DATE: 20
PAGE No

Show that de broglie waves travel with a velocity more than velocity of light.

'v' → particle velocity

$$E = mc^2 = h\nu$$

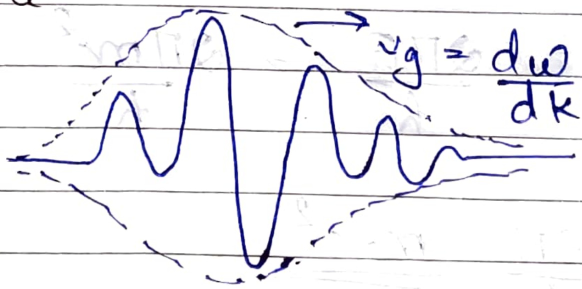
$$\nu = \frac{mc^2}{h}$$

$$\& \ \lambda = \frac{h}{mv}$$

also, $v_p = \lambda \nu = \frac{c^2}{v}$

$$\boxed{v_p = \frac{c^2}{v}} > c$$

Show that the group velocity of the wave packet moves with the velocity of the particle.



$$v_g = \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{d\left(\frac{2\pi}{\lambda}\right)}$$

DATE: 20
PAGE No

$$v_g = \frac{d\nu}{-\frac{1}{\lambda^2} d\lambda} = -\lambda^2 \frac{d\nu}{d\lambda}$$

now, $v = \lambda \nu$

$$\nu = \frac{v}{\lambda}$$

$$\frac{d\nu}{d\lambda} = -\frac{v}{\lambda^2}$$

$$\boxed{v_g = v}$$

OR

$$v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$$

$$E = h\nu = \frac{h\nu \times 2\pi}{2\pi} = \frac{h\omega}{2\pi}$$

$$\omega = \frac{2\pi E}{h} = \frac{2\pi mc^2}{h}$$

$$\omega = \frac{2\pi}{h} \frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}}$$

DATE: 20
PAGE No

$$\frac{d\omega}{dv} = \frac{2\pi m_0 c^2}{h} \cdot \frac{-1}{2}\left(1-\frac{v^2}{c^2}\right)^{-3/2} \times \frac{-2v}{c^2}$$

$$\frac{d\omega}{dv} = \frac{2\pi m_0}{h} \frac{v}{(1-v^2/c^2)^{3/2}} \quad \text{--- (1)}$$

now, $\lambda = \frac{h}{mv}$

$$\frac{\lambda}{2\pi} = \frac{h}{2\pi mv}$$

$$k = \frac{2\pi mv}{h}$$

$$k = \frac{2\pi m_0}{h}\left(\frac{v}{\sqrt{1-v^2/c^2}}\right)$$

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left(\frac{\sqrt{1-v^2/c^2} + \frac{v^2/c^2}{\sqrt{1-v^2/c^2}}}{(1-v^2/c^2)}\right)$$

$$\frac{dk}{dv} = \frac{2\pi m_0}{h} \cdot \frac{1}{(1-v^2/c^2)^{3/2}} \quad \text{--- (2)}$$

$$\boxed{v_g = v}$$

for dispersive medium —

$$\boxed{v_g = v_p - \lambda \frac{dv_p}{d\lambda}} \Rightarrow v_g < v_p$$

Using heisenberg's uncertainty principle, show that an e^- can not stay inside the nucleus.

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

$$10^{-15}\ \Delta p \geq \frac{h}{4\pi}$$

$$mv \simeq \frac{h}{4\pi} \times 10^{15}$$

$$v \simeq 10^{12}\ m/s > c$$

also, Energy using this momentum, $E = \frac{p^2}{2m} = 40 MeV$

but, Energy of β-particles emitted by nucleus $= 4-5$ MeV

Natural Broadening of spectral lines.

in lasers,

$t_3 = 10^{-8} s$ —— excited state

$t_2 = 1 ms$ —— metastable state

$t_1 = \infty s$ —— E_1 grond state

$E_3 \pm \underbrace{\Delta E_3}_{\text{width of a state}}$

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

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

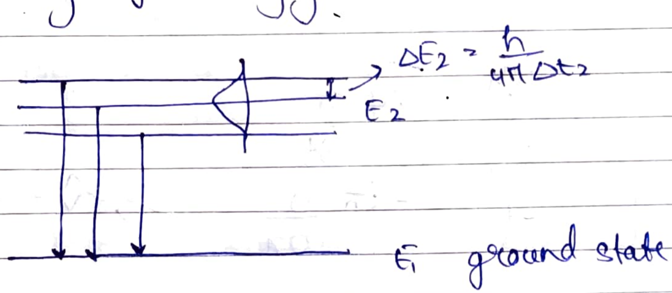
$$\Delta E = \frac{p \Delta p}{m} = \frac{m}{m} v \Delta p$$

$$\Delta E = \frac{\Delta x \cdot \Delta p}{\Delta t}$$

$$\Delta E \cdot \Delta t = \Delta p \cdot \Delta x$$

$$\therefore \boxed{\Delta E \cdot \Delta t \geq \frac{h}{4\pi}}$$

Due to finite life time of states, there is splitting of Energy levels.



- operators are used to calculate a physical quantity.

DATE: 20
PAGE No

Time dependent schrodinger eq^n is valid for free particle or not.

for a free particle, $y = A \sin(kx - \omega t)$

Derive the steady-state form of the schrodinger eq^n.

$$\hat{E} = K.E + U$$
$$\hat{E} = \frac{\hat{p}^2}{2m} + U$$

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

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

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

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}, \quad \hat{v} = -\frac{i\hbar}{m}\frac{\partial}{\partial x}$$

$$\hat{p}^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

KE operator, $\frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

DATE: 20
PAGE No

Hamiltonian, $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$

$$\boxed{\hat{H}\psi(x,t) = \hat{E}\psi(x,t)}$$

→ energy eigenvalue eq^n

$\psi(x,t) \rightarrow$ eigenvectors

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

$$\psi(x,t) = \underbrace{Ae^{ikx}}_{\psi(x)} \cdot e^{-i\omega t}$$

replacing $\psi(x,t)$ by $\psi(x)$ in above eq^n

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - U(x)]\psi(x) = 0}$$

Probability of finding the particle in volume dV -

$$P(x,t) = |\psi(x,t)|^2 dV$$

$$\int_{-\infty}^{\infty} P(x,t)\,dV = \boxed{\int_{-\infty}^{\infty} |\psi(x,t)|^2 dV = 1}$$

→ Normalisation condition

DATE: 20
PAGE No

Postulates of Quantum Mechanics -

(i) To any physical observable quantity, a wave f^n is associated.

(ii) Each observable quantity in quantum mechanics can be assigned a mathematical operator which when operates of the quantity gives a real value.

(iii) Acceptable wave f^n
- finite
- single - valued
- continous
- normalizable

Orthoganity of wave f^ns -

Suppose $\psi_m(x,t)$ & $\psi_n(x,t)$ represents wave f^n, for two physical states, then the condition of orthogonality says -

$$\boxed{\int_{-\infty}^{\infty} \psi_m^*(x,t) \cdot \psi_n(x,t)\, dx = 0}$$

$$\psi(x,t) = A e^{i(kx - \omega t)}$$
$$\psi^*(x,t) = A e^{-i(kx-\omega t)}$$

DATE: 20
PAGE No

Orthonormal wave f^ns -

orthogonal + normalised

$$\int_{-\infty}^{\infty} \psi_m^*(x,t) \cdot \psi_n(x,t)\, dx = \delta_{mn}$$

$$\delta_{mn} = 0 \quad m \neq n$$
$$= 1 \quad m = n$$

Kronecker delta

(iv) Expectation value -

$$\langle \hat{G} \rangle = \frac{\int_{x_1}^{x_2} \psi^*(x,t)\, \hat{G}\, \psi(x,t)\, dx}{\int_{x_1}^{x_2} \psi^*(x,t)\, \psi(x,t)\, dx}$$

Note :- Commutation relation -

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

eg - $[\hat{x}, \hat{p}_x]$

$$[\hat{x}, \hat{p}_x]\psi(x) = \hat{x}\hat{p}_x\psi - \hat{p}_x\hat{x}\psi$$
$$= x\left(-i\hbar \frac{\partial\psi}{\partial x}\right) + i\hbar \frac{\partial}{\partial x}(x\psi)$$
$$= \cancel{-i\hbar x \frac{\partial\psi}{\partial x}} + i\hbar\psi + \cancel{i\hbar x \frac{\partial\psi}{\partial x}}$$

$$\therefore \boxed{[\hat{x}, \hat{p}_x] = i\hbar}$$

eg- $[\hat{y}, \hat{p}_x]$

$= \hat{y}\hat{p}_x\psi - \hat{p}_x\hat{y}\psi$

$= y\left(-i\hbar\frac{\partial\psi}{\partial x}\right) + i\hbar\frac{\partial(y\psi)}{\partial x}$

$= \cancel{-i\hbar y\frac{\partial\psi}{\partial x}} + i\hbar\psi\overset{0}{\cancel{\frac{\partial y}{\partial x}}} + \cancel{i\hbar y\frac{\partial\psi}{\partial x}}$

$\boxed{[\hat{y}, \hat{p}_x] = 0}$

↳ these are non-conjugate pairs & can be measured simultaneously

while

$[\hat{x}, \hat{p}_x] = i\hbar \Rightarrow$ finite

↳ conjugate pair, related to heisenberg uncertainty & cannot be measured simultaneously.

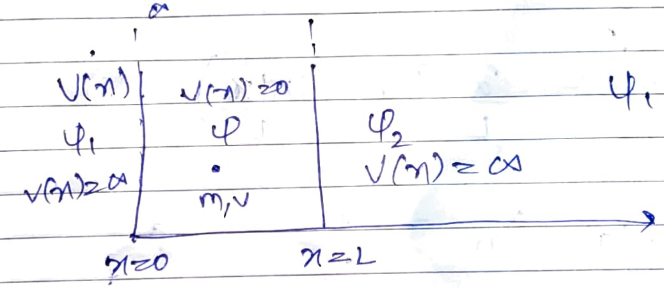
★ **Applications of Schrodinger wave f^n** –

(i) free particle, $y = A\cos(kx-\omega t) = \psi(x,t)$

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

LHS $\neq$ RHS

(ii) **Particle in a box** :-



$\psi_1 = \psi_2 = 0$

$$V(x) = \begin{cases} 0 & ; \ 0 < x \le L \\ \infty & ; \ x < 0, \ x > L \end{cases}$$

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

$k = \sqrt{\frac{2mE}{\hbar^2}}$

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

at $x=0$, $\psi_1(x) = \psi(x)$

at $x=L$, $\psi_2(x) = \psi(x)$

$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{kx}{L}$

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

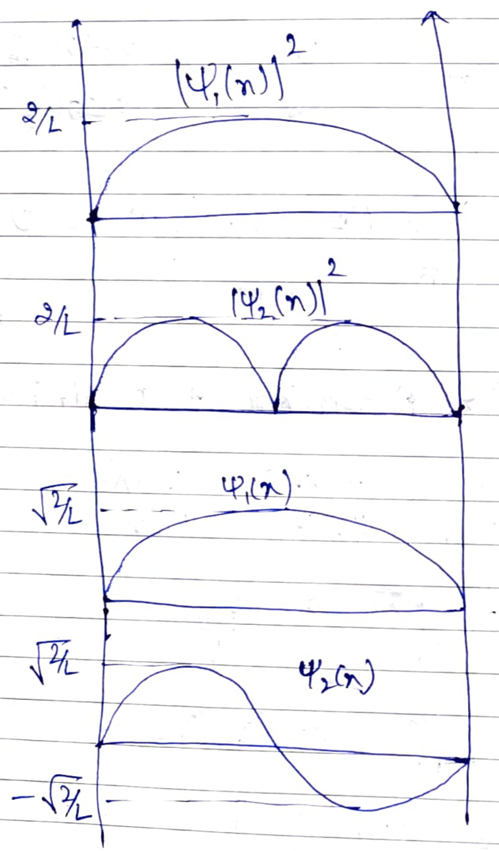
$\psi_1(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$

$\psi_2(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$

$$|\psi_1(x)|^2 = \frac{2}{L}\sin^2\left(\frac{\pi x}{L}\right)$$

$$|\psi_2(x)|^2 = \frac{2}{L}\sin^2\left(\frac{2\pi x}{L}\right)$$

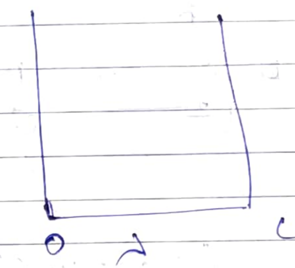
$$E_n, P_n, \lambda_n = ?$$



$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$P = \hbar K$$

&



$$L = \frac{n\lambda}{2}$$

$$\boxed{\lambda_n = \frac{2L}{n}}$$

Q. Derive the eq^n for momentum & energy of a ~~particle~~ e^- in a 1-D box of length 0.1 nm for $n = 1$ & 2.

Q. The wave f^n ψ of a particle is given by

$$\psi = Ae^{-kx}, \quad 0 < x < \infty$$
$$= 0, \quad x < 0$$

Find A in terms of 'k' & Evaluate the probability of finding the particle lying in this region.

Q. For a free particle show that the Schrodinger wave eq^n leads to de broglie relation.

A1)

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2\pi^2h^2}{\pi^2 8mL^2} = \frac{n^2h^2}{8mL^2}$$

$$P_n = \hbar K = \hbar\left(\frac{\sqrt{2mE_n}}{\hbar}\right) = \sqrt{2mE_n}$$

$$P_n = \sqrt{\frac{2m\, n^2 h^2}{8m L^2}} = \frac{nh}{2L}$$

$$E_1 = \frac{h^2}{8m_e L^2} = \frac{(6.626\times10^{-34})^2}{8(9.1\times10^{-31})(10^{-20})}$$

$$= 0.603\times10^{-17}$$

$$= \frac{60.3\times10^{-19}}{1.6\times10^{-19}}\ eV$$

$$= 37.68\ eV$$

$$E_2 = 2^2 E_1 = 4\times37.68$$

$$= 150.72\ eV$$

$$P_n = \frac{nh}{2L}$$

$$P_1 = \frac{h}{2L} = \frac{6.626\times10^{-34}}{2\times10^{-10}}$$

$$P_1 = 3.313\times10^{-24}\ kg\,m/s$$

$$P_2 = 2P_1$$

$$= 6.626\times10^{-24}\ kg\,m/s$$

A2)

$$\psi = Ae^{-kx}, \quad 0<x$$

$$= 0, \quad x<0$$

normalisation –

$$\int_{-\infty}^{\infty}\psi^*\psi\,dx = \int_0^{\infty}|Ae^{-kx}|^2\,dx$$

$$= A^2\int_0^{\infty}e^{-2kx}\,dx$$

$$= \frac{A^2}{-2k}\left[e^{-2kx}\right]_0^{\infty}$$

$$= \frac{-A^2}{2K}[-1] = \frac{A^2}{2K} = 1$$

$$A^2 = 2K$$

$$A = \sqrt{2K}$$

DATE: 20
PAGE No

Ans: $E_n = \frac{n^2h^2}{8mL^2}$

$E_1 = \frac{h^2}{8mL^2} = \frac{p^2}{2m}$

$p^2 = \frac{h^2}{4L^2} \Rightarrow p = \frac{h}{2L}$

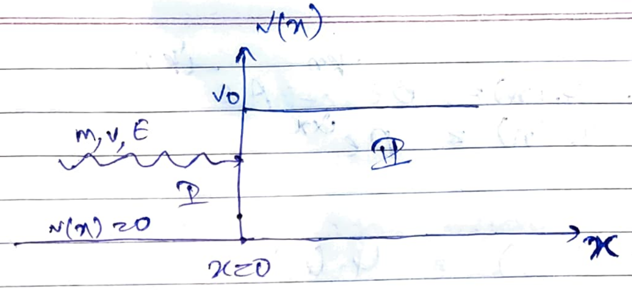
also, $\lambda_1 = 2L$

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

Step Potential Barrier :-

Consider a beam of free particles moving along a straight line when they cross a region of different potential.

DATE: 20
PAGE No



→ Case 1 : $E > V_0$

$V(x) = V_0 \quad 0 \le x$
$\qquad\quad 0 \quad x < 0$

Region - I : $\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_1(x) = 0$ Let $\frac{2mE}{\hbar^2} = k^2$

Region - II : $\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_2(x) = 0$

Let $\frac{2m}{\hbar^2}(E-V_0) = \alpha^2$

Region - I - (Reflected wave, incident wave)

$\psi_1(x) = A\,e^{-ikx} + B\,e^{ikx}$

Region - II - $\psi_2(x) = C\,e^{-i\alpha x} + D\,e^{i\alpha x}$ → transmitted wave

this component cannot exist bcz a wave cannot travel in -ve x dirⁿ in R - II.

at $x = 0$ -

$\psi_1(x) = \psi_2(x)$

& $\frac{d\psi_1(x)}{dx} = \frac{d\psi_2(x)}{dx}$

DATE: 20
PAGE No

$$\therefore \psi_1(x) = Be^{ikx} + Ae^{-ikx}$$
$$\psi_2(x) = De^{i\alpha x}$$

$$\psi_1(0) = \psi_2(0)$$
$$B + A = D$$
$$A + B = D \quad — ①$$

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

$$\left. ikBe^{ikx} - ikAe^{-ikx}\right|_{x=0} = \left. i\alpha De^{i\alpha x}\right|_{x=0}$$

$$ikB - ikA = i\alpha D$$
$$(B-A) = \frac{\alpha}{k}D \quad — ②$$

from ① & ②

$$2B = \left(1 + \frac{\alpha}{k}\right)D$$

$$B = \left(\frac{k+\alpha}{2k}\right)D \quad — ③$$

$$\& A = \left(\frac{k-\alpha}{2k}\right)D \quad — ④$$

$$\psi = e^{ikx}$$
$$\psi^* = e^{-ikx}$$

DATE: 20
PAGE No

Probability Current density, $J = \frac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*)$

now, $J_i \rightarrow$ PCD for incident wave
$J_r \rightarrow$ ——— reflected —
$J_t \rightarrow$ ——— transmitted —

$$J_i = \frac{\hbar}{2im}\left(B^* e^{-ikx}\frac{d(Be^{ikx})}{dx} - Be^{ikx}\frac{d(B^*e^{-ikx})}{dx}\right)$$

$$J_i = \frac{\hbar}{2im}\left[|B|^2(ik) + |B|^2(ik)\right]$$

$$= B^2\frac{\hbar k}{m}$$

$$J_r = \frac{\hbar}{2im}\left(A^2(-ik) - A^2(ik)\right)$$

$$= +|A|^2\frac{\hbar k}{2m}$$

$$J_t = |D|^2\frac{\hbar\alpha}{m}$$

Reflected coefficient, $R = \left|\frac{J_r}{J_i}\right|$

$$R = \frac{A^2}{B^2} = \left(\frac{k-\alpha}{k+\alpha}\right)^2$$

$$\boxed{R + T = 1}$$

DATE: 20
PAGE No

Transmitted coefficient, $T = \left|\frac{J_t}{J_i}\right|$

$$T = \left|\frac{D^2\alpha}{B^2 k}\right| = \frac{4k^2}{(k+\alpha)^2}\left(\frac{\alpha}{k}\right)$$

$$T = \frac{4\alpha k}{(k+\alpha)^2} \qquad \boxed{R + T = 1}$$

Since we know the values of 'α' & 'k'

$$R = \left(\frac{k-\alpha}{k+\alpha}\right)^2 = \frac{k^2+\alpha^2-2k\alpha}{k^2+\alpha^2+2k\alpha}$$

$$R = \frac{\frac{2mE}{\hbar^2} + \frac{2m(E-V_0)}{\hbar^2} - 2\times\sqrt{\frac{4m^2}{\hbar^4}\left(E(E-V_0)\right)}}{\frac{2mE}{\hbar^2} + \frac{2m(E-V_0)}{\hbar^2} + 2\sqrt{\frac{4m^2}{\hbar^4}\left(E(E-V_0)\right)}}$$

$$R = \frac{E + E - V_0 - 2\sqrt{E(E-V_0)}}{E + E - V_0 + 2\sqrt{E(E-V_0)}}$$

$$R = \left(\frac{\sqrt{E} - \sqrt{E-V_0}}{\sqrt{E} + \sqrt{E-V_0}}\right)^2$$

DATE: 20
PAGE No

if $E \gg V_0$, $R \simeq 0$ i.e. no reflection

if $E > V_0$, $R \to$ finite i.e. reflection is possible

also, $$T = \frac{4\times\frac{2m}{\hbar^2}\sqrt{E(E-V_0)}}{\frac{2m}{\hbar^2}\left(E + E - V_0 + 2\sqrt{E(E-V_0)}\right)}$$

$$T = \frac{4\sqrt{E(E-V_0)}}{\left[\sqrt{E} + \sqrt{E-V_0}\right]^2}$$

Q. As $E\uparrow$ w.r.t. V_0 the chances of receiving reflected particle will decrease. Why?
Due to uncertainty principle. The energy of the particle can be $E \pm \Delta E$, so when energy is E & $E + \Delta E$, particle will go unreflected but when energy is $E - \Delta E$, the particle will suffer reflection.

→ Case 2: $E < V_0$

$$V(x) = \begin{cases} V_0, & x \geq 0 \\ 0 & x < 0 \end{cases}$$

R-I: $$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\,\psi_1(x) = 0$$

Let $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

DATE: 20
PAGE No

R-II: $\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_2(x) = 0$

$\because E < V_0$

$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0-E)\psi_2(x) = 0$

Let $\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

$\therefore \psi_2(x) = Ce^{\alpha x} + De^{-\alpha x}$

↳ this term should be zero

$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$

↳ incident ↳ reflected.

$\psi_2(x) = Ce^{\alpha x} + De^{-\alpha x}$

↳ ~~transmitted~~

↳ at $x=\infty$, ψ_2 is not defined

$\therefore C = 0$

at $x=0$ -

$\psi_1(0) = \psi_2(0)$

$A+B = D$

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

$ikAe^{ikx} - ikBe^{-ikx}\Big|_{x=0} = -\alpha De^{\alpha x}\Big|_{x=0}$

$(A-B)ik = \cancel{\alpha C} - \alpha D$

$A-B = +\frac{\alpha i}{k}D$

DATE: 20
PAGE No

$\therefore 2A = \left(1+\frac{\alpha i}{k}\right)D$

$A = \left(\frac{k+i\alpha}{2k}\right)D$

& $B = \left(\frac{k-i\alpha}{2k}\right)D$

$J_i = |A^2|\frac{\hbar k}{m}$

$J_r = -|B|^2\frac{\hbar k}{m}$

~~$J_t = \frac{\hbar}{2im}\left(D^*e^{-\alpha x}\frac{d}{dx}(De^{-\alpha x}) - De^{-\alpha x}\frac{d}{dx}(D^*e^{-\alpha x})\right)$~~

~~$J_t = 0$~~ $J_t = \frac{\hbar}{m}D^*e^{-\alpha x}.De^{-\alpha x} = \frac{\hbar\alpha|D|^2}{m}$

Reflection coefficient, $R = \left|\frac{J_r}{J_i}\right|$

$R = \left(\frac{B}{A}\right)^2 = \left(\frac{k-i\alpha}{k+i\alpha}\right)^2 \neq 1$

Transmission coefficient, $T = \left|\frac{J_t}{J_i}\right|$ ~~$= 0$~~

~~$\therefore R = 1$ i.e. complete reflection.~~

$T = \frac{4k^2}{(k+i\alpha)^2} \neq 0$

DATE: 20
PAGE No

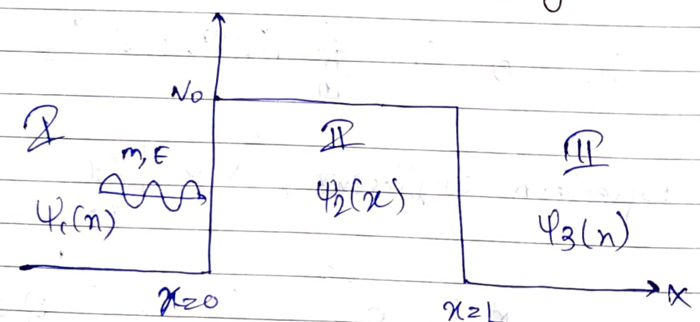
- The current density is defined as the flux of particles crossing per unit area ⊥ to dirⁿ of propagation.

Current density, $J(x,t) = \psi^* \psi \, v$

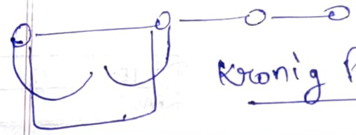
$= \psi^* \psi \left(\frac{\hbar k}{m}\right)$

- Transmission coefficient is ratio of particles transmitted to the particles incident on it.

✱ Quantum Mechanical Tunneling :-



Consider a beam of free particles having mass 'm' & Energy 'E' incident on a rectangular barrier along the +ve x-dirⁿ.



Kronig Penny Model

DATE: 20
PAGE No

$$V(x) = \begin{cases} 0 & , \; x < 0 \\ V_0 & , \; 0 \le x < L \\ 0 & , \; x > L \end{cases}$$

R-I : $\frac{d^2\psi_1(x)}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_1(x) = 0$ $\quad \alpha^2 = \frac{2mE}{\hbar^2}$

R-II : $\frac{d^2\psi_2(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_2(x) = 0$ $\quad \beta^2 = \frac{2m}{\hbar^2}(V_0-E)$

R-III : $\frac{d^2\psi_3(x)}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_3(x) = 0$ $\quad \alpha^2 = \frac{2mE}{\hbar^2}$

$\psi_1(x) = A_1 e^{i\alpha x} + B_1 e^{-i\alpha x}$

$\psi_2(x) = A_2 e^{\beta x} + B_2 e^{-\beta x}$

$\psi_3(x) = A_3 e^{i\alpha x} + \cancel{B_3 e^{-i\alpha x}} \rightarrow 0$

↳ this should be zero bcz no wave can travel in -ve x dirⁿ in R-III

at $x = 0$,

$\psi_1(0) = \psi_2(0)$

$A_1 + B_1 = A_2 + B_2 \quad — (1)$

DATE: 20
PAGE No

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

$$i\alpha(A_1 - B_1) = \beta(A_2 - B_2)$$

$$A_1 - B_1 = \frac{\beta}{i\alpha}(A_2 - B_2) \quad \text{— (2)}$$

Also,

at $x = L$

$$\psi_2(L) = \psi_3(L)$$

$$A_2 e^{\beta L} + B_2 e^{-\beta L} = A_3 e^{i\alpha L} \quad \text{— (3)}$$

& $$\left.\frac{d(\psi_2(x))}{dx}\right|_{x=L} = \left.\frac{d(\psi_3(x))}{dx}\right|_{x=L}$$

$$\left[A_2 \beta e^{\beta x} - B_2 \beta e^{-\beta x}\right]_{x=L} = i\alpha A_3 e^{i\alpha x}\Big|_{x=L}$$

$$A_2 \beta e^{\beta L} - B_2 \beta e^{-\beta L} = i\alpha A_3 e^{i\alpha L} \quad \text{— (4)}$$

DATE: 20
PAGE No

divide all the 4 eq's by A_1 &
put $\frac{B_1}{A_1} = b_1$, $\frac{B_2}{A_1} = b_2$

$\frac{A_2}{A_1} = a_2$, $\frac{A_3}{A_1} = a_3$ & $\frac{\beta}{\alpha} = n$

(1) $\rightarrow$ $1 + b_1 = a_2 + b_2$

(2) $\rightarrow$ $1 - b_1 = \frac{\beta}{i\alpha}(a_2 - b_2)$

(3) $\rightarrow$ $a_2 e^{\beta L} + b_2 e^{-\beta L} = a_3 e^{i\alpha L}$

(4) $\rightarrow$ $\beta(a_2 e^{\beta L} - b_2 e^{-\beta L}) = i\alpha a_3 e^{i\alpha L}$

also, Transmission coefficient,

$$T = \frac{|A_3|^2}{|A_1|^2} = |a_3|^2$$

$$T = \left|\frac{2e^{-i\alpha L}}{\left(\frac{n+i}{2n}\right)e^{-\beta L}(1-in) + \left(\frac{n-i}{2n}\right)e^{\beta L}(1+in)}\right|^2$$

$$T = 8n^2 e^{-2i\alpha L} \left|\frac{1}{[(n^2-1)^2 - 4n^2]\cosh(2\beta L) - 4in(n^2-1)\sinh(2\beta L)}\right|^2$$

DATE: 20
PAGE No

$$a_3 = \frac{4ni\, e^{-i\alpha L}}{(n+i)^2 e^{-\beta L} - (n-i)^2 e^{\beta L}}$$

$$\beta L = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \cdot L >> 1$$

$$\therefore e^{-\beta L} << e^{\beta L}$$

$$a_3 = \frac{-4ni}{(n-i)^2} e^{-i\alpha L} \cdot e^{-\beta L}$$

$$a_3^* = \frac{4ni}{(n+i)^2} e^{i\alpha L} e^{-\beta L}$$

$$T = a_3 \cdot a_3^* = \frac{16n^2}{(n+i)^2(n-i)^2} e^{-2\beta L}$$

$$T = \frac{16n^2}{\underbrace{(n^2+1)^2}_{\approx 1}} e^{-2\beta L}$$

$$\therefore T \approx e^{-2\beta L} \approx \exp\left[-2\sqrt{\frac{2m(V_0-E)}{\hbar^2}} \cdot L\right] \neq 0$$

DATE: 20
PAGE No

Q. Show that change in Probability Density in a region of space is equal to the net change in probability density current in that region.

- Probability density, $\rho = \psi^* \cdot \psi$

Probability density current,

$$\vec{J}(\vec{r}, t) = \frac{i\hbar}{2m}(\psi \nabla \psi^* - \psi^* \nabla \psi)$$

eq.^{n} of continuity, $\boxed{\vec{\nabla} \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0}$

Sol.^{n} –
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \quad \text{— (1)}$$

now, $$\frac{\partial \rho(x,t)}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}$$

taking conjugate,

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

multiplying eq.^{n} (2) by ψ

$$-\frac{\hbar^2}{2m}\psi \frac{\partial^2 \psi^*}{\partial x^2} + V\psi\psi^* = -i\hbar\, \psi \frac{\partial \psi^*}{\partial t} \quad \text{— (3)}$$

multiplying eq.^{n} (1) by ψ^*

$$-\frac{\hbar^2}{2m}\psi^* \frac{\partial^2 \psi}{\partial x^2} + V\psi^*\psi = i\hbar\, \psi^* \frac{\partial \psi}{\partial t} \quad \text{— (4)}$$

DATE: 20
PAGE No

~~Adding (3) & (4)~~ (4) − (3)

$$i\hbar\left[\psi\frac{\partial\psi^*}{\partial t}+\psi^*\frac{\partial\psi}{\partial t}\right]=\frac{\hbar^2}{2m}\left(\psi\frac{\partial^2\psi^*}{\partial x^2}-\psi^*\frac{\partial^2\psi}{\partial x^2}\right)$$

$$\psi^*\frac{\partial\psi}{\partial t}+\psi\frac{\partial\psi^*}{\partial t}=\frac{i\hbar}{2m}\left[\psi^*\frac{\partial^2\psi}{\partial x^2}-\psi\frac{\partial^2\psi^*}{\partial x^2}\right]$$

$$\frac{\partial\rho}{\partial t}=\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial\psi}{\partial x}-\psi\frac{\partial\psi^*}{\partial x}\right]$$

$$\frac{\partial\rho}{\partial t}=-\frac{\partial}{\partial x}J(x,t)$$

$$\boxed{\frac{\partial\rho}{\partial t}+\frac{\partial J}{\partial x}=0}$$

In 3-D –

$$\boxed{\frac{\partial\rho}{\partial t}+\vec{\nabla}\cdot\vec{J}=0}$$

for stationary states, $\vec{\nabla}\cdot\vec{J}=0$

~~$y = A\sin(\omega t - kx)$~~
$y = A\sin(kx - \omega t)$

DATE: 20
PAGE No

Q. Show that the probability density current for a plane wave in a medium is equal to the product of probability density & velocity of particle in the medium

$$J=\rho\cdot v$$

$$v=\frac{\hbar k}{m}$$

$$\rho=\psi\cdot\psi^*$$

$$J=\frac{\hbar}{2im}\left[\psi^*\nabla\psi-\psi\nabla\psi^*\right]$$

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

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

$$J=\frac{\hbar}{2im}\left[|A|^2(ik)-|A|^2(-ik)\right]$$

$$J=\frac{\hbar}{2im}2\left[\psi\cdot\psi^*(ik)\right]$$

$$J=\frac{p}{m}\psi\cdot\psi^*$$

$$\boxed{J=\psi\cdot\psi^*\,v}$$

DATE: 20
PAGE No

Hermitian operators :-

$\hat{A} \rightarrow$ operator

$f, g \rightarrow$ ~~general~~ random wave f^ns

$$\int_{-\infty}^{+\infty} f^*(\hat{A}g)\,dV = \int_{-\infty}^{+\infty} (\hat{A}f)^* g\,dV$$

If operator $\hat{A}$ satisfies the above relation, then it is said to be Hermitian.

→ Bra-ket notations -

$$(f, \hat{A}g) = (\hat{A}f, g)$$

Q. Show that the momentum operator is Hermitian or not?

$$\hat{p} = -i\hbar\,\partial/\partial x$$

LHS-

$$\int_{-\infty}^{\infty} f^*(-i\hbar)\frac{\partial g}{\partial x}\,dx = -i\hbar\int_{-\infty}^{\infty} f^*\frac{\partial g}{\partial x}\,dx$$

$$= -i\hbar\left[f^*[g]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty}\frac{\partial f^*}{\partial x}g\,dx\right]$$

$$- i\hbar\int_{-\infty}^{+\infty}\frac{\partial f^*}{\partial x}g\,dx$$

DATE: 20
PAGE No

$$\int_{-\infty}^{\infty} -\hbar\left(\frac{\partial^2 f^*}{\partial x^2}\right)g$$

$$= \int_{-\infty}^{+\infty}\left(-i\hbar\frac{\partial f}{\partial x}\right)^* g\,dx = (\hat{p}_x f, g) = RHS$$

Q. Check whether $\hat{p}_x^2$ is Hermitian or not?

$$\hat{P}_x = -\hbar\frac{\partial^2}{\partial x^2}$$

LHS-

$$\int_{-\infty}^{\infty} f^* - \hbar\left(\frac{\partial^2}{\partial x^2}g\right)dx = -\hbar\int_{-\infty}^{\infty} f^*\frac{\partial^2 g}{\partial x^2}\,dx$$

$$= -\hbar\left[f^*\left[\frac{\partial g}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial f^*}{\partial x}\cdot\frac{\partial g}{\partial x}\,dx\right]$$

$$= +\hbar\int_{-\infty}^{\infty}\frac{\partial f^*}{\partial x}\cdot\frac{\partial g}{\partial x}\,dx$$

$$= \hbar\left[\frac{\partial f}{\partial x}[g]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial^2 f^*}{\partial x^2}g\,dx\right]$$

$$= \int_{-\infty}^{\infty}\left(-\hbar\frac{\partial^2 f}{\partial x}\right)^* g\,dx$$

→ Yes

Q. Check whether position ($\hat{x}$) & $i\partial/\partial x$ are Hermitian or not?

→ No

DATE: 20
PAGE No

Consequences of Hermitian operators –

(1) The expectation value of a dynamical quantity represented by Hermitian operator is always real.

proof: Let ψ_n be the wave f.n corresponding to nth quantum state for a system.
Let $\hat{A}$ be an operator which is Hermitian in nature. So the eigenvalue eq.n will be –

$$\hat{A}\psi_n = \lambda_n \psi_n$$

Since $\hat{A}$ is Hermitian –

$$\int_{-\infty}^{\infty} \psi_n^* (\hat{A}\psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{A}\psi_n)^* \psi_n\, dx$$

$$(\psi_n, \hat{A}\psi_n) = (\hat{A}\psi_n, \psi_n)$$

$$\text{LHS} = \int_{-\infty}^{\infty} \psi_n^* (\hat{A}\psi_n)\, dx$$

$$= \lambda_n \underbrace{\int_{-\infty}^{\infty} \psi_n^* \psi_n\, dx}$$

$$(\psi_n, \hat{A}\psi_n) = \lambda_n (\psi_n, \psi_n)$$

DATE: 20
PAGE No

$$\text{RHS} = \int_{-\infty}^{\infty} (\hat{A}\psi_n)^* \psi_n\, dx = \lambda_n^* \int_{-\infty}^{\infty} \psi_n^* \psi_n\, dx$$

$$(\hat{A}\psi_n, \psi_n) = \lambda_n^* (\psi_n, \psi_n)$$

$$\therefore \lambda_n(\psi_n, \psi_n) = \lambda_n^* (\psi_n, \psi_n)$$

$$(\lambda_n - \lambda_n^*)(\psi_n, \psi_n) = 0$$

normalisation condition = 1

$$\Rightarrow \boxed{\lambda_n = \lambda_n^*}$$

no imaginary part.

OR

$$\hat{A}\psi_n = \lambda_n \psi_n$$

$$(\psi_n, \hat{A}\psi_n) = (\hat{A}\psi_n, \psi_n)$$

$$\lambda_n(\psi_n, \psi_n) = \lambda_n^*(\psi_n, \psi_n)$$

$$(\lambda_n - \lambda_n^*)(\psi_n, \psi_n) = 0$$

$$\Rightarrow \boxed{\lambda_n = \lambda_n^*}$$

DATE: 20
PAGE No

(2) Two eigen f^{n}s of a Hermitian operator belonging to different eigen ~~st~~ values (states) are orthogonal.

proof: Let ψ_m & ψ_n are two wave f^{n}s corresponding to two diff. eigenstates of a system.

$$\hat{A}\psi_n = \lambda_n \psi_n \qquad \lambda_n \neq \lambda_m$$
$$\hat{A}\psi_m = \lambda_m \psi_m$$

$$(\psi_m, \hat{A}\psi_n) = (\hat{A}\psi_m, \psi_n)$$

$$\lambda_n(\psi_m, \psi_n) = \lambda_m^*(\psi_m, \psi_n)$$

$\because$ Operator $\hat{A}$ is hermitian, $\lambda_m^* = \lambda_m$

$$(\lambda_n - \lambda_m)(\psi_m, \psi_n) = 0$$

$$\lambda_n - \lambda_m \neq 0$$

$$\Rightarrow (\psi_m, \psi_n) = 0$$

$$\boxed{\int_{-\infty}^{\infty} \psi_m^* \cdot \psi_n \, dx = 0}$$

DATE: 20
PAGE No

★ Ehrenfest Theorem - It states that the quantum ~~ne~~ mechanics yields the same result as classical mechanics for the the motion of ~~a~~ wave packets associated with a moving particle if we take the average ~~of~~ (or expectation value) of the dynamical quantities involved.

$$p_x = m v_x$$
$$= \frac{d}{dt}(m \cdot x)$$

(1) $$\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}$$

(2) $$\langle F_x\rangle = -\left\langle \frac{dV}{dx}\right\rangle = \frac{d}{dt}\langle p_x\rangle$$

proof -

(1) $$\text{LHS} = \frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} \psi^* \cdot x\psi \, dx$$

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} \psi^* x \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \cdot x\psi \, dx$$

$$= \int_{-\infty}^{\infty} x\left[\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}\right] dx$$

now, $\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} = \frac{i\hbar}{2m} \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$

$$\therefore \frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} x \frac{i\hbar}{2m}\left[\frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]\right] dx$$

$$= - \int_{-\infty}^{\infty} \frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right] dx$$

$$\cancel{= \int_{-\infty}^{\infty} \frac{i\hbar}{2m} (\psi^*)^2 \left[\frac{\psi^* \partial\psi/\partial x - \psi\, \partial\psi^*/\partial x}{(\psi^*)^2}\right] dx}$$

$$\cancel{= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} (\psi^*)^2 \left[\frac{\psi^* \partial\psi/\partial x - \psi\, \partial\psi^*/\partial x}{(\psi^*)^2}\right] dx}$$

$$\cancel{= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} (\psi^*)^2 \frac{\partial}{\partial x}\left(\frac{\psi}{\psi^*}\right) dx}$$

$$\cancel{= -\frac{i\hbar}{2m} \left[(\psi^*)^2 \left[\frac{\psi}{\psi^*}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} 2(\psi^*) \frac{\partial \psi^*}{\partial x} \left(\frac{\psi}{\psi^*}\right) dx \right]}$$

$$\cancel{= \frac{i\hbar}{m} \int_{-\infty}^{\infty}}$$

DATE: 20
PAGE No

$$= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} (\psi)^2 \left(\frac{\psi^* \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x}}{(\psi)^2}\right) dx$$

$$= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} (\psi)^2 \frac{\partial}{\partial x}\left(\frac{\psi^*}{\psi}\right) dx$$

$$= \frac{i\hbar}{2m} \left[(\psi)^2 \left[\frac{\psi^*}{\psi}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} 2(\psi) \frac{\partial \psi}{\partial x} \times \frac{\psi^*}{\psi} dx \right]$$

$$= -\frac{i\hbar}{2m} \times 2 \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$= \frac{1}{m} \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \psi\right) dx$$

$$= \frac{\langle p_x \rangle}{m} = \text{RHS}$$

(2) LHS $= \langle F_x \rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{i\hbar}{m} \frac{\partial^2}{\partial x^2} \psi\right) dx$

$$= -\frac{i\hbar}{m} \left[\psi^* \left[\frac{\partial \psi}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \cdot \frac{\partial \psi}{\partial x} dx \right]$$

$$= \frac{i\hbar}{m} \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \cdot \frac{\partial \psi}{\partial x} dx$$

DATE: 20
PAGE No

$$= \frac{i\hbar}{m}\left[\frac{\partial \psi}{\partial x}\left[\psi^*\right]_{-\infty}^{\infty} - \int\right.$$

DATE: 20
PAGE No

CLASSICAL MECHANICS

★ Generalised coordinates :-

$$f(r_1, r_2, r_3, \ldots, r_N; t) = 0$$ Holonomic Constraint

$\neq 0$ non-

$$f(x_1, y_1, z_1; x_2, y_2, z_2; \ldots; x_N y_N z_N; t) = 0$$

$f(r, \dot{r}, t) = 0$ Bilateral → differential $(f(r, \dot{r}, t)) = 0$

→ Geometric

$f(r, \dot{r}, t) \geq 0$ Unilateral

$$f(\vec{r}, \dot{\vec{r}}, t) = 0 \rightarrow$$

$$f(r, \dot{\vec{r}}) = 0 \rightarrow$$

⊙ Note :- Virtual work done by forces in contraint motion is zero.

★ Generalised velocity :-

$$\vec{r} = r(q_1, q_2, q_3, \ldots, q_{3N}; t)$$

Euler's theorem -

$$X = x(x_1, x_2, x_3)$$

$$\delta X = \frac{\partial x}{\partial x_1}\delta x_1 + \frac{\partial x}{\partial x_2}\delta x_2 + \frac{\partial x}{\partial x_3}\delta x_3$$

displacement, $\delta \vec{r} = \sum_{j=1}^{3N} \frac{\partial \vec{r}}{\partial q_j} \delta q_j$

velocity, $\vec{v_i} = \frac{\partial \vec{r}}{\partial t} = \sum_{j=1}^{3N} \frac{\partial \vec{r_i}}{\partial q_j} \dot{q_j} + \frac{\partial \vec{r_i}}{\partial t}$

acc^n, $\vec{a_i} = \ddot{\vec{r_i}} = \frac{d}{dt}(\vec{v_i})$

$\ddot{\vec{r_i}} = \sum_j \frac{\partial \vec{r_i}}{\partial q_j} \dot{q_j} + \frac{\partial \vec{r_i}}{\partial t}$

$$\vec{a_i} = \sum_{j=1}^{3N} \left[\sum_{k=1}^{3N} \frac{\partial}{\partial q_j} \left(\frac{\partial r_i}{\partial q_k} \dot{q_k} + \frac{\partial r_i}{\partial t} \right) \dot{q_j} + \frac{\partial}{\partial t} \left(\sum_k \frac{\partial r_i}{\partial q_k} \dot{q_k} \right) \right]$$

$$\vec{a_i} = \sum_{j,k} \frac{\partial^2 r_i}{\partial q_j \partial q_k} \dot{q_j} \dot{q_k} + \sum_j \frac{\partial^2 r_i}{\partial q_j \partial \cancel{t}} \dot{q_j} + \sum_k \frac{\partial^2 r_i}{\partial q_k \partial t} \dot{q_k} + \frac{\partial^2 r_i}{\partial t^2}$$

Since 'j' is dummy index

$$\vec{a_i} = \ddot{\vec{r_i}} = \sum_{j,k} \frac{\partial^2 r_i}{\partial q_j \partial q_k} \dot{q_j} \dot{q_k} + 2 \sum_j \frac{\partial^2 r_i}{\partial q_j \partial t} \dot{q_j} + \frac{\partial r_i}{\partial t^2}$$

$\frac{1}{2} m v^2$

$\frac{1}{2} m (\dot{x}^2 + \dot{y}^2)$

Generalised K.E -

in classical mechanics, $T = \frac{1}{2} m_i (\dot{\vec{r_i}})^2$

$$KE = \frac{1}{2} \sum m_i (\dot{\vec{r_i}} \cdot \dot{\vec{r_i}})$$

$$= \frac{1}{2} \sum_i m_i \left[\sum_j \frac{\partial \vec{r_i}}{\partial q_j} \dot{q_j} + \frac{\partial \vec{r_i}}{\partial t} \right] \left[\sum_k \frac{\partial \vec{r_i}}{\partial q_k} \dot{q_k} + \frac{\partial \vec{r_i}}{\partial t} \right]$$

$$KE = \frac{1}{2} \sum_i \sum_j \sum_k m_i \frac{\partial^2 r_i}{\partial q_j \partial q_k} \dot{q_j} \dot{q_k} + \sum_i \sum_j m_i \frac{\partial^2 r_i}{\partial q_j \partial t} \dot{q_j} + \frac{1}{2} \sum_i m_i \left(\frac{\partial r_i}{\partial t} \right)^2$$

$$T = T^{(2)} + T^{(1)} + T^{(0)}$$

$T = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2)$

$x = r \cos\theta \qquad r^2 = x^2 + y^2$

$y = r \sin\theta \qquad \theta = \tan^{-1} y/x$

$\frac{\partial x}{\partial r} = \cos\theta, \quad \frac{\partial y}{\partial r} = \sin\theta$

$\frac{\partial x}{\partial \theta} = -r \sin\theta, \quad \frac{\partial y}{\partial \theta} = r \cos\theta$

$$T = \frac{1}{2} m \left[\left(\frac{\partial \vec{r}}{\partial r} \right) \left(\frac{\partial \vec{r}}{\partial r} \right) \dot{r} \dot{r} + \left(\frac{\partial \vec{r}}{\partial \theta} \right) \left(\frac{\partial \vec{r}}{\partial \theta} \right) \dot{\theta} \dot{\theta} + 2 \left(\frac{\partial \vec{r}}{\partial r} \right) \left(\frac{\partial \vec{r}}{\partial \theta} \right) \dot{r} \dot{\theta} \right]$$

DATE: 20
PAGE No

$$T = \frac{1}{2}m\Big[\Big(\frac{\partial(x\hat{i}+y\hat{j})}{\partial r}\Big)\cdot\Big(\frac{\partial(x\hat{i}+y\hat{j})}{\partial r}\Big)\dot{r}\dot{r} +$$

$$\frac{\partial(x\hat{i}+y\hat{j})}{\partial\theta}\cdot\frac{\partial(x\hat{i}+y\hat{j})}{\partial\theta}\dot{\theta}\dot{\theta} +$$

$$2\frac{\partial(x\hat{i}+y\hat{j})}{\partial r}\cdot\frac{\partial(x\hat{i}+y\hat{j})}{\partial\theta}\dot{r}\dot{\theta}\Big]$$

$$\therefore T = \frac{1}{2}m\left[\dot{r}^2 + r^2\dot{\theta}^2\right]$$

for i^{th} particle :- $T = \frac{1}{2}m_i\dot{x}_i^2$

$$p_{x_i} = m_i\dot{\vec{x}_i}$$

$$\boxed{p_{x_i} = \frac{\partial T}{\partial \dot{\vec{x}_i}}} \Rightarrow p_i = \frac{\partial T}{\partial \dot{q}_j}$$

Generalised force -

$$\delta W = \vec{F}\cdot\vec{dr}$$

$$\delta W = \sum_i \vec{F_i}\cdot\sum_j \frac{\partial \vec{r_i}}{\partial q_j}\cdot\delta q_j$$

$$\delta W = \sum_{i=1}^{N}\vec{F_i}\cdot\sum_{j=1}^{3N}\frac{\partial\vec{r_i}}{\partial q_j}\cdot\delta q_j$$

DATE: 20
PAGE No

$$\boxed{\delta W = \sum_j Q_j\cdot\delta q_j}$$

$\to$ Generalised force

$$Q_j = \sum_i \vec{F_i}\cdot\frac{\partial\vec{r_i}}{\partial q_j}\delta q_j$$

* D'Alembert's law :-

when the system is in eqlbm -

$$\delta W = \sum_i \vec{F_i}\cdot\delta\vec{r_i} = 0$$

$$\Rightarrow \sum_i \vec{F_i}^{(a)}\delta\vec{r_i} + \underbrace{\sum_i \vec{f_i}\cdot\delta\vec{r_i}}_{0} = 0$$

work done by constrained forces is zero

$$\Rightarrow \sum_i \vec{F_i}^{(a)}\cdot\delta\vec{r_i} = 0 \quad \to \text{in static eqlbm}$$

$i \to 1$ to N
$j \to 1$ to $3N$

for dynamical eqlbm -

$$\delta W = \sum_i(\vec{F_i} - \dot{\vec{p_i}})\cdot\delta\vec{r_i} = 0 \quad [\vec{F_i} = \vec{F_i}^{(a)}]$$

now, $\sum_{i,j}\dot{\vec{p_i}}\frac{\partial r_i}{\partial q_j}\delta q_j = \sum_i\dot{\vec{p_i}}\cdot\delta\vec{r_i}$

$$\therefore \sum_i\dot{\vec{p_i}}\cdot\delta\vec{r_i} = \sum_{i,j} m_i\ddot{r_i}\frac{\partial r_i}{\partial q_j}\delta q_j$$

$$= \sum_{i,j} \left[\frac{d}{dt}\left(m_i \dot{r}_i \frac{\partial r_i}{\partial q_j}\right) - m_i \dot{r}_i \frac{d}{dt}\left(\frac{\partial r_i}{\partial q_j}\right)\right] \delta q_j$$

$$= \sum_{i,j} \left[\frac{d}{dt}\left(m_i \dot{r}_i \frac{\partial r_i}{\partial q_j}\right) - m_i \dot{r}_i \frac{\partial \dot{r}_i}{\partial q_j}\right] \delta q_j$$

$$\sum_i \dot{\vec{p}}_i \cdot \delta \vec{r}_i = \sum_{i,j} \left[\frac{d}{dt}\left(m_i \vec{v}_i \frac{\partial \vec{r}_i}{\partial q_j}\right) - m_i \vec{v}_i \frac{\partial \vec{v}_i}{\partial q_j}\right] \delta q_j$$

now, $v_i = \frac{\partial r_i}{\partial q_j} \cdot \dot{q}_j$

differentiating both sides by $\dot{q}_j$

$$\frac{\partial v_i}{\partial \dot{q}_j} = \frac{\partial r_i}{\partial q_j}$$

$$\therefore \sum_i \dot{\vec{p}}_i \cdot \delta \vec{r}_i = \sum_{i,j} \left[\frac{d}{dt}\left[m_i \vec{v}_i \frac{\partial \vec{v}_i}{\partial \dot{q}_j}\right] - m_i \vec{v}_i \frac{\partial \vec{v}_i}{\partial q_j}\right] \delta q_j$$

$$= \sum_{i,j} \left[\frac{d}{dt}\left(\frac{\partial}{\partial \dot{q}_j}\left(\sum_i \frac{1}{2} m_i v_i^2\right)\right) - \frac{\partial}{\partial q_j}\left(\sum_i \frac{1}{2} m_i v_i^2\right)\right] \delta q_j$$

$$\sum_i \dot{\vec{p}}_i \cdot \delta \vec{r}_i = \sum_j \left[\frac{\partial}{\partial t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right] \delta q_j$$

DATE: 20
PAGE No

$$\therefore \delta W = \sum_j \left(Q_j - \left[\frac{\partial}{\partial t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right]\right) \delta q_j = 0$$

$$\Rightarrow Q_j \cdot \delta q_j = \left[\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right] \delta q_j$$

$$\therefore \boxed{Q_j = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}}$$

Lagrange's eq^n of motion

for conservative forces

$$Q_j = -\frac{\partial V}{\partial q_j}$$

$$\therefore -\frac{\partial V}{\partial q_j} = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial}{\partial q_j}(T - V) = 0$$

$ma = ka$

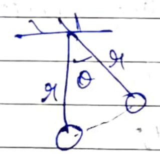
$$\because \frac{\partial V}{\partial q_i} = 0$$

$$\therefore \frac{d}{dt}\left(\frac{\partial (T-V)}{\partial \dot{q}_i}\right) - \frac{\partial}{\partial q_i}(T-V) = 0$$

Let $L = T - V$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

for a simple pendulum –



$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2)$$

$x = r\cos\theta$
$y = r\sin\theta$

$$\dot{x} = \frac{\partial x}{\partial t} = \dot{r}\cos\theta - r\sin\theta\,\dot{\theta}$$

$$\dot{y} = \frac{\partial y}{\partial t} = \dot{r}\sin\theta + r\cos\theta\,\dot{\theta}$$

$\dot{x}$ $\quad \frac{\partial\left(\frac{\partial x}{\partial t}\right)}{\partial q}$

$$T = \frac{1}{2}m[\dot{x}^2 + \dot{y}^2]$$
$$= \frac{1}{2}m\left[\dot{r}^2\cos^2\theta + r^2\sin^2\theta(\dot{\theta}^2) + \dot{r}^2\sin^2\theta + r^2\cos^2\theta(\dot{\theta})^2\right]$$

$$T = \frac{1}{2}m[\dot{r}^2 + r^2(\dot{\theta})^2]$$

$$V = mgr(1-\cos\theta)$$

$$L = T - V$$
$$L = \frac{1}{2}m[\dot{r}^2 + r^2(\dot{\theta})^2] - mgr(1-\cos\theta)$$

$$\frac{\partial L}{\partial r} = \frac{1}{2}m[2r(\dot{\theta})^2] - mg(1-\cos\theta)$$

$$\frac{\partial L}{\partial \theta} = \frac{1}{2}m[0] - mgr\sin\theta = -mgr\sin\theta$$

$$\frac{\partial L}{\partial \dot{r}} = m\dot{r}$$

$$\frac{\partial L}{\partial \dot{\theta}} = mr^2(\dot{\theta})$$

now, $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}}\right) - \frac{\partial L}{\partial r} = 0$

& $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0$

Problems on Lagrange's eqⁿ +

DATE: 20
PAGE No

for central forces -

$L = T - V$

$L = T - V(r)$

$L = \frac{1}{2} m (\dot{r}^2 + r^2 (\dot{\theta})^2) - V(r)$

$\frac{\partial L}{\partial r} = m r (\dot{\theta})^2 - V'(r)$

$\frac{\partial L}{\partial \dot{\theta}} = m r^2 (\dot{\theta})$

$\frac{\partial L}{\partial \dot{r}} = m \dot{r}$

$\boxed{\frac{\partial L}{\partial \theta} = 0}$

↳ cyclic coordinates

✱ Reyleigh's dissipation f^n -

frictional force ∝ velocity

$\vec{F}_{fx} = -[k_x v_{ix} \hat{i} + k_y v_{iy} \hat{j} + k_z v_{iz} \hat{k}]$

Let reyleight dissipation f^n be -

$\vec{\mathcal{F}} = \frac{1}{2} [k_x v_x^2 + k_y v_y^2 + k_z v_z^2]$

$\frac{\partial}{\partial \dot{q}_j}$

DATE: 20
PAGE No

$F_f = -\vec{\nabla}_v \cdot \mathcal{F}$

↳ velocity different operator

↳ $\hat{i}\left(\frac{\partial}{\partial v_x}\right) + \hat{j}\left(\frac{\partial}{\partial v_y}\right) + \hat{k}\left(\frac{\partial}{\partial v_z}\right)$

work done by frictional force -

$dw = -\vec{F}_f \cdot d\vec{r}$

$= -\vec{F}_f \cdot v\,dt$

$\frac{dw}{dt} = -\vec{F}_f \cdot \vec{v}$

$= [k_x v_{ix} \hat{i} + k_y v_{iy} \hat{j} + k_z v_{iz} \hat{k}] \cdot [v_x \hat{i} + v_y \hat{j} + v_z \hat{k}]$

$= k_x v_x^2 + k_y v_y^2 + k_z v_z^2$

$\boxed{\frac{dw}{dt} = 2\mathcal{F}}$

$Q_j = \sum_i F_i^{(a)} \cdot \delta \vec{r}_i$

$= \sum_i -\vec{\nabla}_v \cdot \mathcal{F} \cdot \frac{\partial \vec{r}}{\partial q_i} \cdot \delta q_i$

$= \sum_i -\vec{\nabla}_v \cdot \mathcal{F} \cdot \frac{\partial \vec{r}}{\partial q_j} \delta q_i$

DATE: 20
PAGE No

$$Q_j = -\sum_i \frac{\partial F}{\partial \dot{q}_j}\, \delta q_j$$

now, according to Lagrange's eqn

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = Q_j$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} + \frac{\partial F}{\partial \dot{q}_j} = 0$$

$$\frac{d}{dt}\left(\frac{\partial (T+F)}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = 0$$

$$\frac{d}{dt}\left(\frac{\partial}{\partial \dot{q}_j}(T-V)\right) - \frac{\partial (T-V)}{\partial q_j} = Q_j$$

★ Charged particle motion in EM field:

Lagrangian –

$$\vec{\nabla}\cdot\vec{E} = q/\epsilon_0$$

$$\vec{\nabla}\cdot\vec{B} = 0 \quad \Rightarrow \vec{B} = \vec{\nabla}\times\vec{A}$$

$$\vec{\nabla}\times\vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla}\times\vec{B} = \mu_0 \vec{J} + \mu_0\epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

DATE: 20
PAGE No

$$\vec{F} = q(\vec{v}\times\vec{B} + \vec{E})$$

now, $\vec{\nabla}\times\vec{E} = -\frac{\partial}{\partial t}(\vec{\nabla}\times\vec{A})$

$$\vec{\nabla}\times\vec{E} = -\vec{\nabla}\times\frac{\partial \vec{A}}{\partial t}$$

$$\therefore \vec{\nabla}\times\left(\vec{E} + \frac{\partial \vec{A}}{\partial t}\right) = 0$$

$$\Rightarrow \vec{E} + \frac{\partial \vec{A}}{\partial t} = -\vec{\nabla}\phi$$

$$\therefore \vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}$$

now, $\vec{F} = q\left[-\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} + \vec{v}\times(\vec{\nabla}\times\vec{A})\right]$

$$F_x = q\left[-\frac{\partial \phi}{\partial x} - \frac{\partial A_x}{\partial t} + \left[\vec{v}\times(\vec{\nabla}\times\vec{A})\right]_x\right]$$

now, $\vec{\nabla}\times\vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ A_x & A_y & A_z \end{vmatrix}$

$$= \hat{i}\left[\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right] - \hat{j}\left[\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right] + \hat{k}\left[\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right]$$

now, $\vec{\nabla} \times (\vec{\nabla} \times \vec{A}) = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ v_x & v_y & v_z \\ \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} & \frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial z} & \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \end{vmatrix}$

$$\vec{v} \times (\vec{\nabla} \times \vec{A}) = \hat{i}\left[v_y\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) - v_z\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\right]$$

$$[\vec{v} \times (\vec{\nabla} \times \vec{A})]_x = v_y\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) + v_z\left(\frac{\partial A_y}{\partial z} - \frac{\partial A_z}{\partial y}\right)$$

$$A_x = A_x(x, y, z, t)$$

$$\frac{dA_x}{dt} = \frac{\partial A_x}{\partial x}\frac{dx}{dt} + \frac{\partial A_x}{\partial y}\frac{dy}{dt} + \frac{\partial A_x}{\partial z}\frac{dz}{dt} + \frac{\partial A_x}{\partial t}$$

$$= v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_x}{\partial y} + v_z\frac{\partial A_x}{\partial z} + \frac{\partial A_x}{\partial t}$$

$$\frac{dA_x}{dt} - \frac{\partial A_x}{\partial t} = v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_x}{\partial y} + v_z\frac{\partial A_x}{\partial z} \quad \text{--- (1)}$$

→ Adding & Subtracting $v_x\frac{\partial A_x}{\partial x}$

$$[\vec{v} \times (\vec{\nabla} \times \vec{A})]_x = \left[v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_y}{\partial x} + v_z\frac{\partial A_z}{\partial x}\right] - \left[v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_x}{\partial y} + v_z\frac{\partial A_x}{\partial z}\right]$$

$$[\vec{v} \times (\vec{\nabla} \times \vec{A})]_x = \frac{\partial(\vec{v}\cdot\vec{A})}{\partial x} - \frac{dA_x}{dt} + \frac{\partial A_x}{\partial t}$$

now $$\vec{F} = q\left[-\frac{\partial\phi}{\partial x} - \frac{\partial A_x}{\partial t} + \frac{\partial(\vec{v}\cdot\vec{A})}{\partial x} - \frac{dA_x}{dt} + \frac{\partial A_x}{\partial t}\right]$$

$$\vec{F} = q\left[\frac{\partial}{\partial x}[\vec{v}\cdot\vec{A} - \phi] - \frac{dA_x}{dt}\right]$$

$$\vec{F} = q\left[-\frac{\partial}{\partial x}[\phi - \vec{v}\cdot\vec{A}] - \frac{d}{dt}\left(\frac{\partial(\vec{v}\cdot\vec{A})}{\partial v_x}\right)\right]$$

$$\vec{F} = q\left[-\frac{\partial}{\partial x}[\phi - \vec{v}\cdot\vec{A}] + \frac{d}{dt}\left(\frac{\partial}{\partial v_x}(\phi - \vec{v}\cdot\vec{A})\right)\right]$$

$$\because \frac{\partial\phi}{\partial v_x} = 0$$

Let $q(\phi - \vec{v}\cdot\vec{A}) = U$

$$\vec{F} = \frac{d}{dt}\left(\frac{\partial U}{\partial v_x}\right) - \frac{\partial}{\partial x}(U)$$

$$Q_j = -\frac{\partial U}{\partial q_j} + \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right)$$

$$= -\left[\frac{\partial U}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{q}_j}\right)\right] = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}$$

DATE: 20
PAGE No

$$\therefore \boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0}$$

where $L = T - U$

$$L = \frac{1}{2}mv^2 - q\phi + q\,\vec{v}\cdot\vec{A}$$

First integrals of Motion : Conservation Theorem

Calculate ~~Langrian~~ Lagrangian & its eq.^{n} for a particle moving in central forces (in 2-D).

$$U = V(r)$$

$$T = \frac{m}{2}(\dot{x}^2 + \dot{y}^2)$$

$$T = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2)$$

$$L = T - V(r)$$

$$= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r)$$

eq^{n}s –

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}}\right) - \frac{\partial L}{\partial r} = 0 \quad \text{— (1)}$$

DATE: 20
PAGE No

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0 \quad \text{— (2)}$$

for (1) –

$$\frac{d}{dt}(m\dot{r}) - mr\dot{\theta}^2 - V'(r) = 0$$

$$m\ddot{r} - mr\dot{\theta}^2 - \frac{\partial V}{\partial r} = 0$$

for (2) –

$$\frac{d}{dt}(mr^2\dot{\theta}) - 0 = 0$$

$$mr^2\ddot{\theta} = 0 \Rightarrow mr^2\dot{\theta} \rightarrow \text{constant}$$

- When a generalised coordinate is not present in the Lagrangian of the system, then the corresponding momentum of the system will be a constant. Such coordinates are known as cyclic coordinates.

$$L = T - V$$

$$\frac{d}{dt}\left(\frac{\partial (T-V)}{\partial \dot{q}_i}\right) - \frac{\partial (T-V)}{\partial q_i} = 0$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) + \frac{\partial V}{\partial q_j} = 0$$

$$\because \frac{\partial V}{\partial \dot{q}_j} = \frac{\partial T}{\partial q_j} = 0$$

if q_j is not present i.e. $\frac{\partial V}{\partial q_j} = 0$

$$\therefore \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) = 0$$

$$\therefore \frac{\partial T}{\partial \dot{q}_j} = p_j = \text{constant}$$

Conservation of Linear momentum -

if the displacement coordinate is cyclic i.e. translation of the system has no effect on description of the system remains invariant under such translation, then the corresponding linear momentum of the system is conserved.

$$d\vec{q_j} = \hat{n}\, d\vec{r_i}$$

now, $\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) + \frac{\partial V}{\partial q_j} = 0$

for angular momentum, $\hat{n} = \vec{r_i} \times \vec{n}$

$$\frac{d}{dt}(p_j) = -\frac{\partial V}{\partial q_j}$$

or $\dot{p}_j = -\frac{\partial V}{\partial q_j} = Q_j = 0$

$$\because Q_j = \sum_i \vec{F_i} \cdot \frac{\partial \vec{r_i}}{\partial q_j} = \sum_i \vec{F_i} \cdot \hat{n}$$

$$p_j = \sum_i \vec{p_i} \cdot \frac{\partial \vec{r_i}}{\partial q_j} = \sum_i \vec{p_i} \cdot \hat{n}$$

$$\dot{p}_j = 0$$

$$\Rightarrow p_j = \text{constant.}$$

Conservation of Energy -

$$L = L(q_i, \dot{q}_i)$$

$$\frac{dL}{dt} = \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt}$$

from Lagrange's eq^n of motion -

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$$

$$\therefore \frac{dL}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt}$$

DATE: 20
PAGE No

$$\frac{dL}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \cdot \dot{q}_j\right)$$

$$\because \frac{dL}{d\dot{q}_j} = p_j$$

$$\therefore \frac{d}{dt}(\dot{q}_j p_j) = \frac{d}{dt}(-L + \dot{q}_j p_j) = 0$$

$$\Rightarrow -L + \dot{q}_j p_j = \text{constant} = H \text{ (say)}$$

$$T = \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k \quad [\text{if 't' is not present}]$$

⊙ Euler theorem –
we have a f^n 'f' of the order 'n' which depends upon q_j coordinate, then euler's theorem says that –

$$\sum_n q_j \frac{\partial f}{\partial q_j} = nf$$

$$\rightarrow f = T, \quad n = 2$$

$$\sum_{n=2} \dot{q}_j \frac{\partial T}{\partial \dot{q}_j} = 2T = \sum_{n=2} \dot{q}_j p_j$$

now, $H = \dot{q}_j p_j - L$

$$H = 2T - (T - V)$$

$\boxed{H = T + V = E}$ → Energy is conserved

DATE: 20
PAGE No

Q. Setup Hamitonian for a particle in central field.

$$L = T - V$$
$$= \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) - V(r)$$

$$H = \dot{q}_j p_j - L$$

$$H = \dot{r} p_r + \dot{\theta} p_\theta - L$$

$$p_r = \frac{\partial T}{\partial \dot{r}} = m\dot{r}$$

$$\& \; p_\theta = \frac{\partial T}{\partial \dot{\theta}} = m r^2 \dot{\theta}$$

$$\therefore H = m\dot{r}^2 + m r^2 \dot{\theta}^2 - L$$

$$H = m\dot{r}^2 + m r^2 \dot{\theta}^2 - \frac{m\dot{r}^2}{2} - \frac{m r^2 \dot{\theta}^2}{2} + V(r)$$

$$H = \frac{1}{2} m\dot{r}^2 + \frac{1}{2} m r^2 \dot{\theta}^2 + V(r)$$

$$H = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) + V(r)$$

$$\boxed{H = T + V}$$

DATE: 20
PAGE No

(Hamilton's)

Hamiltonian's canonical eq^n of Motion :-

$$H = \sum_j \dot{q}_j p_j - L(q_j, \dot{q}_j, t)$$

$\because H = H(q_i, p_i, t)$

$$\Rightarrow dH = \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt \quad \text{--- (1)}$$

for $L = L(q_i, \dot{q}_i, t)$

$$dL = \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial t} dt$$

$$dH = \sum_j \dot{q}_j dp_j + \sum_j d\dot{q}_j \cdot p_j - dL$$

using (1)

$$\frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt = \sum_j \dot{q}_j dp_j + \sum_j d\dot{q}_j \cdot p_j - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i - \frac{\partial L}{\partial t} dt$$

using eq^n -

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

$$\& \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$$

DATE: 20
PAGE No

$$\frac{d}{dt}(p_i) = \frac{\partial L}{\partial q_i}$$

$$\dot{p}_i = \frac{\partial L}{\partial q_i}$$

now,

$$\frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial t} dt = \sum \dot{q}_i dp_i + \sum_i \cancel{\frac{\partial L}{\partial \dot{q}_i}} d\dot{q}_i - \frac{\partial L}{\partial q_i} dq_i - \cancel{\frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i} - \frac{\partial L}{\partial t} dt$$

on comparing coefficients -

$$\boxed{\begin{aligned} \frac{\partial H}{\partial q_i} &= -\frac{\partial L}{\partial q_i} = -\dot{p}_i \\ \frac{\partial H}{\partial p_i} &= \dot{q}_i \\ \& \quad \frac{\partial H}{\partial t} &= -\frac{\partial L}{\partial t} \end{aligned}} \rightarrow \text{Hamiton's eq}^n\text{s}$$

$\vec{\tau} = r \times F$

Central forces :- radially directive

$$f(r) = \pm \frac{K}{r^n}, \quad n \geq 0, \quad K = +ve$$

+ → repulsive
− → attractive

For a particle moving under central forces –
(i) Angular momentum is conserved
(ii) Areal velocity ⟶

Angular momentum –

$$L = \vec{r} \times \vec{p}$$

$$= r\hat{e}_r \times m\left(\frac{dr}{dt}\hat{e}_r + r\frac{d\theta}{dt}\hat{e}_\theta\right)$$

$$L = mr^2\frac{d\theta}{dt}(\hat{e}_r \times \hat{e}_\theta)$$

$$|L| = mr^2\dot{\theta}$$

from Lagrange's eqn

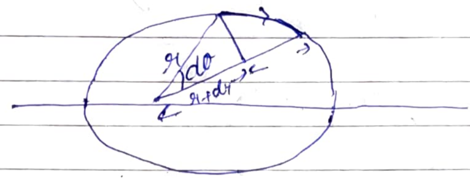
$$\frac{d}{dt}(mr^2\dot{\theta}) = 0$$

$mr^2\dot{\theta}$ → constant

L ⇒ constant

DATE: 20
PAGE No

Areal velocity conservation –



Areal velocity is defined as the surface area swept out by the radius vector '$\vec{r}$' per unit time during the planar motion of the particle under the influence of a central force.

$$dA = \frac{1}{2}\vec{r} \times d\vec{r} \quad \text{(in vector form)}$$

$$= \frac{1}{2}(r\hat{e}_r \times r\,d\theta\,\hat{e}_\theta)$$

$$= \frac{1}{2}r^2 d\theta\,\underbrace{(\hat{e}_r \times \hat{e}_\theta)}_{\hat{n}}$$

$$dA = \frac{1}{2}r^2 d\theta\,\hat{n}$$

Areal velocity, $\frac{dA}{dt} = \frac{1}{2}r^2\frac{d\theta}{dt}\hat{n} = \frac{L}{2m}\hat{n}$ → constant

DATE: 20
PAGE No

General eq^n of orbits under the influence of central force (Inverse square force) (attractive) -

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r)$$

$$r(t),\ \theta(t)$$

for $\theta(t) \Rightarrow$ $l = mr^2\dot{\theta}$

$$\dot{\theta} = \frac{L}{mr^2(t)}$$

$$\frac{d\theta}{dt} = \frac{L}{mr^2(t)}$$

$$\Rightarrow \boxed{\int d\theta = \int_0^t \frac{L}{mr^2(t)}\,dt}$$

for $r(t) \Rightarrow$ $E = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + V$

$$E = \frac{1}{2}m\dot{r}^2 + \left[\frac{l^2}{2mr^2} + V\right]$$ $\rightarrow$ effective potential

$$\frac{1}{2}m\dot{r}^2 = E - \frac{l^2}{2mr^2} - V$$

$$\dot{r}^2 = \frac{2}{m}\left[E - V - \frac{l^2}{2mr^2}\right]$$

DATE: 20
PAGE No

$$\dot{r} = \frac{dr}{dt} = \sqrt{\frac{2}{m}}\left(E - V - \frac{L^2}{2mr^2}\right)^{1/2}$$

$$\boxed{\int_0^t dt = \int_{r_0}^{r} \frac{dr}{\sqrt{2/m}\left(E - V - \frac{L^2}{2mr^2}\right)^{1/2}}}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}}\right) - \frac{\partial L}{\partial r} = 0$$

$$\frac{d}{dt}(m\dot{r}) - mr\dot{\theta}^2 + \frac{dV}{dr} = 0$$

$$m\ddot{r} - mr\dot{\theta}^2 + \frac{dV}{dr} = 0$$

$$\cancel{m\ddot{r} - \frac{L^2}{mr^3} + \frac{dV}{dr} = 0}$$

$$m\ddot{r} = -\frac{d}{dr}\left[\frac{l^2}{mr^3} + V\right]$$

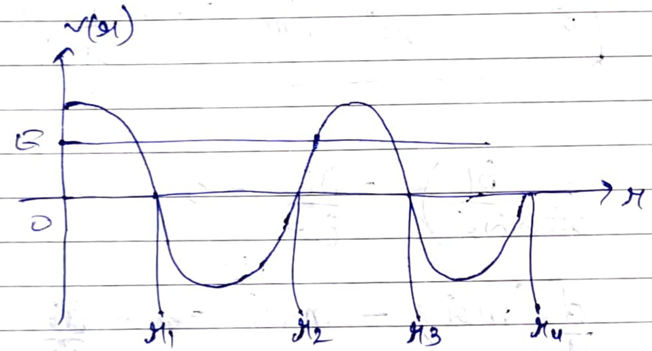
$$\frac{l^2}{mr^3} = \frac{m(r\dot{\theta})^2}{r} = \frac{mv_\theta^2}{r}$$

$\hookrightarrow$ fictitious force

DATE: 20
PAGE No

• for stable & unstable eqlbm.

$$\left.\frac{d^2V}{dr^2}\right|_{r=a} < 0 \qquad \left.\frac{d^2V}{dr^2}\right|_{r=a} > 0$$



$r < r_1 \to$ forbidden region

$r_1 \to r_2 \to$ apsidal distances

$\Rightarrow$ particle is trapped

<u>eqn of orbits</u> -

$$F_r = ma_r$$

$$-\frac{c}{r^2} = ma_r \qquad , c>0$$

$$-\frac{c}{r^2} = m\left[\frac{d^2r}{dt^2} - r\left(\frac{d\theta}{dt}\right)^2\right]$$

DATE: 20
PAGE No

using $\vec{L} = mr^2\dot{\theta}$

$|L| = mr^2\dot{\theta}$

$$\therefore \dot{\theta} = \frac{L}{mr^2} = \frac{k}{r^2} = ku^2 \text{ where } k = \frac{L}{m}$$

$$\& \quad r = \frac{1}{u} \Rightarrow \frac{dr}{dt} = -\frac{1}{u^2}\frac{du}{dt}$$

$$= -\frac{1}{u^2}\frac{du}{d\theta}\cdot\frac{d\theta}{dt}$$

$$\frac{dr}{dt} = -\frac{1}{u^2}\cdot ku^2\frac{du}{d\theta} = -k\frac{du}{d\theta}$$

$$\& \quad \frac{d^2r}{dt^2} = -k\frac{d}{dt}\left(\frac{du}{d\theta}\right)$$

$$= -k\left[\frac{d}{d\theta}\left(\frac{du}{d\theta}\right) * \frac{d\theta}{dt}\right]$$

$$\frac{d^2r}{dt^2} = -k\left[\frac{d^2u}{d\theta^2} * ku^2\right]$$

$$= -k^2u^2\frac{d^2u}{d\theta^2}$$

$$\text{now, } -cu^2 = m\left[-k^2u^2\frac{d^2u}{d\theta^2} - \frac{1}{u}(ku^2)^2\right]$$

$$-cu^2 = m\left[-k^2u^2\frac{d^2u}{d\theta^2} - k^2u^3\right]$$

DATE: 20
PAGE No

$$C = mh^2\left[\frac{d^2u}{d\theta^2} + u\right]$$

$$\frac{d^2u}{d\theta^2} + u = \frac{C}{mh^2} = A \text{ (say)}$$
[constant]

$$\frac{d^2u}{d\theta^2} + (u-A) = 0$$

$$\frac{d^2(u-A)}{d\theta^2} + (u-A) = 0$$

$$\therefore u - A = B\cos(\theta-\theta_0)$$

$$\frac{1}{r} = A + B\cos(\theta-\theta_0)$$

$$\frac{1}{r} = A\left[1 + \frac{B}{A}\cos(\theta-\theta_0)\right]$$

$$\boxed{\frac{p}{r} = 1 + e\cos(\theta-\theta_0)}$$

where $p = 1/A$ & $e = B/A$

unbounded ←
for
$e > 1$ → hyperbola
$e = 1$ → parabola

bounded ←
$e = 0$ → ~~ellipse~~ circle
$e < 1$ → ~~circle~~ ellipse

DATE: 20
PAGE No

perigee → $\frac{p}{r_{min}} = 1+e$, $\theta = 0$

apogee → $\frac{p}{r_{max}} = 1-e$, $\theta = \pi$

DATE: 20
PAGE No

DATE: 20
PAGE No

#

* Time independent Perturbation Theory -
(non-degenerate system)

⇒ Dirac Bra-ket notation -

ket vector : $|\phi\rangle = \phi(x,t)$
Bra vector : $\langle\phi| = \phi^*(x,t)$

$$\phi_i = \sum_i C_i \psi_i(x,t)$$

DUAL vector space → Hilbert vector space

Expectation value -

$$\langle\hat{A}\rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

$$\langle\hat{A}\rangle = \frac{(\psi, \hat{A}\psi)}{(\psi, \psi)} = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}$$

orthogonality condn $= \int_{-\infty}^{\infty} \psi_m^* \hat{A} \psi_n \, dx = 0$

$$\Rightarrow \langle\psi_m|\hat{A}|\psi_n\rangle = 0$$

orthonormality = $\int_{-\infty}^{\infty} \psi_m^* \hat{A} \psi_n \, dx = \delta_{mn}$

$\Rightarrow \langle \psi_m | \hat{A} | \psi_n \rangle = \delta_{mn}$

Hermitian operator -

$$\int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx = \int_{-\infty}^{\infty} (\hat{A}\psi)^* \psi \, dx$$

$$(\psi, \hat{A}\psi) = (\hat{A}\psi, \psi)$$

$$\langle \psi | \hat{A} | \psi \rangle = |\langle \psi | \hat{A} | \psi \rangle^*|$$

Perturbation theory -

for equilibm system / unperturbed system -

$$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$\frac{p^2}{2m} + V(x)$; $\psi_n^{(0)}$ unperturbed wave f^n ; $E_n^{(0)} \to$ unperturbed Energy

for particle in a box -

$$\psi_n^{(0)} = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$E_n^{(0)} = \frac{n^2 h^2}{8mL^2}$$

λ = perturbation parameter

$(\lambda^0, \lambda^1, \lambda^2, \ldots)$ $\to$ order of perturbation

now, system in slightly disturbed from its mean position.

$H\psi_n = E_n \psi_n$ perturbed Hamiltonian eq^n

$H = H_0 \lambda^0 + H' \lambda'$

$$\psi_n = \psi_n^{(0)} \lambda^0 + \psi_n^{(1)} \lambda' + \psi_n^{(2)} \lambda^2 + \ldots$$

$$E_n = E_n^{(0)} \lambda^0 + E_n^{(1)} \lambda' + E_n^{(2)} \lambda^2 + \ldots$$

substituting in above eq^n -

$$\Rightarrow (H_0 \lambda^0 + H'\lambda')(\psi_n^{(0)} \lambda^0 + \psi_n^{(1)} \lambda' + \psi_n^{(2)} \lambda^2 + \ldots)$$

$$= (E_n^{(0)} \lambda^0 + E_n^{(1)} \lambda' + E_n^{(2)} \lambda^2 + \ldots)(\psi_n^{(0)} \lambda^0 + \psi_n^{(1)} \lambda' + \psi_2^{(2)} \lambda^2)$$

$$\Rightarrow H_0 \psi_n^{(0)} + (H_0 \psi_n^{(1)} + H' \psi_n^{(0)}) \lambda + (H_0 \psi_n^{(2)} + H' \psi_n^{(1)}) \lambda^2 + \ldots$$

$$= E_n^{(0)} \psi_n^{(0)} + (E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}) \lambda + (E_n^{(0)} \psi_2^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}) \lambda^2 + \ldots$$

comparing coefficient of -

$\lambda^0 \to H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$

$\lambda' \to H_0 \psi_n^{(1)} + H' \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$

$\lambda^2 \to H_0 \psi_n^{(2)} + H' \psi_n^{(1)} = E_n^{(0)} \psi_2^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}$

$$\therefore \boxed{H_0\psi_n^{(j)} + H'\psi_n^{(j-1)} = E_n^{(0)}\psi_n^{(j)} + E_n^{(1)}\psi_n^{(j-1)} + \dots + E_n^{(j)}\psi_n^{(0)}}$$

$\hookrightarrow$ generalised perturbation eq^n

$$\boxed{\begin{aligned}\psi_n &= \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} \\ E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)}\end{aligned}}$$

$\hookrightarrow$ 2nd order correction in energy eigenvalues

** Correction for first order perturbation eq^n -

$$H_0\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$$

$$(H_0 - E_n^{(0)})\psi_n^{(1)} + (H' - E_n^{(1)})\psi_n^{(0)} = 0$$

pre multiply by $\psi_n^{(0)*}$ both sides & integrate over the volume 'V'.

$$\int_V \psi_n^{(0)*}(H_0 - E_n^{(0)})\psi_n^{(1)}\,dV + \int_V \psi_n^{(0)*}(H' - E_n^{(1)})\psi_n^{(0)}\,dV = 0$$

$$\langle \psi_n^{(0)} | H_0 - E_n^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_n^{(0)} | (H' - E_n^{(1)}) | \psi_n^{(0)} \rangle = 0 \quad \text{---} (1)$$

$\hookrightarrow$ H_0 is Hermitian in nature

$$\therefore \langle \psi_n^{(0)} | H_0 | \psi_n^{(1)} \rangle = \langle \psi_n^{(1)} | H_0 | \psi_n^{(0)} \rangle^*$$

now, $\langle \psi_n^{(1)} | H_0 | \psi_n^{(0)} \rangle^*$

we know $H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$

& $E_n^{(0)} = E_n^{(0)*}$

$$\therefore \langle \psi_n^{(1)} | H_0 | \psi_n^{(0)} \rangle^* = \langle \psi_n^{(1)} | E_n^{(0)}\psi_n^{(0)} \rangle^*$$

$$= E_n^{(0)*} \langle \psi_n^{(1)} | \psi_n^{(0)} \rangle$$

~~for~~ from eq^n (1)

$$\circledast \quad \langle \psi_n^{(0)} | H_0 - E_n^{(0)} | \psi_n^{(1)} \rangle = \langle \psi_n^{(0)} | E_n^{(0)} - E_n^{(0)} | \psi_n^{(1)} \rangle = 0$$

now, using eq^n (1)

$$\langle \psi_n^{(0)} | H' - E_n^{(1)} | \psi_n^{(0)} \rangle = 0$$

$$\langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle - E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle = 0$$

$$\therefore E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle = \int \psi_n^{(0)*} H' \psi_n^{(0)} dx$$

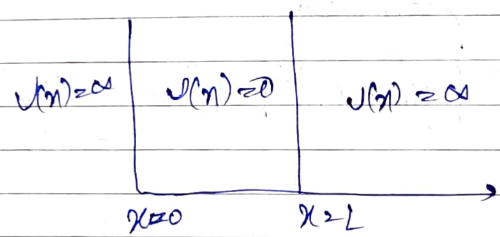
$$E_n^{(1)} = H'_{nn}$$

$$E_n = E_n^{(0)} + E_n^{(1)} \qquad \lambda = 1$$

Q. Consider an infinite 1-D potential well of length 'L' with walls at $x=0$ & $x=L$, that is modified at the bottom by a perturbation -

$$V_p(x) = \begin{cases} V_0 & 0 \le x \le L/2 \\ 0 & \text{otherwise} \end{cases}$$

Using 1st order perturbation theory, calculate E_n.



$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$E_n^{(0)} = \frac{n^2 h^2}{8mL^2}$$

now, correction, $E_n^{(1)} = \int \psi_n^{(0)*} V_0 \psi_n^{(0)} dx$

$$E_n^{(1)} = \int_0^{L/2} \left(\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\right) V_0 \left(\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\right) dx$$

$$E_n^{(1)} = \frac{2V_0}{L} \int_0^{L/2} \sin^2 \frac{n\pi x}{L} \, dx$$

$$= \frac{2V_0}{L} \int_0^{L/2} \left(\frac{1-\cos\frac{2n\pi x}{L}}{2}\right) dx$$

$$= \frac{V_0}{L} \left[x - \frac{\sin 2n\pi x/L}{\frac{2n\pi}{L}} \right]_0^{L/2}$$

$$= \frac{V_0}{L}\left[\frac{L}{2}\right] = V_0/2$$

now, $E_n = \frac{n^2h^2}{8mL^2} + \frac{V_0}{2} = E_n^{(0)} + E_n^{(1)}$

** Correction ~~of~~ for 2nd order perturbation eq.^{n} —

$$H_0 \psi_n^{(2)} + H' \psi_n^{(1)} = E_n^{(0)} \psi_n^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}$$

$$(H_0 - E_n^{(0)}) \psi_n^{(2)} + (H' - E_n^{(1)}) \psi_n^{(1)} = E_n^{(2)} \psi_n^{(0)}$$

pre multiply by $\psi_n^{(0)*}$ & integrate over the volume 'V'.

$$\int_V \psi_n^{(0)*} (H_0 - E_n^{(0)}) \psi_n^{(2)} dV + \int_V \psi_n^{(0)*} (H' - E_n^{(1)}) \psi_n^{(1)} dv = \int_V \psi_n^{(0)*} E_n^{(2)} \psi_n^{(0)} dV$$

DATE: 20
PAGE No

$$\Rightarrow \cancel{\langle \psi_n^{(0)} | H_0 - E_n^{(0)} | \psi_n^{(2)} \rangle} + \langle \psi_n^{(0)} | H' - E_n^{(1)} | \psi_n^{(1)} \rangle = E_n^{(2)} \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle$$

$$\therefore E^{(2)} = \frac{\langle \psi_n^{(0)} | H' - E_n^{(1)} | \psi_n^{(1)} \rangle}{\cancel{\langle \psi_n^{(0)} | \psi_n^{(0)} \rangle} \to 1}$$

$$E^{(2)} = \langle \psi_n^{(0)} | H' - E_n^{(1)} | \psi_n^{(1)} \rangle \quad \text{— (A)}$$

for 2nd order correction in energy we need to know first order corrected wave f^n.

Rayleigh Schrodinger method :-
The perturbed wave f^{n}s are expanded as orthonormal set of basis f^{n}s of unperturbed wave f^{n}s.

$$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$$\psi_n^{(1)} = \sum_k a_{nk}^{(1)} \psi_k^{(0)}$$

$$\psi_n^{(2)} = \sum_k a_{nk}^{(2)} \psi_k^{(0)}$$

The eq^n of the perturbed Hamiltonian-

$$H_0 \psi_n^{(1)} + H' \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$$

$$(H_0 - E_n^{(0)}) \psi_n^{(1)} + (H' - E_n^{(1)}) \psi_n^{(0)} = 0$$

DATE: 20
PAGE No

premultiply by $\psi_l^{(0)*}$ & integrating over 'v'

$$\Rightarrow \langle \psi_l^{(0)} | H_0 - E_n^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_l^{(0)} | H' - E_n^{(1)} | \psi_n^{(0)} \rangle = 0$$

$$\Rightarrow \langle \psi_l^{(0)} | H_0 - E_n^{(0)} | \sum_k a_{nk}^{(1)} \psi_k^{(0)} \rangle + \langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle - E_n^{(1)} \langle \psi_l^{(0)} | \psi_n^{(0)} \rangle = 0$$

$$\Rightarrow (E_l^{(0)} - E_n^{(0)}) \sum_l a_{nl}^{(1)} + H'_{ln} - E_n^{(1)} \delta_{ln} = 0$$

if $\delta_{ln} = 1$ i.e. $l = n$

$$H'_{nn} = E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

if $\delta_{ln} = 0$ i.e. $l \neq n$

$$(E_l^{(0)} - E_n^{(0)}) a_{nl}^{(1)} + H'_{ln} = 0$$

$$a_{nl}^{(1)} = \sum_{l \neq n} \frac{H'_{ln}}{E_n^{(0)} - E_l^{(0)}}$$

$$\therefore \boxed{\psi_n^{(1)} = \sum_{l \neq n} \frac{H'_{ln}}{E_n^{(0)} - E_l^{(0)}} \psi_n^{(0)}}$$

DATE: 20
PAGE No

second order perturbed eq^n -

$$H_0 \psi_n^{(2)} + H' \psi_n^{(1)} = E_n^{(0)} \psi_n^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}$$

$$(H_0 - E_n^{(0)}) \psi_n^{(2)} + (H' - E_n^{(1)}) \psi_n^{(1)} = E_n^{(2)} \psi_n^{(0)}$$

premultiply by $\psi_l^{(0)*}$ & integrate

$$\Rightarrow \langle \psi_l^{(0)} | H_0 - E_n^{(0)} | \psi_n^{(2)} \rangle + \langle \psi_l^{(0)} | H' - E_n^{(1)} | \psi_n^{(1)} \rangle = \langle \psi_l^{(0)} | E_n^{(2)} | \psi_n^{(0)} \rangle$$

$$\Rightarrow (E_l^{(0)} - E_n^{(0)}) \sum_l a_{nl}^{(2)} + \langle \psi_l^{(0)} | H' | \sum_k a_{nk}^{(1)} \psi_k^{(0)} \rangle$$

$$- \langle \psi_l | E_n^{(1)} | \psi_n^{(1)} \rangle = E_n^{(2)} \langle \psi_l^{(0)} | \psi_n^{(0)} \rangle$$

$$\Rightarrow (E_l^{(0)} - E_n^{(0)}) \sum_l a_{nl}^{(2)} + H'_{lk} a_{nk}^{(1)} - E_n^{(1)} a_{nl}^{(1)} = E_n^{(2)} \delta_{ln}$$

if $l = n$:

$$H'_{nk} a_{nk}^{(1)} - E_n^{(1)} a_{nn}^{(1)} = E_n^{(2)}$$

$$\therefore E_n^{(2)} = H'_{nk} a_{nk}^{(1)} - H'_{nn} a_{nn}^{(1)}$$

$$E_n^{(2)} = \sum_{n \neq k} H'_{nk} a_{nk}^{(1)}$$

$$\boxed{E_n^{(2)} = \sum_{n \neq k} H'_{nk} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}}}$$

DATE: 20
PAGE No

if $l \neq n$

$$(E_l^{(0)} - E_n^{(0)}) \sum a_{nl}^{(2)} + H'_{lk} a_{nk}^{(1)} = E_n^{(1)} a_{nl}^{(1)}$$

$$a_{nl}^{(2)} = \frac{E_n^{(1)} a_{nl}^{(1)} - H'_{lk} a_{nk}^{(1)}}{E_l^{(0)} - E_n^{(0)}}$$

$$a_{nl}^{(2)} = \frac{H'_{nn} a_{nl}^{(1)} - H'_{lk} a_{nk}^{(1)}}{E_l^{(0)} - E_n^{(0)}}$$

$$a_{nl}^{(2)} = \sum_{l \neq n} \frac{H'_{nn} H'_{nl}}{[E_l^{(0)} - E_n^{(0)}]^2} - \frac{H'_{lk} H'_{nk}}{(E_l^{(0)} - E_n^{(0)})(E_n^{(0)} - E_k^{(0)})}$$

$$\therefore \psi_n^{(2)} = \sum_k a_{nk}^{(2)} \psi_k^{(0)}$$

★ Variational Methods :-

$$E_1 \leq \langle \phi | H | \phi \rangle$$

$$E_1 \leq \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

$\to$ Rayleigh's Ratio

$$\langle H \rangle = \langle \phi | H | \phi \rangle$$

$$\phi = \sum_i c_i | \psi_i \rangle$$

Bra vector → j
Ket vector → i

$$\langle H \rangle = \sum_i \sum_j c_j^* \langle \psi_j | H c_i | \psi_i \rangle$$

$$= \sum_i \sum_j c_j^* c_i \langle \psi_j | H | \psi_i \rangle$$

$$\langle H \rangle = \sum_{i,j} c_j^* c_i E_i \langle \psi_j | \psi_i \rangle$$

$$= \sum_j |c_j|^2 E_j$$

$$E_j = E_1 + \Delta E_j$$

$$\langle H \rangle = \sum_j |c_j|^2 E_1 + \sum_j |c_j|^2 \Delta E_j$$

$$= E_1 \sum_j |c_j|^2 + \sum_j |c_j|^2 \Delta E_j$$

$$\sum_j |c_j|^2 = 1, \quad \Delta E_j \to +ve$$

$$\therefore \boxed{\langle H \rangle \geq E_1}$$

Q. The schrodinger eq^n of a particle confined to x-axis is given by

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

$$\psi(0) = 0, \quad \psi(x) = 0 \quad \text{at } x \to \infty$$

Use trial f^n $\phi(x) = x e^{-\alpha x}$ to obtain the best value.

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + mgx$$

$$\langle H \rangle = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

now, $\langle \phi | \phi \rangle = \int_0^\infty x e^{-\alpha x} \cdot x e^{-\alpha x} dx$

$$= \int_0^\infty x^2 \cdot e^{-2\alpha x} dx$$

$$= \left[x^2 \frac{e^{-2\alpha x}}{-2\alpha} + \frac{1}{\alpha} \int x e^{-2\alpha x} dx \right]_0^\infty$$

$$= \frac{1}{4\alpha^3}$$

DATE: 20
PAGE No

now, $\langle \phi | H | \phi \rangle = \int_0^\infty x e^{-\alpha x} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} (x e^{-\alpha x}) \right) dx$

$+ \int_0^\infty x e^{-\alpha x} (mgx) x e^{-\alpha x} dx$

now, $\frac{d^2}{dx^2} (x e^{-\alpha x}) = ?$

$\frac{d}{dx} (x e^{-\alpha x}) = x(-\alpha) e^{-\alpha x} + e^{-\alpha x}(1)$

$= e^{-\alpha x} [1 - \alpha x]$

$\frac{d^2}{dx^2} (x e^{-\alpha x}) = e^{-\alpha x} [-\alpha] + (1-\alpha x)(-\alpha) e^{-\alpha x}$

$= e^{-\alpha x} [(1-\alpha x)(-\alpha) - \alpha]$

$= -\alpha e^{-\alpha x} [\cancel{1} - \alpha x + \cancel{1}]$

$= \alpha e^{-\alpha x} [\alpha x - 2]$

~~now, $\langle \phi | H | \phi \rangle = \int_0^\infty x e^{-\alpha x} \left(-\frac{\hbar}{2m} \right) \alpha x e^{-\alpha x} dx$~~

~~$+ \int_0^\infty x e^{-\alpha x} (mg x) x e^{-\alpha x} dx$~~

DATE: 20
PAGE No

now, $\langle \phi | H | \phi \rangle = \int_0^\infty x e^{-\alpha x} \left(-\frac{\hbar^2}{2m} \right) (\alpha e^{-\alpha x} (\alpha x - 2)) dx$

$+ \int_0^\infty x e^{-\alpha x} (mgx) x e^{-\alpha x} dx$

$= -\frac{\hbar^2}{2m} \int_0^\infty \alpha x e^{-2\alpha x} (\alpha x - 2) dx$

$+ mg \int_0^\infty x^3 e^{-2\alpha x} dx$

$\langle H \rangle = \frac{\hbar^2 \alpha^2}{2m} + \frac{3}{2} \frac{mg}{\alpha}$

$\frac{d}{d\alpha} \langle H \rangle = \frac{2\hbar^2 \alpha}{2m} - \frac{3}{2} \frac{mg}{\alpha^2} = 0$

$\frac{\hbar^2 \alpha}{m} - \frac{3}{2} \frac{mg}{\alpha^2} = 0$

$\Rightarrow \alpha = \left(\frac{3m^2 g}{2\hbar^2} \right)^{1/3}$