SCHRÖDINGER EQUATION

EINSTEIN, 1905, PHOTOELECTRIC EFFECT THEORY

PHOTONS: $E = h\nu$ $\left(E = \frac{h}{2\pi} 2\pi\nu \equiv \hbar\omega \right)$

$\hbar \equiv \frac{h}{2\pi}$

$\omega \equiv 2\pi\nu$

$\nu \equiv \frac{1}{T}$ → PERIOD

EINSTEIN, 1905, RELATIVITY THEORY

PARTICLES $\frac{|\vec{p}|}{E} = \frac{v}{c^2}$ ⇒ PHOTONS $\frac{|\vec{p}|}{E} = \frac{1}{c}$

$\Rightarrow |\vec{p}| = \frac{E}{c}$

DE BROGLIE 1923 (?)

SINCE FOR PHOTONS $|\vec{p}| = \frac{h\nu}{c} = \frac{h}{\lambda} = \hbar k$

$k \equiv \frac{1}{2\pi\lambda}$

$\lambda = \frac{c}{\nu} = cT$

leng. of wave

WE ASSUME THIS TO BE TRUE ALSO FOR PARTICLES

$$|\vec{p}| = \frac{h}{\lambda}$$

⇒ EACH PARTICLE IS DESCRIBED BY THE WAVE

$$\psi(t,x) = e^{i\left(\frac{\vec{p}}{\hbar}\cdot\vec{x} - \frac{E}{\hbar}t\right)} \qquad \left(\cos\left(\frac{\vec{p}}{\hbar}\cdot\vec{x} - \frac{E}{\hbar}t\right) \dots \right)$$

SCHRÖDINGER 1925 SAID:

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

WE CALL $\boxed{\hat{p} = -i\hbar\frac{\partial}{\partial x}}$

$$\Rightarrow \quad \boxed{\hat{E} = i\hbar \frac{\partial}{\partial t}}$$

$p^2 = \vec{p} \cdot \vec{p}$

BUT

$$E = \frac{1}{2} m v^2 + U(x)$$

$$\vec{p} = m\vec{v} \qquad \vec{v} = \frac{\vec{p}}{m} \Rightarrow v^2 = \frac{p^2}{m^2}$$

$$\Rightarrow \quad E = \frac{p^2}{2m} + U(x)$$

SCHRÖDINGER ASSUMED AN EQUATION FOR ψ

$$\hat{E}\,\psi(t,\vec{x}) = \frac{\hat{p}^2}{2m}\psi + U(x)\,\psi(t,x)$$

1D

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

3D

$$\hat{p} = -i\hbar\left(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right)\psi(t,x) =$$

$$-i\hbar\,\vec{\nabla}\psi$$

$$\Rightarrow \quad p^2 = \hbar^2\,\vec{\nabla}\cdot\vec{\nabla}\psi = \hbar^2\nabla^2\psi \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

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

NOTE

IF $$i\hbar \frac{\partial}{\partial t'}\psi(t',x') = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\psi(t',x') + U(x')\psi(t',x')$$

$$t = \frac{t'}{\hbar} \Rightarrow t' = t\hbar \Rightarrow \frac{\partial}{\partial t'} = \frac{\partial}{\partial t}\frac{\partial t}{\partial t'} = \frac{\partial}{\partial t}\frac{1}{\hbar}$$

$$x = \frac{x'}{\hbar} \Rightarrow x' = x\hbar \Rightarrow \frac{\partial}{\partial x'} = \frac{\partial}{\partial x}\frac{\partial x}{\partial x'} = \frac{\partial}{\partial x}\frac{1}{\hbar}$$

$$\Rightarrow i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2m}\frac{\partial^2}{\partial x^2}\psi(t,x) + U(x)\psi(t,x)$$

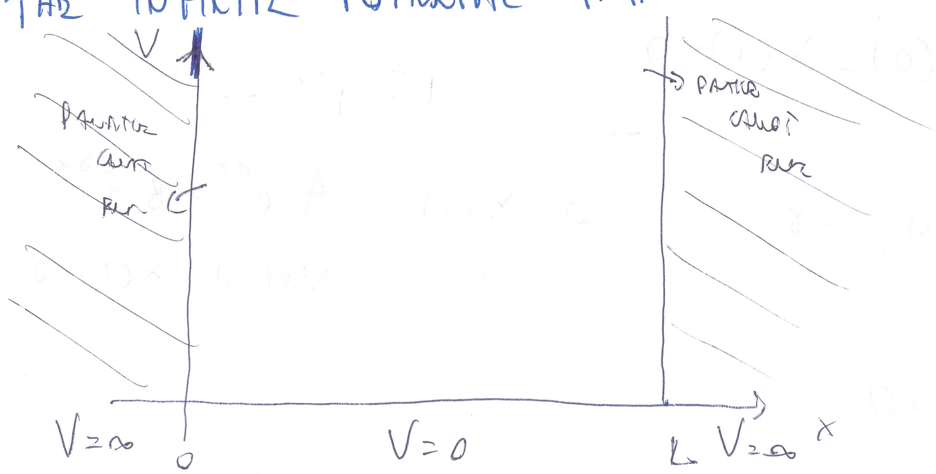
$$\Rightarrow S = \underbrace{m v^2}_{E} \cdot t = m\frac{L^2}{T^2}\cdot T = \cancel{m\frac{L'^2}{T'} = \ldots}$$

$$= m\frac{L^2}{T} = m\frac{L'^2}{T'}\cdot\frac{1}{\hbar}$$

$$= S'/\hbar$$

$$\boxed{\Rightarrow S \text{ IS MEASURED IN UNITS OF } \hbar \text{ / OR } \hbar = 1}$$

THE "INFINITE POTENTIAL TRAP"



$\psi(t,0) = 0$

$\Rightarrow$ $\psi(t,L) = 0$

PARTICLE NOT THERE

SEPARATION OF VARIABLES (USING $\hbar$)

$$\psi(t,x) = T(t)\,X(x)$$

$$\frac{i\hbar \frac{\partial}{\partial t} T(t)}{T(t)} = \frac{-\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} X(x)}{X(x)} = C$$

FOR $0 < x < L$

$\psi(t,x) = 0$ FOR $x \leq 0$, $x \geq L$

WE HAVE $i\hbar \frac{\partial}{\partial t} T(t) = C\, T(t)$

BUT $i\hbar \frac{\partial}{\partial t} \equiv \hat{E}$

WE CALL $C = E$, THE ENERGY OF THE PARTICLE

$\Rightarrow$ $T(t) = e^{-i\frac{E}{\hbar}t}$

$$\Rightarrow \; -\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} X(x) = E\,X(x)$$

$$\Rightarrow \; \frac{\partial}{\partial x^2} = \frac{-E\,2m}{\hbar^2} X(x) \equiv -\lambda^2 X(x)$$

WITH $X(0) = X(L) = 0$

IF $\lambda < 0$, $\lambda = \gamma$ $\Rightarrow$ $X(x) = A e^{\gamma x} + B e^{-\gamma x}$

IMPOSSIBLE $X(0) = 0$, $X(L) = 0$

$\Rightarrow$ $\lambda > 0$

$$X(x) = A\sin(\lambda x) + B\cos(\lambda x)$$

$$X(0) = 0 \Rightarrow X(x) = A\sin(\lambda x)$$

$$X(L) = 0 \Rightarrow X(x) = A\sin\left(\frac{\pi n}{L}x\right) \Rightarrow \lambda = \frac{\pi n}{L}$$

$$\Rightarrow \psi(t,x) = \sum_n A_n e^{-i\frac{E_n}{\hbar}t}\sin\left(\frac{\pi n}{L}x\right)$$

$$E_n = \frac{\lambda^2\hbar^2}{2m} = \frac{\pi^2 n^2\hbar^2}{L^2 2m} = n^2\frac{h^2}{L^2 8m} \equiv n^2 E_0$$

PARTICLES IN THE BOX MAY ASSUME ONLY ENERGIES

$n^2 E_0$

[A CLASSICAL PARTICLE WOULD HAVE ANY ENERGY $\frac{1}{2}mv^2$, WHERE v IS THE INITIAL ENERGY, BOUNCING BACK AND FORTH (INERTIA, POT ⇒ $v \to -v$)]

NOTE

$m = 1\,kg \quad h \simeq 6\cdot 10^{-34}\,J\cdot s \quad L = 1\,m$

$E_0 \sim 10^{-67}\,J$ TOO SMALL TO BE NOTICED!

$m = 10^{-30} \quad L = 10^{-10} \qquad E_0 \sim \frac{10^{-68}}{10^{-30}10^{-20}} \sim 10^{-17}$

COMPARABLE TO ELECTRON ENERGY IN ATOMS!

NOR 2

IF $\hbar = 1$

$$\Rightarrow \quad E_0 = \frac{(\pi)^2}{L^2 m} \quad \Rightarrow \quad [E_0] = \frac{1}{[L^2][M]}$$

BUT

$$E = \frac{ML^2}{T^2} \Rightarrow \quad E_0 = \frac{(\pi)^2 \hbar^k}{L^2 m}$$

INUSUAL UNITS

WHERE

$$\frac{(E \cdot T)^k}{L^2 M} = \frac{M^k L^{2k} T^k}{T^{2k} L^2 M} = M^{k-1} L^{2k-2} T^{-k}$$

$$\Rightarrow \quad k-1 = 1 \quad \Rightarrow k = 2 \quad \Rightarrow \quad \frac{M L^2}{T}$$

WE RECOVER THE EXPRESSION WITH $\hbar$

SCH. IN 3D (CUBIC TRAP)

$$\psi(t,x) = T(t)\, X(x)\, Y(y)\, Z(z)$$

$$XYZ\, i\hbar \frac{\partial}{\partial t} T = -\frac{\hbar^2}{2m}\left(TYZ \frac{\partial^2 X}{\partial x^2} + TXZ \frac{\partial^2 Y}{\partial y^2} + TXY \frac{\partial^2 Z}{\partial x^2} \right)$$

DIVIDE BY

$$\frac{1}{XYZT}$$

$$\Rightarrow \quad \frac{i\hbar \frac{\partial T}{\partial t}}{T} = -\frac{\hbar^2}{2m}\left(\frac{\frac{\partial^2 X}{\partial x}}{X} + \frac{\frac{\partial^2 Y}{\partial y}}{Y} + \frac{\frac{\partial^2 Z}{\partial^2 z}}{Z} \right)$$

$= E$

$\Rightarrow$

$$T(t) = e^{-i\frac{E}{\hbar}t}$$

AND

$$E + \frac{\hbar^2}{2m}\frac{\partial_z^2 Z}{Z} = -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2 X}{X} + \frac{\partial_y^2 Y}{Y}\right)$$

$$\equiv E_{xy}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial_z^2 Z}{Z} = E - E_{xy} \equiv E_z$$

$$Z(0) = Z(L_z) = 0 \quad \Rightarrow \quad E_z > 0, \quad E_z = n_z^2 E_0^z$$

$$Z(z) \propto \sin\left(\frac{\cancel{2}\pi n_z}{L_z} z\right) \qquad E_0^z = \frac{h^2}{L_z^2 8m}$$

$\Rightarrow$

$$E_{xy} + \frac{\hbar^2}{2m}\frac{\partial_y^2 Y}{Y} = -\frac{\hbar^2}{2m}\frac{\partial_x^2 X}{X} \equiv E_x$$

$$X(0) = X(L_x) = 0 \quad \Rightarrow \quad E_x = n_x^2 E_0^x > 0$$

$$X(x) \propto \sin\left(\frac{\cancel{2}\pi n_x}{L_x} x\right) \qquad E_0^x = \frac{h^2}{L_x^2 8m}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial_y^2 Y}{Y} = E_{xy} - E_x \equiv E_y$$

$y(0) = y(L_y) = 0$

$\Rightarrow \quad E_y = n_y^2 E_0^y > 0 \qquad E_0^y = \frac{h^2}{L_y^2 \, 2m}$

$y(y) \propto \sin\left(\frac{\pi n_x}{L_x} x\right)$

$\Rightarrow \quad E = n^2 E_0, \qquad n^2 \equiv n_z^2 + n_y^2 + n_x^2$

$n = 1, 2, 3, \ldots$

(IF $\exists$ $n = 0$ (EX $n_x = 0$) $\Rightarrow X(x) = 0 \quad \forall x$

$\Rightarrow \psi = 0$ NO PARTICLE!)