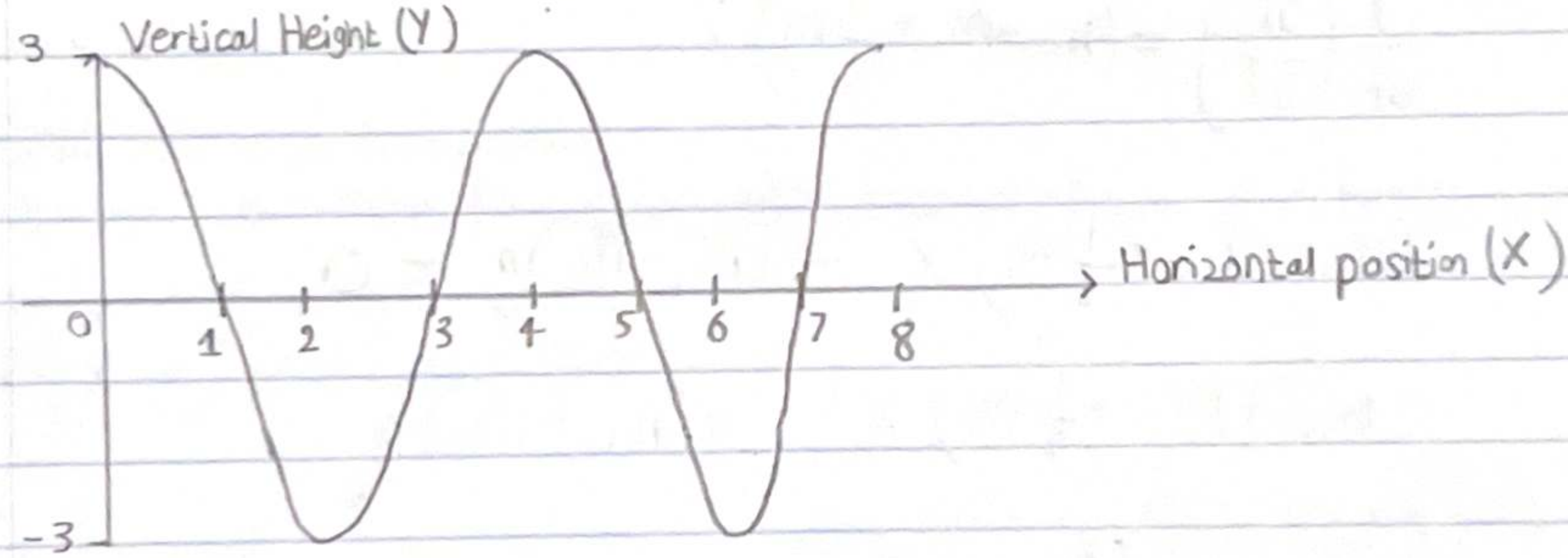
Hamiltonian
Hilbert Space
Wave function / wave equation ✓ Eigenvalue / Eigenvector
Schrödinger Equation ✓ Contour plots
Central Potential. Standing waves. P. kinetics,
Immunity

Wave Equation. (Classical)

- Function describing a wave (as a function of time and position)

Consider :



Time independant wave - equation

Consider the above diagram as a Snapshot of the wave profile.

Equation : y should be a function of x
Value of x Should give height (y)

$Y(x) = A\,Cos(x)$ ✗ (Can also be Sin)

↑ this causes function to reset after 2π. (Not valid for other waves)

$Y(x) = A\,Cos\left(\frac{2\pi}{\lambda}x\right)$ ← Inclusion of λ ensures function will complete whole cycle and predict whole wave)

λ is the distance wave takes to reset.
(how far to travel in x direction to reset.)
(Predicts whole wave)

This makes x depend on λ.

P. kinetics
H. Mechanics
E. vector

Immensity
Nature-wiring

$$\frac{\partial L}{\partial x} = m_1 g - m_2 g = (m_1 - m_2) g$$

$$\frac{\partial L}{\partial \dot{x}} = 2\left(\frac{1}{2} m_1 + \frac{1}{2} m_2 + \frac{1}{4} m\right)\dot{x}$$

$$= \left(m_1 + m_2 + \frac{1}{2} m\right)\dot{x}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \left(m_1 + m_2 + \frac{1}{2} m\right)\ddot{x}$$

$$\left(m_1 + m_2 + \frac{1}{2} m\right)\ddot{x} - (m_1 - m_2) g = 0$$

$$\left(m_1 + m_2 + \frac{1}{2} m\right)\ddot{x} = (m_1 - m_2) g$$

$$\ddot{x} = \frac{(m_1 - m_2)}{\left(m_1 + m_2 + \frac{1}{2} m\right)} g$$

$$a = \frac{m_1 - m_2}{m_1 + m_2 + \frac{1}{2} m} g \longleftarrow (m_1 > m_2)$$

Check

$$y(0) = 3\overset{\cos}{}\left(\frac{2\pi}{\cancel{4}} \times \cancel{4}\right)$$
$$= 3\cos(2\pi)$$
$$= 3 \leftarrow$$

$$y(1) = 3\cos\left(\frac{2\pi}{4} \times 1\right)$$
$$= 3\cos\left(\frac{\pi}{2}\right)$$
$$= 0 \leftarrow$$

Time - dependent wave equation. $\qquad 2^{4}$

However, Wave move throughout time (function changes with time)

$$y(x,t) = A\cos\left(\frac{2\pi}{\lambda} x + \phi\right)$$

Causes wave to Shift to the left

$\cos(\theta) = \sin(90 - \theta)$

$$y(x,t) = A\cos\left(\frac{2\pi}{\lambda} x - \phi\right)$$

Causes wave to shift to right.

This does not work as wave does not just move and stops.
Wave keeps on shifting
phase shift must depend on time
As time increases, Wave must continue to shift

$T \rightarrow$ Period $\rightarrow$ Time wave takes to reset.

Wave will look exactly the same after reset.

function needs to reset after wavelength and period.

$$Y(X,t) = A\cos\left(\frac{2\pi}{\lambda}x - \frac{2\pi}{T}t\right)$$

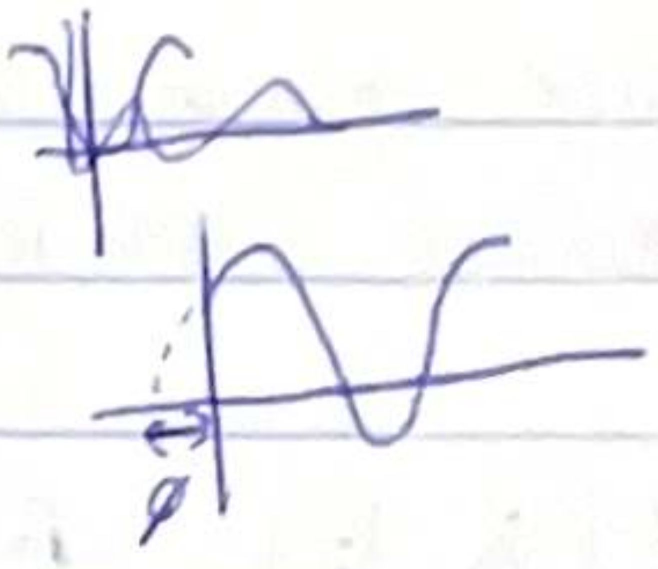
-ve causes right shift

or can be + / or can be −

$$Y(X,t) = A\cos\left(\frac{2\pi}{\lambda}x - \frac{2\pi}{T}t \mp \phi\right)$$

accounts for wave starting at other position

eg.



$-3 \leq Y(X,t) \leq 3$

in this case.

Since perfect cosine wave $\phi = 0$

Check

$$y(x,t) = 3\cos\left(\frac{2\pi}{4}x - \frac{2\pi}{T}t\right)$$

$\phi = 90^\circ$ for sin & cos.

phase shift or phase difference

Consider V of wave $= 0.5\,m/s$

$V = f\lambda = \frac{\lambda}{T}$

$T = \frac{\lambda}{V} = \frac{4}{0.5} = 8\,s$

$$Y(X,t) = 3\cos\left(\frac{2\pi}{4}x - \frac{2\pi}{8}t\right)$$

$$Y(3, 5.2) = 3\cos\left(\frac{2\pi}{4}(3) - \frac{2\pi}{8}(5.2)\right)$$

Vertical posn of wave at $X = 3\,M$ and $t = 5.2\,s$

since λ is constant

Can be written as

$$y(x,t) = A\cos(kx - \omega t)$$

Since $\frac{2\pi}{T} = \omega$

The standard wave equation in 1 Dimension.

$$\boxed{\frac{\partial^2 y}{\partial^2 x} = \frac{1}{V^2}\frac{\partial^2 y}{\partial^2 t}}$$

$$y(x,t) = A\cos(kx - \omega t)$$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{V^2}\frac{\partial^2 y}{\partial t^2}}$$

$\checkmark$

$$\frac{\partial y}{\partial x} = A(-\sin(kx - \omega t) \times K)$$
$$= -KA\sin(kx - \omega t)$$

$$\frac{\partial^2 y}{\partial^2 x} = -K^2 A\cos(kx - \omega t) \leftarrow$$
$$= -K^2 y$$

$$\frac{\partial y}{\partial t} = A(-\sin(kx - \omega t) \times (-\omega))$$

$$= +\omega A\sin(kx - \omega t)$$

$$\frac{\partial^2 y}{\partial x^2} = \omega A\cos(kx - \omega t)(\times -\omega)$$
$$= -\omega^2 A\cos(kx - \omega t) \leftarrow$$
$$= -\omega^2 y$$

From $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$

$$\cancel{-}k^2\cancel{y} = \frac{1}{v^2} \times \cancel{-}\omega^2 \cancel{y}$$

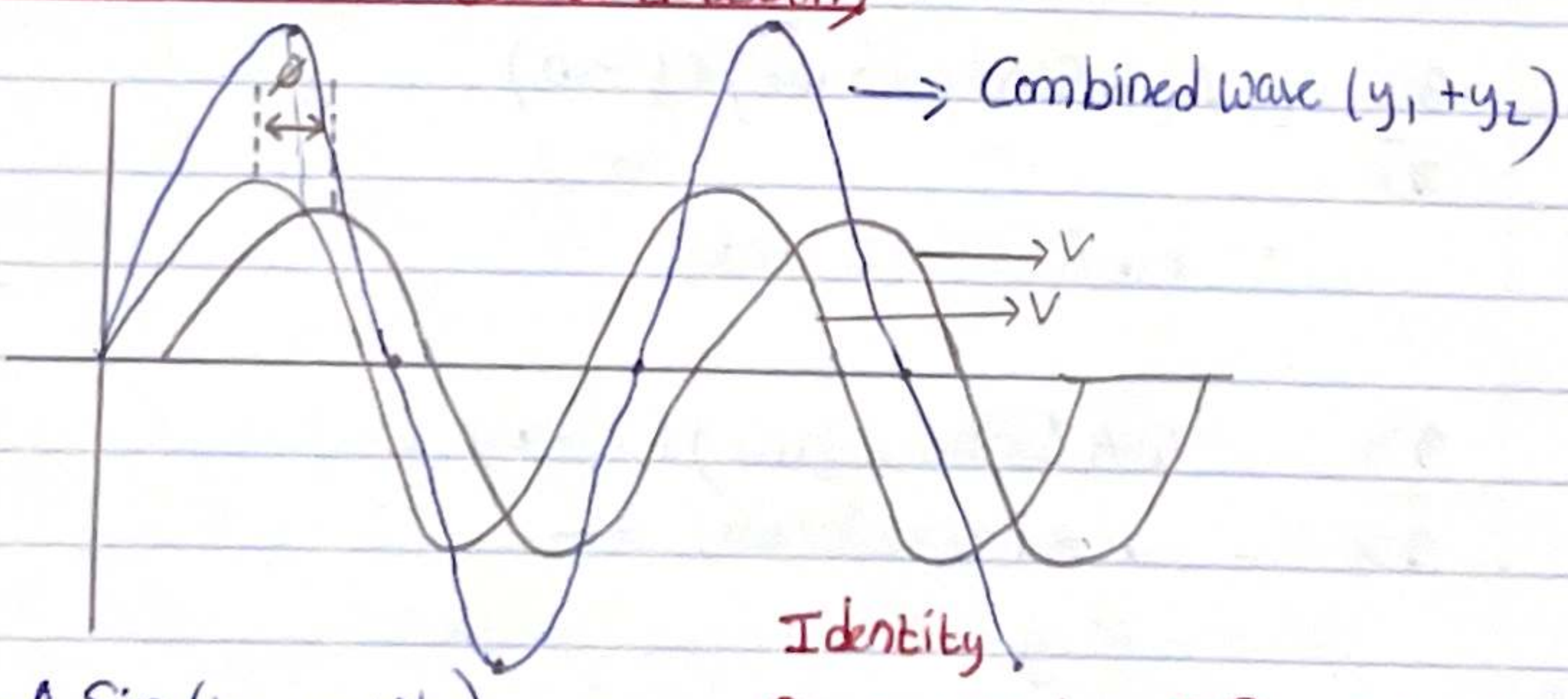
$$k^2 = \frac{1}{v^2} \times \omega^2$$ Is is true? If yes, $A\cos(kx - \omega t)$ is a proper wave equation.

$k = \frac{2\pi}{\lambda}$ $\quad \omega = \frac{2\pi}{T} = 2\pi f$ $\quad v = f\lambda$

$$\frac{4\pi^2}{\lambda^2} = \frac{1}{\cancel{f^2}\lambda^2} \times 4\pi^2 \cancel{f^2}$$

$$\frac{4\pi^2}{\lambda^2} = \frac{4\pi^2}{\lambda^2}$$ ← Wave equation is true.

Interference of waves (Same direction)



Identity

$\sin a + \sin b = 2\sin\frac{1}{2}(a+b)\cos\frac{1}{2}(a-b)$

$y_1 = A\sin(kx - \omega t)$

$y_2 = A\sin(kx - \omega t - ø)$

Same Amplitude, Same Velocity ~~isn~~ Since $(kx - \omega t)$ is same for both

But y_2 is ahead of y_1 by ø

Equivalent of $F = ma$ for quantum mechanics.

Schrödinger equation

$E_{total} = PE + KE$

$= V + \frac{1}{2}mv^2$

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

momentum

$P = mv$

$\frac{1}{2}\cancel{m(mx)} = \frac{pm}{2}$

$\cancel{\frac{m^2v^2}{2}}$

$KE = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m}$

$= \frac{1}{2} \times \frac{m^2v^2}{m} = \frac{(mv)^2}{2m}$

$= \frac{p^2}{2m}$

General form of wave equation

$\boxed{\psi = e^{i(kx - \omega t)}}$

$= \cos(kx - \omega t) + i\sin(kx - \omega t)$

This wave equation can take complex soln s.

$\frac{d\psi}{dx} = ike^{i(kx - \omega t)}$

$\frac{d^2\psi}{dx^2} = i^2k^2e^{i(kx - \omega t)}$

$= -1k^2\psi$

$= -k^2\psi \quad -1$

$\lambda = \frac{h}{p}$ De Broglie relation

$\frac{p}{h} = \frac{1}{\lambda}$

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

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

$\Rightarrow \frac{p}{h} = \frac{1}{\lambda}$

$$y_1 + y_2 = A\sin(kx-\omega t) + A\sin(kx-\omega t-\phi)$$

$$= A\left[\sin(\underbrace{kx-\omega t}_{a}) + \sin(\underbrace{kx-\omega t-\phi}_{b})\right]$$

$a = kx - \omega t$

$b = kx - \omega t - \phi$

$$= A\left[2\sin\tfrac{1}{2}(kx-\omega t+kx-\omega t-\phi)\cos\tfrac{1}{2}(kx-\omega t-(kx-\omega t-\phi))\right]$$

$$= A\left[2\sin\tfrac{1}{2}(kx-\omega t+kx-\omega t-\phi)\cos\tfrac{1}{2}(\cancel{kx}-\cancel{\omega t}-\cancel{kx}+\cancel{\omega t}+\phi)\right]$$

$$= A\left[2\sin\tfrac{1}{2}(2kx-2\omega t-\phi)\cos\tfrac{1}{2}(\phi)\right]$$

$$= 2A\sin\left(kx-\omega t-\frac{\phi}{2}\right)\cos\left(\frac{\phi}{2}\right)$$ ← Eqn of Combined wave

or $\cos(+\frac{\phi}{2})$

$$= \underbrace{2A\cos\left(\frac{\phi}{2}\right)}\sin\left(kx-\omega t-\frac{\phi}{2}\right)$$

Combined wave:

- Amplitude is bigger
- peak occurs $\frac{\phi}{2}$ further to right
- $kx - \omega t$ is same. So, same λ and frequency (and velocity)

When phase difference between 2 waves $= 180^\circ$ or π $\cos(\frac{\pi}{2}) = \cos(90)^\circ = 0$

→ Cancel out

Complete destructive interference when $\phi = \pi$ rad.

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

$$h = 2\pi\hbar$$

$$\frac{p}{2\pi\hbar} = \frac{1}{\lambda}$$

$$\frac{p}{\hbar} = \left(\frac{2\pi}{\lambda}\right) \longrightarrow = k$$

$$K = \frac{p}{\hbar} \quad — (11)$$

(11) in (1)

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$$

$$-\hbar^2 \frac{d^2\psi}{dx^2} = p^2\psi$$

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

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

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

$$= \frac{1}{2m} \times p^2\psi + V\psi$$

$$E\psi = \frac{1}{2m} \times -\hbar^2 \frac{d^2\psi}{dx^2} + V\psi$$

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

$\hat{\psi} =$

KE associated with electron (Particle)

PE associated with electron. (Particle)

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

$$\frac{-h}{8\pi^2 m}\left[\frac{d^2\Psi}{dx^2} + \left(\frac{2}{x}\right)\frac{d\Psi}{dx}\right] + V\Psi(x) = E\Psi$$

Wave function

Total energy electron (particle) is allowed to have

(Hamiltonian) ??

Determining Ionisation Energy of the Hydrogen atom from the time independent Schrödinger Equation.

$$E\Psi(x) = \frac{-h^2}{4\pi^2 \times 2m}\frac{d^2\Psi(x)}{dx^2} + V\Psi(x)$$

$$= \frac{-h^2}{8\pi^2 m}\left[\frac{d^2\Psi(x)}{dx^2}\right] + V\Psi(x) \quad \text{— (1)}$$

electron and proton have Same charge magnitude.

$$V\Psi(x) = \frac{-e^2}{4\pi\varepsilon_0 x}\Psi$$

potential energy due to attraction of a single proton at distance r. (or x).

-ve as potential energy is -ve

Bohr radius (radius at which electrons orbit proton)

multiply both side of equation (1) by $-\frac{8\pi^2 m}{h^2}$ and put $a_0 = \frac{\varepsilon_0 h^2}{\pi m e^2}$

$$\left(\frac{-8\pi^2 m}{h^2}E\right)\Psi = \frac{d^2\Psi}{dx^2} + \left(\frac{2}{r}\right)\frac{d\Psi}{dx} + \frac{2}{a_0 r}\Psi$$

$$\frac{d\Psi}{dx} = \frac{-\Psi}{a_0}$$

$$\cancel{\frac{d^2\psi}{dx^2}}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{d}{dx}\left(\frac{-\psi}{a_0}\right) = \frac{\psi}{a_0^2}$$

$$\frac{1}{a_0^2}\cancel{\psi} = \left(\frac{-8\pi^2 m}{h^2}E\right)\cancel{\psi}$$

$$E = \frac{-h^2}{8\pi^2 m a_0^2}$$

$h = 6.626 \times 10^{-34}$ Js
$m = 9.109 \times 10^{-31}$ Kg
$a_0 = 5.292 \times 10^{-11}$ m

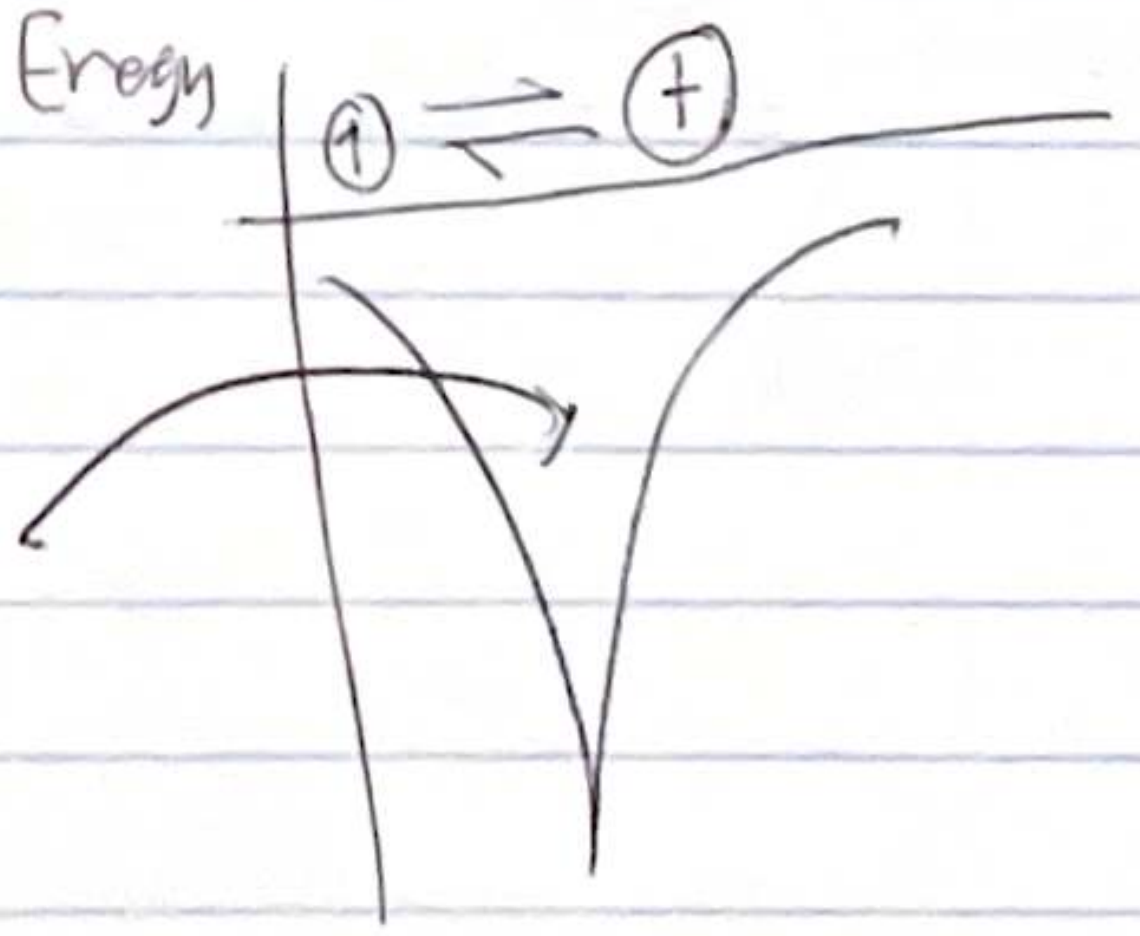
E = Energy of 1 electron in 1S orbital.
$= -2.18 \times 10^{-18}$ J
X by N_A
$= -1312.6$ kJ ← Ionisation energy of hydrogen atom.

Time dependant Schrödinger Equation.

$$i\hbar \Psi(r,t) = \left[\frac{-\hbar}{2\mu}\nabla^2 + V(r,t)\right]\Psi(r,t).$$

$$\underbrace{E\Psi(x)}_{\text{Total Energy}} = \underbrace{\frac{-h^2}{2m}\frac{d^2\Psi(x)}{dx^2}}_{\text{Kinetic Energy}} + \underbrace{V\Psi(x)}_{\text{Potential Energy.}}$$

Potential Energy between Proton and electron



$$\frac{e^2}{4\pi\varepsilon_0 r^2} \Longleftarrow$$ Potential well (-ve)

$$\cancel{\frac{e^2}{4\pi\varepsilon_0 r}}$$

pendent Schrodinger Equation

$$\boxed{H\Psi = E\Psi}$$

Wave function. → for hydrogen Atom.

Hamiltonian $(T + V)$

Energy eigenvalue

$H = E_K + V$ ← Potential energy

E_K: Kinetic energy

$$H = \frac{p^2}{2m} + V$$

from classical wave equation,

$$\Psi = e^{i(kx - \omega t)}$$

differentiate w.r.t position

$$\frac{d\Psi}{dx} = k i e^{i(kx - \omega t)} = ik\Psi$$

$$\frac{d^2\Psi}{dx^2} = k^2 i^2 e^{i(kx - \omega t)} = -k^2\Psi$$

$k = \frac{2\pi}{\lambda}$, from De Broglie's equation

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

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

$$\frac{\hbar}{p} = \frac{1}{k}$$

$$\Rightarrow k = \frac{p}{\hbar}$$

$$\frac{d^2\Psi}{dx^2} = -\frac{p^2}{\hbar^2}\Psi$$

$$H = \frac{p^2}{2m} + V$$

$$\frac{1}{2m}\frac{d^2\Psi}{dx^2} = -\frac{1}{\hbar}\frac{p^2}{2m}\Psi$$

$$\Rightarrow \frac{p^2}{2m} = E_K = \frac{-\hbar}{2m}\frac{d^2\Psi}{dx^2}$$

$$\Rightarrow \boxed{E\Psi = -\frac{\hbar}{2m}\frac{d^2\Psi}{dx^2} + V_{(x)}\Psi}$$

Time-dependant Schrodinger Equation

$E = hf$

$\omega = 2\pi f$

$f = \frac{\omega}{2\pi}$

$\Rightarrow E = \frac{h\omega}{2\pi}$

$$\boxed{E = \hbar\omega}$$

From classical wave equation,

$\psi = e^{i(Kx - \omega t)}$

$\Big\downarrow$ Differentiate w.r.t time

$\frac{d\psi}{dt} = -i\omega\psi \longrightarrow \omega\psi = -\frac{1}{i}\frac{d\psi}{dt}$

$E = \hbar\omega$

$E\psi = \hbar\omega\psi$

$E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt} \longrightarrow E\psi = -\frac{\hbar}{i}\frac{d\psi}{dt}\left(\frac{-i}{-i}\right)$ $\quad * \; -i \times i = -i^2 = -(-1) = 1$

$$\boxed{E\psi = i\hbar\frac{d\psi}{dt}}$$

$\Big\downarrow$ Substitute in TISE

$$\boxed{i\hbar\frac{d\psi}{dt} = -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + V_{(x)}\psi}$$

$-\frac{i}{\hbar}E\psi = \frac{d\psi}{dt}$

$E\psi = \hbar\omega\psi$

$= -i\omega\psi$

... to 1S Orbital energy

$H\Psi = E\Psi$ ← wave function

↓ Hamiltonian $E_k + E_p$; ↑ Energy eigenvalue

Potential

$\Rightarrow$ ~~$E\Psi = E_k(r) +$~~

$$E\Psi(r) = \underbrace{E_k \Psi(r)}_{E_k} + \overbrace{V(r)\Psi(r)}^{\text{Potential}}$$

General form of wave equation : $\Psi = e^{i(kr - \omega t)}$

$$\frac{d\Psi}{dr} = ik e^{i(kr-\omega t)}$$
$$= ik\Psi$$

$$\frac{d^2\Psi}{dr^2} = i^2 k^2 e^{(kr-\omega t)}$$
$$= -k^2\Psi$$

AND ~~OR~~ $E_k = \frac{p^2}{2m}$

$$\Rightarrow E\Psi = \underbrace{\frac{p^2\Psi}{2m}} + V\Psi$$

From wave equation $k = \frac{2\pi}{\lambda}$ path difference

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

$$\Rightarrow \frac{d^2\Psi}{dr^2} = \frac{p2\pi}{h}$$

$$\frac{p}{h} = \frac{1}{\lambda} \rightarrow \cancel{\times} 2\pi$$

$= 2\pi\hbar \leftarrow h$

$$\frac{p}{\cancel{2\pi}\hbar} = \left(\frac{2\pi}{\lambda}\right) = k$$

$$= k = \frac{p}{\hbar}$$

$$\Rightarrow \frac{d^2\Psi}{dr^2} = \frac{-p^2}{\hbar^2}\Psi \Rightarrow -\hbar^2\nabla^2\Psi = p^2$$