PHI-101

Schrödinger's Eqn

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

$\psi \rightarrow$ Wave function: contains all the information about particle's properties like position, velocity, momentum, etc

Newton's laws of classical mechanics are special cases of the more general Quantum Mechanics.

Any 1D wave can be defined by: $\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$

General solⁿ: $y = Ae^{i(kx-\omega t)}$

$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} \Rightarrow p = \hbar k$

$\omega = 2\pi\nu$, $E = h\nu = \hbar\omega$

$\boxed{\begin{array}{l} p = \hbar k \\ E = \hbar\omega \end{array}}$ Fundamental Postulates

$y = Ae^{i(px-Et)/\hbar}$

$E = KE + PE = \frac{p^2}{2m} + V(x,t)$

For conservative system, $F = -\frac{dV(x,t)}{dx}$

Ψ should satisfy the form $Ae^{i(px-Et)/\hbar}$

where $E = \frac{p^2}{2m} + V(x,t)$

Ψ should also be linear as suggested by the interference and superposition experiments.

We assume a free particle, so $F = 0$

as $F = -\frac{dV(x,t)}{dx}$ $\rightarrow$ $V(x,t)$: constant

$\hookrightarrow$ p & E are constant

$$\Psi(x,t) = Ae^{i(px-Et)\hbar}$$

$$\frac{\partial \Psi}{\partial x} = \frac{Aip}{\hbar} e^{i/\hbar(px-Et)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = A\left(\frac{ip}{\hbar}\right)^2 e^{i/\hbar(px-Et)} = \frac{-p^2}{\hbar^2}\Psi$$

$$p^2\Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \quad -1$$

$$\frac{\partial \Psi}{\partial t} = A\left(\frac{-iE}{\hbar}\right) e^{\frac{i}{\hbar}(px-Et)}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\frac{E^2}{\hbar^2}\Psi \Rightarrow E\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

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$$E = \frac{p^2}{2m} + V(x,t)$$

$$\Rightarrow E\Psi = \frac{p^2\Psi}{2m} + V(x,t)\Psi$$

$$\Rightarrow \underbrace{i\hbar \frac{\partial \Psi}{\partial t}}_{\text{Total Energy}} = \underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}}_{KE} + \underbrace{V(x,t)\Psi}_{PE}$$

For time independent schrödinger's eqn:

$V(x,t) = V(x)$

$\Psi(x,t) = \psi(x)\phi(t) \rightarrow$ seperation of variables

$$\Rightarrow \frac{1}{\psi(x)}\left[\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right] = \frac{1}{\phi(t)} i\hbar \frac{d\phi(t)}{dt} = \text{const}$$

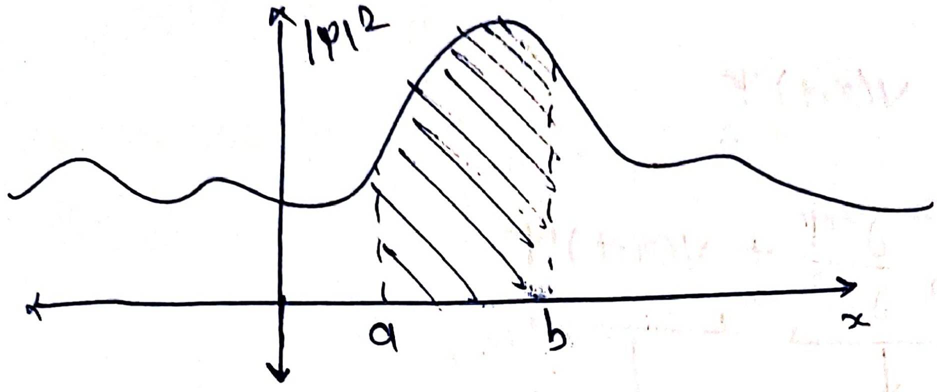
$$i\hbar \frac{d\phi(t)}{dt} = c\phi(t) \Rightarrow i\hbar \int \frac{d\phi(t)}{\phi(t)} = \frac{1}{c}\int dt$$

$$\Rightarrow \phi(t) = e^{-ict/\hbar}$$

By planck einstein, we know $E = \hbar\omega$ where ω is the angular frequency in time,

so $c = E \Rightarrow \phi(t) = e^{-iEt/\hbar}$

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



$$P_{ab} = \int_a^b \psi^*\psi \, dx$$ $\Rightarrow$ Probability of finding the particle in $a \le x \le b$

ψ should be continuos, differentiable and also square integrable.

$\psi \rightarrow N\psi$ ↳ Normalised wavefunction

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

$$\langle x \rangle = \frac{\int \psi^* x \psi \, dx}{\int \psi^* \psi \, dx}$$

For a normalised wavefunction : $\int \psi^* \psi \, dx = 1$

$$\langle x \rangle = \int \psi^* x \psi \, dx$$

$$\langle v \rangle = \frac{d\langle x \rangle}{dt} = \int x \frac{d}{dt}(\psi^*\psi) \, dx$$

$$= \int x \left(\psi^* \frac{d\psi}{dt} + \psi \frac{d\psi^*}{dt} \right) dx$$

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

$E = \hbar\omega \Rightarrow \omega = E/\hbar$

$p = \hbar k \Rightarrow k = p/\hbar$

$$\Psi(x,t) = Ae^{i(px-Et)/\hbar}$$

$$\frac{d\Psi}{dx} = A\left(\frac{ip}{\hbar}\right)e^{i(px-Et)/\hbar} = \frac{ip}{\hbar}\Psi$$

$$\Rightarrow p\Psi = -i\hbar\frac{d\Psi}{dx} \Rightarrow \boxed{\hat{p} = -i\hbar\frac{d}{dx}}$$

$$\frac{d\Psi}{dt} = A\left(\frac{-iE}{\hbar}\right)e^{i(px-Et)/\hbar} = -\frac{iE}{\hbar}\Psi$$

$$\Rightarrow E\Psi = i\hbar\frac{d\Psi}{dt} \Rightarrow \boxed{\hat{E} = i\hbar\frac{d}{dt}}$$

$TE = KE + PE$

$$\hat{E}\Psi = \frac{\hat{p}^2\Psi}{2m} + V(x,t)\Psi$$

$$i\hbar\frac{d\Psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x,t)\Psi$$ → Schrödinger's Eqn (TDSE)

$$i\hbar\frac{d\phi}{dt}.\psi = \frac{-\hbar^2}{2m}\phi\frac{d^2\psi}{dx^2} + V(x,t)\phi\psi$$

$$\Rightarrow \frac{i\hbar}{\phi}\frac{d\phi}{dt} = \frac{-\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x,t) = c$$

$$\frac{i\hbar}{\phi}\frac{d\phi}{dt} = c \Rightarrow i\hbar\int\frac{d\phi}{\phi} = c\int dt$$

$$\Rightarrow i\hbar \ln\phi = ct$$

$$\Rightarrow \phi = e^{\frac{-ict}{\hbar}} = e^{-iEt/\hbar}$$

$$\Psi(x,t) = Ae^{i(px-Et)/\hbar}$$

$$= \underbrace{Ae^{ipx/\hbar}}_{\psi(x)} \cdot \underbrace{e^{-iEt/\hbar}}_{\phi(t)}$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}\frac{1}{\psi} + V(x,t) = c$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x,t)\psi = E\psi$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + [V(x,t)-E]\psi = 0 \rightarrow \text{TISE}$$

$$\boxed{\langle\hat{O}\rangle = \int\psi^*\hat{O}\psi\, dx}$$

Ehrenfest Theorem : $\frac{d}{dt}\langle p\rangle = \langle -\frac{dV}{dx}\rangle = \langle F(x)\rangle$

$$F(x) = F(\langle x \rangle) \mp (x - \langle x \rangle) F'(\langle x \rangle) + \frac{1}{2}(x - \langle x \rangle)^2 F''(\langle x \rangle)$$

$$\langle F(x) \rangle = F(\langle x \rangle) - \langle x - \langle x \rangle \rangle F'(\langle x \rangle) + \frac{1}{2} \langle (x - \langle x \rangle)^2 \rangle F''(\langle x \rangle)$$

$\downarrow$

$F(\langle x \rangle)$ is a const

so $\langle F(\langle x \rangle) \rangle = F(\langle x \rangle)$

$$\langle x - \langle x \rangle \rangle = \int \psi^* (x - \langle x \rangle) \psi \, dx$$

$$= \int \psi^* x \psi \, dx - \langle x \rangle \int \psi^* \psi \, dx = 0$$

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

$$\langle F(x) \rangle = F(\langle x \rangle) + \frac{1}{2} \sigma_x^2 F''(\langle x \rangle)$$

For harmonic oscillators, $F(x) \propto x$

$F''(x) = 0$

So, $\langle F(x) \rangle = F(\langle x \rangle)$

$$F(\langle x \rangle) = -\frac{dV(\langle x \rangle)}{d\langle x \rangle}$$

$$\boxed{\vec{J} = \frac{i\hbar}{2m}\left(\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx}\right)}$$

$$\hat{E}\Psi = \frac{\hat{p}^2}{2m}\Psi + V(x,t)\Psi$$

$$i\hbar \frac{d\Psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x,t)\Psi \quad -①$$

$$-i\hbar \frac{d\Psi^*}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi^*}{dx^2} + V(x,t)\Psi^* \quad -②$$

$① \times \Psi^* - \Psi \times ②$

$$i\hbar \frac{d\Psi}{dt}\Psi^* + i\hbar \Psi \frac{d\Psi^*}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}\Psi^* + \frac{\hbar^2}{2m}\Psi\frac{d^2\Psi^*}{dx^2}$$

$$i\hbar \frac{d(\Psi^*\Psi)}{dt} = \frac{\hbar^2}{2m}\left[\Psi\frac{d^2\Psi^*}{dx^2} - \Psi^*\frac{d^2\Psi}{dx^2}\right]$$

$$= \frac{\hbar^2}{2m}\frac{d}{dx}\left(\Psi\frac{d\Psi^*}{dx} - \Psi^*\frac{d\Psi}{dx}\right)$$

$$\frac{d(\Psi^*\Psi)}{dt} = \frac{-i\hbar}{2m}\frac{d}{dx}\left(\Psi\frac{d\Psi^*}{dx} - \Psi^*\frac{d\Psi}{dx}\right)$$

$$\frac{d\rho}{dt} = -\nabla\left(\underbrace{\frac{i\hbar}{2m}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)}_{J}\right)$$

$$\boxed{\frac{d\rho}{dt} + \nabla J = 0}$$

$\psi(x,t) \xrightarrow{FT} \phi(p,t)$

$\underbrace{\psi(x,t)}_{\text{Position space}}$ $\quad$ $\underbrace{\phi(p,t)}_{\text{Momentum space}}$

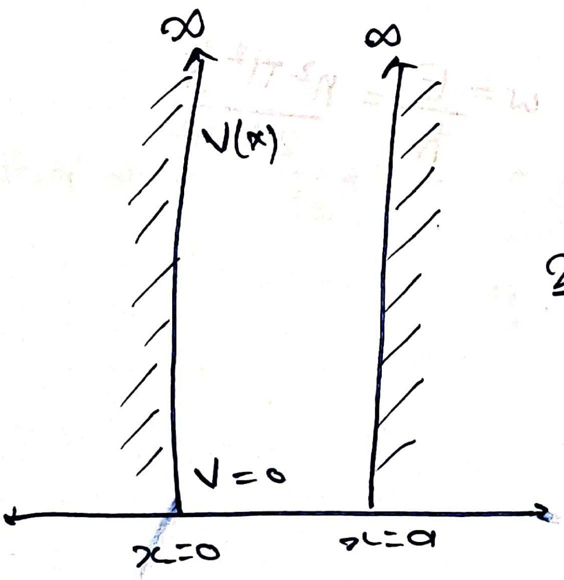
~~$\psi(x,t)$~~

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-\frac{ipx}{\hbar}} dx$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) e^{\frac{ipx}{\hbar}} dp$$

Position space	Momentum space
$\langle x \rangle = \int \psi^* x \psi \, dx$	$\langle p \rangle = \int \phi^* p \phi \, dp$
$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{d}{dx}\right) \psi \, dx$	$\langle x \rangle = \int \phi^* \left(-i\hbar \frac{d}{dp}\right) \psi \, dp$

* Infinite well



$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \cancel{V\psi}^{\,0}$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{2mE}{\hbar^2} = \frac{2m}{\hbar^2} \cdot \frac{p^2}{2m} = \left(\frac{p}{\hbar}\right)^2 = k^2$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \Rightarrow \psi = Ae^{ikx} + Be^{-ikx}$$

or $\psi = A\sin(Kx) + B\cos(Kx)$

$$\psi(0) = \psi(a) = 0$$

$\psi(0) = 0 \Rightarrow B = 0$

$\psi(a) = 0 \Rightarrow A\sin(Ka) = 0 \quad (A \neq 0)$

$$ka = n\pi \Rightarrow k = \frac{n\pi}{a}$$

$$\Rightarrow k^2a^2 = n^2\pi^2$$

$$\Rightarrow \frac{p^2a^2}{\hbar^2} = n^2\pi^2 \Rightarrow \frac{2mE\,a^2}{\hbar^2} = n^2\pi^2$$

$$\Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2} \longrightarrow \text{Discrete Energy levels}$$

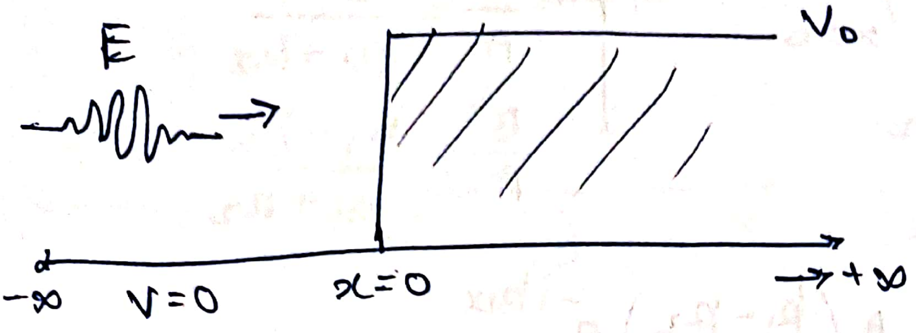
Normalisation: $\displaystyle\int_{-\infty}^{+\infty} \psi^*\psi\,dx = 1$

$$\Rightarrow \int_0^a |A|^2 \sin(Kx)\,dx = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

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

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-i\omega t} \qquad \omega = \frac{E}{\hbar} = \frac{n^2\pi^2\hbar}{2ma^2}$$

* Step Potential ($E > V_0$)



$$\hat{E}\psi = \frac{\hat{p}^2}{2m}\psi + V\psi$$

$$\cancel{i\hbar\frac{d\psi}{dt}} \quad E\psi = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi$$

$$\frac{d^2\psi}{dx^2} + \overbrace{\frac{2mE}{\hbar^2}}^{k_1^2}\psi = 0 \longrightarrow \text{for region I}$$

$$\frac{d^2\psi}{dx^2} + \underbrace{\frac{2m(E-V_0)}{\hbar^2}}_{k_2^2}\psi = 0 \longrightarrow \text{for region II}$$

Region I: $\psi_1(x) = \underbrace{Ae^{ik_1x}}_{\text{Incident}} + \underbrace{Be^{-ik_1x}}_{\text{Reflected}}$

Region II: $\psi_2(x) = \underbrace{Ce^{ik_2x}}_{\text{Transmitted}}$

$$\psi_1(0) = \psi_2(0) \Rightarrow A + B = C$$

$$\left.\frac{d\psi_1}{dx}\right)_{x=0} = \left.\frac{d\psi_2}{dx}\right)_{x=0}$$

$$\Rightarrow Ak_1 - Bk_1 = Ck_2$$

$$\rightarrow \frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

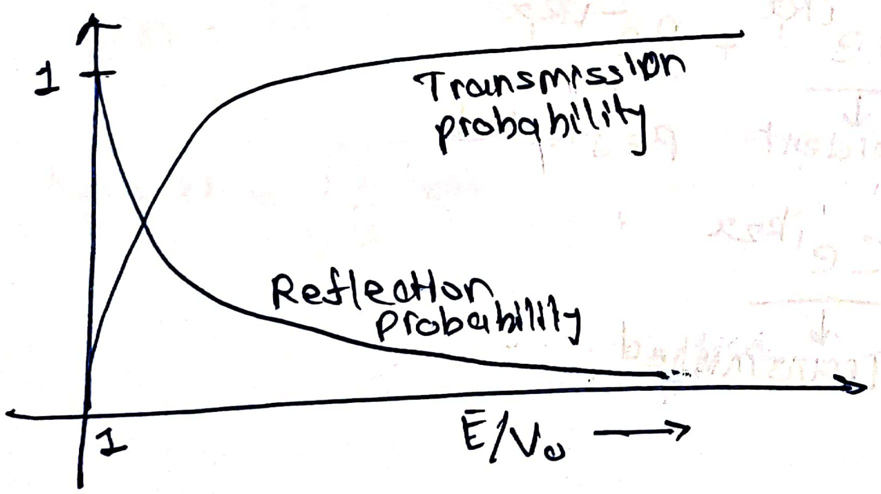
$$\psi_1(x) = Ae^{ik_1 x} + A\left(\frac{k_1 - k_2}{k_1 + k_2}\right)e^{-ik_1 x}$$

$$\psi_2(x) = A\left(\frac{2k_1}{k_1 + k_2}\right)e^{ik_2 x}$$

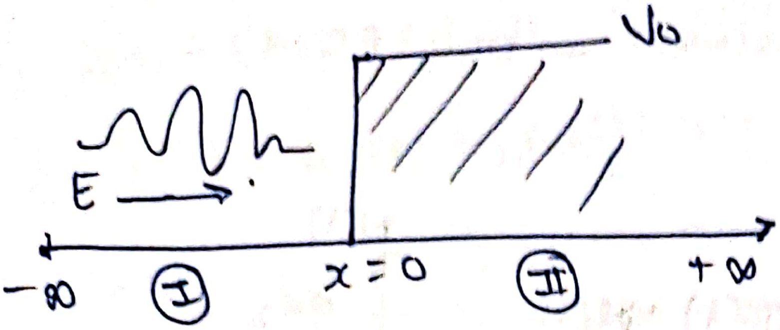
$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$$R = \frac{J_{ref}}{J_{inc}} = \left|\frac{B}{A}\right|^2 = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}$$

$$T = \frac{J_{tran}}{J_{inc}} = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1} = \frac{4\sqrt{E(E - V_0)}}{(\sqrt{E} + \sqrt{E - V_0})^2}$$



* Step Potential ($E < V_0$)



Region I: $$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0 \Rightarrow \psi = \underbrace{Ae^{ik_1x}}_{\text{Incident}} + \underbrace{Be^{-ik_1x}}_{\text{Reflected}}$$

Region II: $$\frac{d^2\psi}{dx^2} - \frac{2m(V_0-E)}{\hbar^2}\psi = 0$$

$$\frac{d^2\psi}{dx^2} - k_2^2\psi = 0 \Rightarrow \psi = \underbrace{Ce^{-k_2x}}_{\text{Transmitted}}$$

$$\psi_1(0) = \psi_2(0) \Rightarrow A + B = C$$

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0} \Rightarrow A - B = \frac{ik_2}{k_1}C$$

$$\frac{C}{A} = \left(\frac{2k_1}{k_1+ik_2}\right) \qquad \frac{B}{A} = \left(\frac{k_1-ik_2}{k_1+ik_2}\right)$$

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1-ik_2}{k_1+ik_2}\right|^2 = 1$$