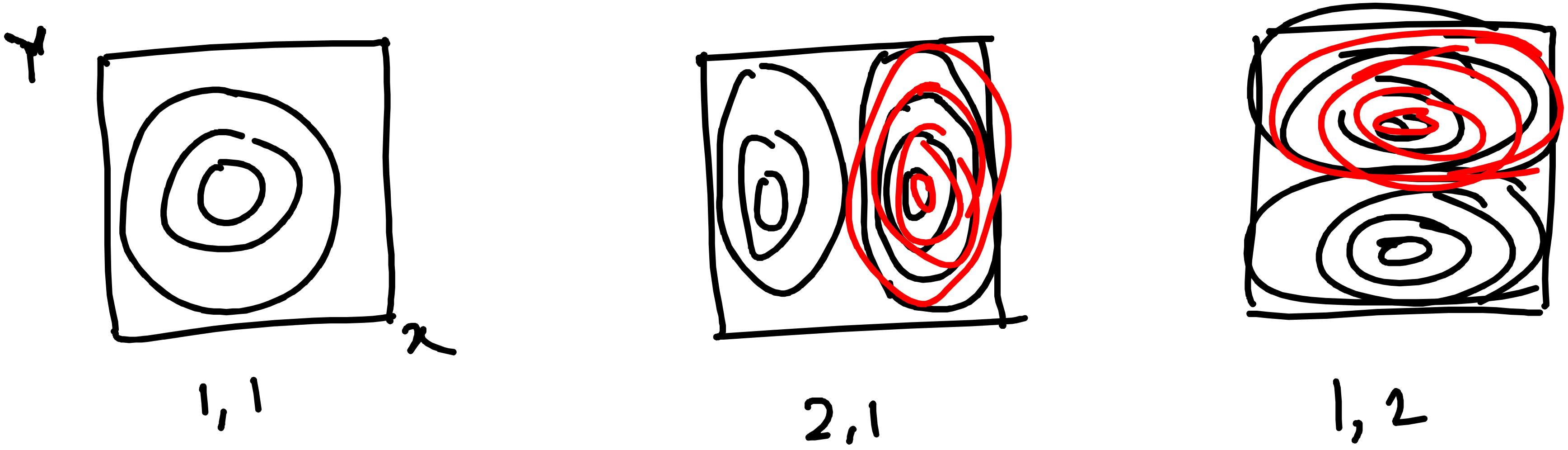




Lifting

$$E_{12} = E_{21}$$

$$a = b$$



3D box

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}$$

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

$$= -\frac{\hbar^2}{2m}\nabla^2$$

∇^2

Laplace operator

Laplacian.