Shrodinger equation in 3-D coordinates

Spherical polar coordinates

$$\underbrace{H\psi = E\psi}_{} \; ; \; \underbrace{H\psi = i\hbar \frac{\partial \psi}{\partial t}}_{\text{Time dependant shrodinger equation}}$$

hamiltonian & wave function [Kinetic & potential energy]

Total conserved energy

Time dependant shrodinger equation

Time independant shrodinger equation

$$H = \frac{1}{2}mv^2 + V = \boxed{\frac{p^2}{2m}} + V = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V$$

$$p^2 = (p_x^2 + p_y^2 + p_z^2)$$

$$p_x = -i\hbar \frac{\partial}{\partial x} \qquad p_y = -i\hbar \frac{\partial}{\partial y} \qquad p_z = -i\hbar \frac{\partial}{\partial z}$$

$$\vec{p} = -i\hbar \vec{\nabla}$$

$$\vec{\nabla} = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}$$

$$p^2 = \vec{\nabla}^2 \quad \text{where} \quad \vec{\nabla}^2 = \vec{\nabla} \cdot \vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\underbrace{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi}_{\text{Time independant}} \qquad \underbrace{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial \psi}{\partial t}}_{\text{Time dependant shrodinger equation}}$$

$[\Psi, V]$ functions of $\vec{r}, t$

$\Psi(r,t) = \Psi(x,y,z,t)$

r = space derivative
t = time derivative

Wave function is dependent on space derivative set as $r\,[x,y,z]$ and time derivative $[t]$

- $\int |\psi|^2 \, dx\, dy\, dz$ [normalised in space ONLY]

$$\int |\psi|^2 d^3 r = \oint |\psi|^2 d\tau = 1$$

$d\tau$ → volume

- $\Psi, V \neq \vec{r}, t$ V :- potential :- only space dependant

Ψ :- space & time dependant

- $$\underbrace{\Psi_n(\vec{r},t)}_{\text{stationary state}} = \Psi_n(r)\, \underbrace{e^{\frac{-iE_n t}{\hbar}}}_{\text{Time dependant}}$$

$\Psi_n(r)$ → normalised stationary state
→ Time independent shrodinger wave equation

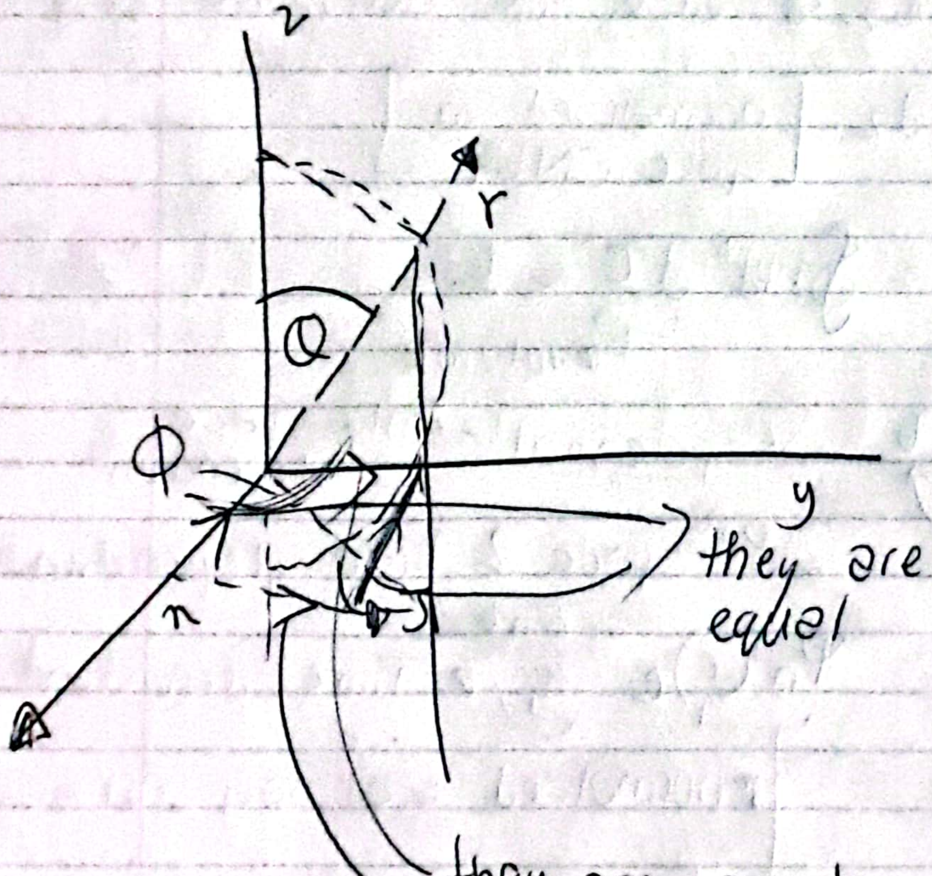
- $$\boxed{\Psi(\vec{r},t) = \sum_n C_n \Psi_n(r)\, e^{\frac{-iE_n t}{\hbar}}}$$

This space and time dependant wavefunction, will give the total wave function which will fulfill the time dependant shrodinger wave equation

spherical polar coordinates

$r = (x, y, z), t \;:\; \Psi(r, \theta, \phi)$

$r \to [0 - \infty]$ $\quad x = r\sin(\theta)\cos(\phi)$
$\theta \to [0 \to \pi]$ $\quad y = r\sin(\theta)\sin(\phi)$
$\phi \to [0 \to 2\pi]$ $\quad z = r\cos(\theta)$



$\to \underbrace{\Psi(r, \theta, \phi)}_{\downarrow} = \underbrace{R(r)}_{\downarrow} \underbrace{Y(\theta\phi)}_{\to}$ angle function dependant on angle only

Wave function dependant on space & angle

Space function dependant on space only

$$-\frac{h^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$$

$$\Big[\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin(\theta)\left(\frac{\partial}{\partial\theta}\right)\right)$$

$$+\frac{1}{r^2}\sin^2\theta\frac{\partial^2}{\partial\phi^2}\Big]$$

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