→ Schrodinger's wave equation

Total energy = Potential + Kinetic

$$\hat{H}\psi = \hat{V}\psi + \hat{E}\psi \qquad \frac{p^2}{2m} \rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi$$

$$E\psi = V(x,y,z)\psi - \frac{\hbar^2}{2m}\nabla^2\psi$$

→ Particle moving in 1D

Side track → ψ the solution of a differential eqⁿ

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

$$\frac{\partial\psi}{\partial x} = k(A\cos(kx) - B\sin(kx))$$

$$\frac{\partial^2\psi}{\partial x^2} = k^2(-A\sin(kx) - B\cos(kx))$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$$

① Free Particle : $V(x) = 0$

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

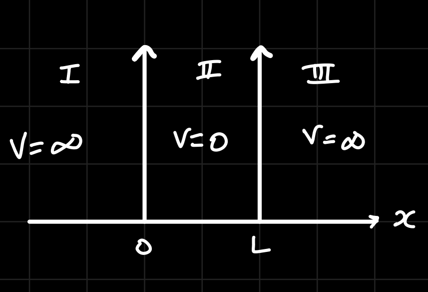
$$E = \frac{\hbar^2 k^2}{2m} \quad \text{—— ①}$$

Total energy depends on wavenumber

POTENTIAL WELL

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

Schrodinger's time independent equation



Boundary conditions →

R → I and III : $\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \infty\psi = E\psi$

V=∞ (particle cannot be present) → $|\psi|^2 = 0$ → ψ must be zero in Regions I and III

R → II : $\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + 0 = E\psi$

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

BOUNDARY CONDITIONS →

let $\psi = A\sin(kx) + B\cos(kx)$

at $x = 0$ → $\psi = 0 + B$
and since $\psi = 0$, the constant $B = 0 \ \forall x$

now we have $\psi = A\sin(kx)$

at $x = L$ → $\psi = A\sin(kL)$
we know, $\psi = 0$ for $x = L$
but $A \neq 0$ because $\psi \neq 0 \ \forall x$

$$\sin(kL) = 0$$
$$kL = n\pi \qquad (n \geq 1)$$
$$k = \frac{n\pi}{L}$$

from ①, we know $k \propto E$

So, we can conclude that energy is discrete / quantized

And,

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

using probability density formula,

$$\int_{-\infty}^{\infty} |\psi^2|\, dx = 1$$

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

$$\left\{\begin{aligned} \sin^2(x) &= 1 - \cos^2(x) \\ \cos(A+B) &= \cos A\cos B - \sin A\sin B \\ \cos(2A) &= \cos^2 A - \sin^2 A \\ \cos(2A) &= 2\cos^2 A - 1 \\ \cos^2(A) &= \frac{\cos(2A)+1}{2} \end{aligned}\right\}$$

$$\frac{A^2}{2}\int_0^L \left(\cos\left(\frac{2n\pi x}{L}\right) + 1\right) dx = 1$$

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

$$\sin(2n\pi)\cdot\frac{2n\pi}{L} + L - 0 - 0 = \frac{2}{A^2}$$

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

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

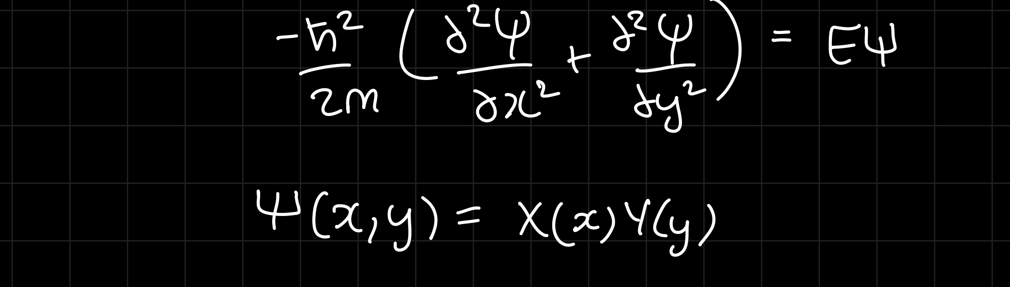
allowed energies → $E_n = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$

$E \neq 0$ ever
that would mean $\psi = 0 \ \forall x$
(not allowed)

and E_{min} = ZPE lowest energy of the particle

$$E_n \propto \frac{n^2}{L^2}$$

$n \equiv$ number of times curve cuts x-axis



Particle in a 2d box

center region →

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

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

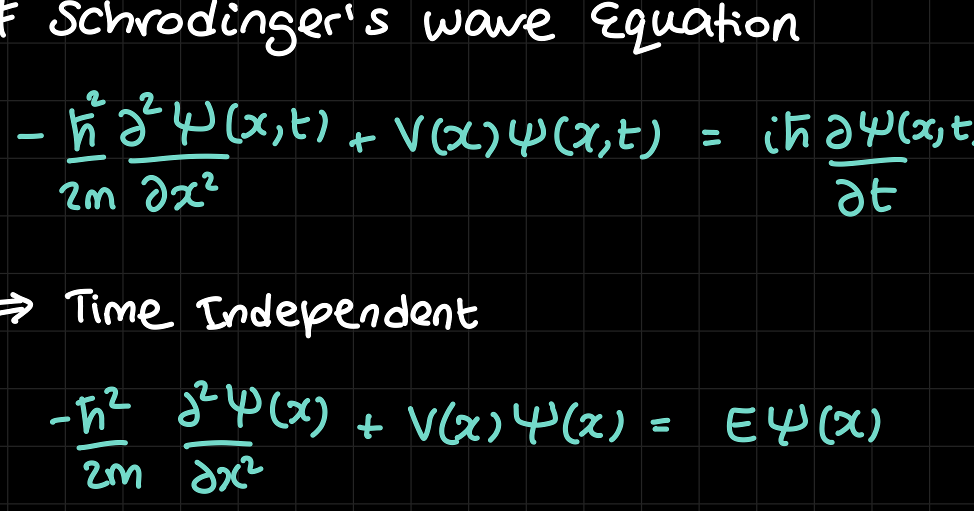
$$\frac{-\hbar^2}{2m}\frac{\partial^2 X}{\partial^2 x} = E_x X, \qquad \frac{-\hbar^2}{2m}\frac{\partial^2 Y}{\partial^2 y} = E_y Y$$

$$X = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n_x\pi x}{L_x}\right), \qquad Y = \sqrt{\frac{2}{L_y}}\sin\left(\frac{n_y\pi y}{L_y}\right)$$

$$\psi = \sqrt{\frac{4}{L_y L_x}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)$$

$$E = \frac{h^2}{8m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right]$$

Quantum Tunelling


The external potential term in the Schrodinger equation:

$$V(x) = \begin{cases} 0, x \leq 0 \\ V, x \in (0,L) \\ 0, x \geq L \end{cases}$$

Region I: the potential $V = 0$; hence Schrodinger's equation reduces to that of a free particle. Therefore, the its wave function

$$\Psi_I = \Psi_{I,i} + \Psi_{I,r} = Ae^{ikx} + Be^{-ikx} \qquad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Region II: finite potential barrier V

$$\frac{\hbar^2}{2m}\frac{\partial^2\Psi_{II}}{\partial x^2} = (V - E)\Psi_{II}$$

Therefore, its wave function is

$$\Psi_{II} = Ce^{-k'x} + De^{k'x} \qquad \text{where} \quad k' = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Region III: the potential $V = 0$ and the transmitted particle is moving towards the right and has a positive momentum

$$\Psi_{III} = Fe^{ikx}$$

Transmission coefficient $T = \frac{(\Psi^*\Psi)_{transmitted}}{(\Psi^*\Psi)_{incident}} = \frac{|F|^2}{|A|^2}$

Tunneling probability:

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V^2\sinh^2(k'L)}{4E(V-E)}}$$

Schrodinger's wave Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

⇒ Time Independent

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

⇒ Time dependent

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

* BORN'S Interpretation (CRITERIAS)

NOPE

(a) ψ must be continuous (no breaks)

(b) $\nabla\psi = \frac{\partial\psi}{\partial x}$ must be continuous (no kinks)
gradient of Psi — we will have a divergence if gradient is discontinuous — same for (a) — and so it will → ∞ ↳ violates (d)

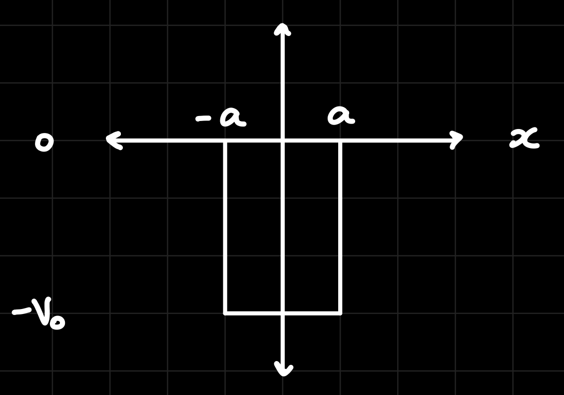
(c) ψ must have a single value at any pt. in space

(d) ψ must be finite everywhere

(e) ψ cannot be zero everywhere

2024: Quiz-1

Q1)



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

at $x = |a|$: $V(x) = 0$

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

$$\frac{\partial^2\psi}{\partial x^2} - \left(\frac{2m}{\hbar^2}.E\right)\psi = 0$$

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

$$\frac{\partial^2\psi(x)}{\partial x^2} = -k^2\psi$$

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

in the region II :

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - V_0\psi(x) = E\psi(x)$$

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + (V_0+E)\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(V_0+E)\psi = 0$$

let $\psi(x) = Ce^{-kx} + De^{kx}$

for $x < -a \rightarrow \psi \neq \infty$

so, $C = 0$

for $x > a \rightarrow \psi \neq \infty$

so, $D = 0$

$$\text{So, } \psi = \begin{cases} De^{kx} & : x < -a \\ A\sin(k'x) + B\cos(k'x) & : -a < x < a \\ Ce^{-kx} & : x > a \end{cases}$$

at $x = -a \rightarrow$ $\psi(x)$ and $\frac{\partial\psi(x)}{\partial x}$ must be continuous

$$-A\sin(k'a) + B\cos(k'a) = De^{-ka} \quad \text{—(2)}$$
$$+k'A\cos(k'a) + k'B\sin(k'a) = k.De^{ka} \quad \text{—(3)}$$

at $x = a \rightarrow$

$$A\sin(k'a) + B\cos(k'a) = Ce^{-ka} \quad \text{—(4)}$$
$$k'A\cos(k'a) - k'B\sin(k'a) = -kCe^{-ka} \quad \text{—(5)}$$

(2) + (4)

$$2B\cos(k'a) = (C+D)e^{-ka}$$

(2) − (4)

$$2A\sin(k'a) = (C-D)e^{-ka}$$