

Classical AND Quantum Mechanics

of Schrödinger Equation $\xrightarrow{\text{Independent / Steady state}}$ $\xrightarrow{\text{Time dependent}}$

Q Metal wave associated with the moving Particles travels with a speed more than velocity of light?

Ans It is true,

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

v = Particle velocity

$$v_p = v\lambda$$

$$= \frac{mc^2}{h} \times \frac{h}{mv}$$

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

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

De-Broglie eq.

$$hv = mc^2$$

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

Wave Packet \rightarrow Superposition of all monochromatic wave.

$$\lambda \pm d\lambda$$

Need of SEL:

\rightarrow apply on IInd law of Newton ($F = ma$)

\rightarrow valid for all particle whose velocity less than moving instant of time.

$$\left| \frac{d^2y}{dt^2} = v^2 p \frac{d^2y}{dx^2} \right. \quad v \text{ wave eq}$$

$$y(x, t) = y = A \sin [i(kx - \omega t)]$$

$$k = \text{wave no.} = \frac{2\pi}{\lambda}$$

$$\omega = \text{angular frequency}$$

$y \rightarrow$ function of
pressure & density

$$\Psi(x, t) = A e^{i(kx - \omega t)} \Rightarrow \frac{d\Psi(x, t)}{dx} = A e^{i(kx - \omega t)} \cdot ik$$

$$\Rightarrow \frac{d\Psi(x, t)}{dx} = ik\Psi(x, t)$$

$$= i\frac{\hbar}{\hbar} \hat{p} \Psi(x, t)$$

$$-i\hbar \frac{\partial}{\partial x} \Psi(x, t) = \hat{p}\Psi(x, t)$$

$-i\hbar \frac{\partial}{\partial x} = \hat{p}$ → Momentum operator

Energy operator

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

K.E. & Operator

* Wave Function

- (1) Complex function
- (2) operator
- (3) Expectation value
- (4) Hamilton operator - $H\Psi(x, t) = E\Psi(x, t)$
Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \quad [H = \frac{p^2}{2m} + V]$$

- (5) wave fun. should be in a boundary condition

Particle is moving free in space $V=0$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = i\hbar \frac{\partial \Psi}{\partial t}$$

$$E = \frac{me^4}{8E_0^2 h^2}$$

* Schrodinger equation : (Steady - state form)

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} \quad (\text{uncertainty principle}) \quad (\hbar = \frac{\hbar}{2\pi}) \quad \left| \begin{array}{l} \Delta E \Delta t \geq \hbar \\ \Delta E = \frac{\hbar}{\Delta t} \end{array} \right.$$

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

$$\hat{L} \psi(n,t) = g \psi(n,t)$$

eigen value
of operator \hat{L}

$$\hat{L} = \frac{d^2}{dx^2} e^{2x} = 4e^{2x}$$

$$\therefore \psi(n,t) = e^{2x}$$

(eigen value) $g = 4$

$$\Psi(n,t) = A \cdot e^{ikx - \omega t}$$

$$\frac{d\Psi(n,t)}{dt} = ik \cdot \Psi(n,t)$$

$$= \frac{i\hbar}{\hbar} \psi(n,t)$$

$$-i\hbar \frac{d(\psi(n,t))}{dt} = p \psi(n,t)$$

$$-i\hbar \frac{d}{dt} = \hat{p}$$

$$\hat{L} \psi(n,t) = \frac{\hbar^2}{2m} \psi(n,t) + V(n) \psi(n,t)$$

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

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

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

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

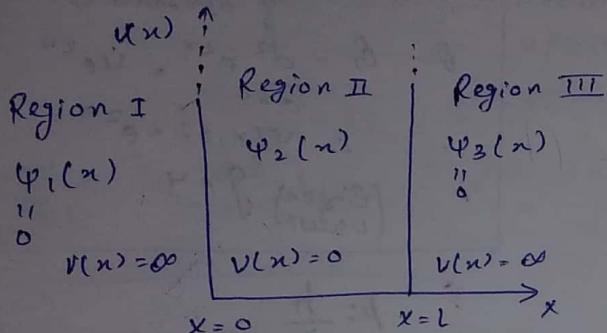
$$p \rightarrow -i\hbar \frac{d}{dx}$$

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

Probability in a small volume dv = $|\Psi(x,t)|^2 dv$

Total Prob. of finding particle in universe = $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$

* Particle trapped in 1-D box with impenetrable walls:



$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

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

$$\Psi(x,t) = A e^{(ikx - i\omega t)}$$

$$\Psi(x,t) = \Psi(x) \cdot e^{-i\omega t}$$

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \Psi(x) = 0 \quad (\text{Steady form})$$

$$\frac{d^2\Psi_1}{dx^2} + \frac{2m}{\hbar^2} (E - \infty) \Psi_1 = 0 \quad \text{Region I}$$

$$\frac{d^2\Psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - 0) \Psi_2 = 0 \quad \text{Region II}$$

$$\frac{d^2\Psi_3}{dx^2} + \frac{2m}{\hbar^2} (E - \infty) \Psi_3 = 0 \quad \text{Region III}$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad (\text{Region II}) \quad \left(k^2 = \frac{2mE}{\hbar^2} \right)$$

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

Boundary conditions \rightarrow wave function should be finite
 \rightarrow " " " " , single value
 \rightarrow " " " " continuous

for boundary condition ① $\psi(x) \rightarrow$ finite

$$\textcircled{2} \quad \begin{aligned} \text{at } x=0 & \quad \psi(x)=0 \\ x=L & \quad \psi(x)=0 \end{aligned}$$

$$A \sin 0 + B \cos 0 = 0 \quad B=0$$

$$A \sin kL = 0 \quad A \neq 0 \Rightarrow \sin kL = 0$$

$$kL = n\pi \quad \boxed{k = \frac{n\pi}{L}}$$

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

$$\psi_n(x) = A \sin \frac{n\pi}{L} x$$

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = 1$$

$$k = \frac{n\pi}{L}$$

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

$$\int_{-\infty}^{+\infty} \psi_1(x)^2 dx + \int_0^L \psi_2(x)^2 dx + \int_L^{+\infty} \psi_3(x)^2 dx = 1$$

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

1. Plot 1st 3 wave fun.

$$\textcircled{2} \quad |\psi_n(x)|^2$$

(3) Momentum values

(4) Energy Eigenvalues

$$\textcircled{1} \quad A^2 \int_0^L \sin^2 kx dx = 1$$

$$\int_0^L (k - \cos 2kx) dx = 1$$

$$A^2 [L - \sin 2kL] = 1$$

$$\frac{A^2}{2} [L - \sin^2 \left(\frac{n\pi}{L} \cdot L \right)] = 1$$

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

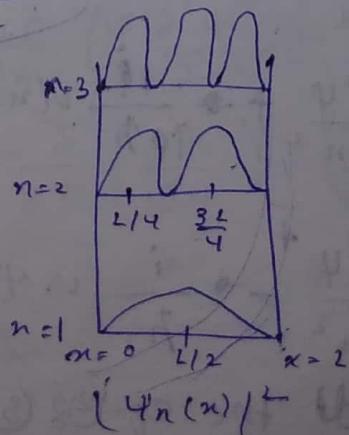
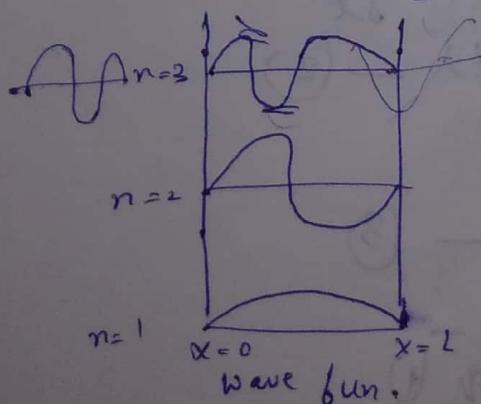
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

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

$$A^2 = \frac{2}{L}$$

$$|\psi_n(x)|^2 = \frac{2}{L} \sin^2 \frac{n\pi x}{L}, \quad n = 1, 2, 3, \dots$$

$$A = \sqrt{\frac{2}{L}}$$



$$|\psi_3(x)|^2$$

$$|\psi_2(x)|^2$$

$$E_2 = \frac{4\hbar^2}{8mL^2}$$

3D Schrödinger eq. -

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(n,t) + v(n) \psi(n,t) = i\hbar \frac{\partial \psi(n,t)}{\partial t}$$

* Probability Density and current density

$$P(n,t) = \psi^*(n,t) \psi(n,t)$$

$$S(x,t) = \frac{i\hbar}{2m} \left[\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right] \quad - 1 - D$$

$$-\frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad - 3 D$$

$$\Psi = \psi(r,t)$$

Ques Show that change in probability density in a region of space is equal to the ~~region of~~ net change in probability current density into that region.

$$\frac{d}{dt} \int_{n_1}^{n_2} P dx = S(n_1, t) - S(n_2, t)$$

Ans

$$\int_{n_1}^{n_2} P dx = \int_{n_1}^{n_2} \psi^* \psi dx$$

$$\frac{d}{dt} \int_{n_1}^{n_2} \psi^* \psi dx = \int_{n_1}^{n_2} \frac{d\psi^*}{dt} \psi dx + \int_{n_1}^{n_2} \psi^* \frac{d\psi}{dt} dx \quad ①$$

Schrodinger eq. $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(n,t)}{\partial n^2} + v(n) \psi(n,t) = i\hbar \frac{\partial \psi(n,t)}{\partial t}$

$$\frac{d\psi}{dt} = \frac{-i\hbar^2}{2m} \frac{\partial^2 \psi}{\partial n^2} + \frac{i\hbar}{m} v(n) \psi(n,t) \quad - (2)$$

$$\frac{\partial \psi^*}{\partial t} = \frac{-i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial n^2} - \frac{i}{\hbar} v \cdot \psi^* \quad - (3)$$

Add the eq. (2) & (3) in eq. ①

$$\frac{d}{dt} \int_{x_1}^{x_2} \psi^* \psi dx = \int_{x_1}^{x_2} -\frac{i\hbar}{2m} \cdot \frac{\partial^2 \psi^* \psi}{\partial x^2} + \frac{i}{\hbar} v \psi^* dx + \left[\int_{x_1}^{x_2} \psi^* + \frac{\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{i\hbar} v(x) \psi(x, t) dx \right]$$

$$\begin{aligned} \frac{d}{dt} \int_{x_1}^{x_2} \psi^* \psi dx &= \frac{i\hbar}{2m} \int_{x_1}^{x_2} \left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} \right) dx \\ &= \frac{i\hbar}{2m} \int_{x_1}^{x_2} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) dx \end{aligned}$$

$$= -S(x_2, t) + S(x_1, t) \quad \underline{\text{Hence Proved}}$$

$\frac{d}{dt} \int_{x_1}^{x_2} P dx$ is the Probability density b/w the x_1, x_2 . It indicating the total particle present in x_1 to x_2 . Time of rate change of probability b/w two points x_1 & x_2 at any instant of time is equal to the change in probability current density.

Difference b/w the Prob. Current density x_2 & Prob. flowing out at x_2

$$\frac{dP}{dt} = \frac{d}{dt} (\psi^* \psi)$$

$$\frac{dP}{dt} = \frac{d\psi^* \psi}{dt} + \psi^* \frac{d\psi}{dt}$$

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

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

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

$$P = S(x_1, t)$$

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

$$\frac{\partial P}{\partial t} + \frac{\partial J(x,t)}{\partial x} = 0 \quad \text{--- 1D}$$

$$\frac{\partial P}{\partial t} + \vec{\nabla} \cdot \vec{J}(x,t) = 0 \quad \text{3-D}$$

Q Show that the Probability density current for a plane wave in a medium is equal to the prob. density multiplied by the velocity of particle in that region.

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

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

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

$$\text{viewed } \partial J(x,t) = \frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right)$$

$$= \frac{i\hbar}{2m} \left[\psi \left(A k e^{i(kx - \omega t)} \right)^* - \psi^* \left(A k e^{i(kx - \omega t)} \right) \right]$$

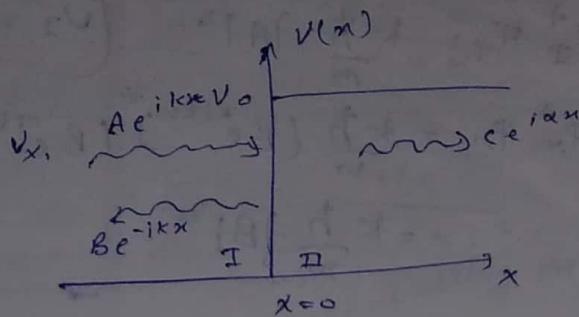
$$= \frac{i\hbar k}{m} \psi (\psi^* \psi)$$

$$= v_{\text{particle}} (\psi^* \psi)$$

$$\left[\left(\frac{\psi^*}{\psi} \psi - \frac{\psi^* \psi}{\psi} \right) \frac{d\psi}{dx} \right] \frac{d}{dt} = \frac{d}{dt}$$

$$\left(\frac{\psi^*}{\psi} \psi - \frac{\psi^* \psi}{\psi} \right) \frac{d\psi}{dx} = 0$$

Step Potential



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

Case I $E > V_0$ Region I

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_1 = 0$$

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

$$\therefore \frac{d^2\psi_1}{dx^2} + k^2 \psi_1 = 0$$

$$\psi_1(x) = \underbrace{A e^{ikx}}_{\text{incident beam}} + \underbrace{B e^{-ikx}}_{\text{reflected wave}}$$

$$(D^2 + k^2) \psi_1 = 0$$

$$D = \pm ik$$

Region II

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

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

$$\therefore \frac{d^2\psi_2}{dx^2} + \alpha^2 \psi_2 = 0$$

$$\psi_2 = \underbrace{C e^{i\alpha x}}_{\text{transmitted wave}} + \underbrace{D e^{-i\alpha x}}_{\text{no reflected wave}}$$

$D e^{-i\alpha x} = 0$
There is no boundary in Reg. 2, so that there is no reflected wave.

Reflectance / Reflected current density (J_R)

Transmittance / Transmitted current density (J_t)

$E > V_0$

To Prove : $J_R + J_t = J_I$ $(J_I \rightarrow \text{incident current density})$

$$R + T = 1 \quad \text{---} \quad \textcircled{I}$$

$$\frac{J_R}{J_I} + \frac{J_t}{J_I} = 1$$

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

$$J_I = v_I \psi_I^* \psi_I = \frac{\kappa \hbar}{m} |A|^2 \quad (v_I = \frac{\kappa \hbar}{m})$$

$$\begin{aligned} J_R &= v_R \psi_R^* \psi_R = \frac{\kappa \hbar}{m} (B e^{ikx})^* (B e^{-ikx}) \quad (\psi_R = B e^{ikx}) \\ &= \frac{\kappa \hbar}{m} |B|^2 \end{aligned}$$

$$\begin{aligned} J_T &= v_T \psi_T^* \psi_T = \frac{\alpha \hbar}{m} (C e^{ixn})^* (C e^{ixn}) \quad (\psi_T = C e^{-ixn}) \\ &= \frac{\alpha \hbar}{m} |C|^2 \quad (v = \frac{\alpha \hbar}{m}) \end{aligned}$$

$$R = \frac{J_R}{J_I} = \frac{|B|^2}{|A|^2} = ? \quad , \quad T = \frac{J_T}{J_I} = \frac{\alpha}{\kappa} \frac{|C|^2}{|A|^2}$$

Boundary condition,

$$\rightarrow x = \pm \infty, \text{ finite everywhere} \rightarrow A e^{ikx} + B e^{-ikx} = C e^{ixn} \quad \text{Putting } n=0$$

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

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \Rightarrow ik(A - B) = i\alpha C$$

$$A + B = C \quad \text{--- (1)}$$

$$A - B = \frac{\alpha}{\kappa} C \quad \text{--- (2)}$$

Solving eq. (1) & (2)

$$A - (C - A) = \frac{\alpha}{\kappa} C \quad \text{--- (1)}$$

$$A - C + A = \frac{\alpha}{\kappa} C \Rightarrow 2A - C = \frac{\alpha}{\kappa} C$$

$$\frac{\alpha}{\kappa} + C = 2A$$

$$C \left(\frac{\alpha + \kappa}{\kappa} \right) = 2A$$

$$C = 2A \left(\frac{\kappa}{\alpha + \kappa} \right)$$

Similarly

$$\therefore \boxed{T =}$$

Case II

$$\kappa^2 = \frac{2mE}{\hbar^2}$$

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

$$\frac{d^2\psi_1}{dx^2}$$

$$\psi_1(n) =$$

$$J_I$$

$$J_R =$$

$$J_T$$

$$\text{Similarly, } B = \left(\frac{k-\alpha}{k+\alpha} \right) A$$

$$\therefore \left[R = \frac{J_T}{J_I} = \frac{|B|^2}{|A|^2} = \left(\frac{k-\alpha}{k+\alpha} \right)^2 \right]$$

$$\left[T = \frac{J_t}{J_I} = \frac{\alpha |C|^2}{k |A|^2} = \frac{4\alpha k}{(k+\alpha)^2} \right]$$

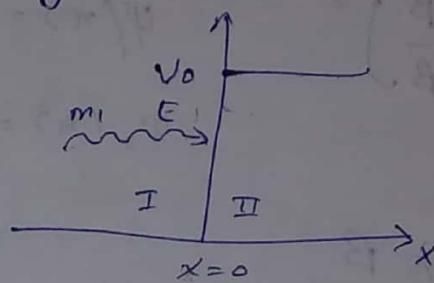
By putting the value of R & T in Q.I
we proved the eq

Case II $E < V_0$

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

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

$$V(x) = 0 \quad x < 0 \\ = V_0 \quad x > 0$$



$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2} (E - 0) \psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + k^2 \psi_1 = 0$$

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

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

$$\frac{d^2\psi_2}{dx^2} - \beta^2 \psi_2 = 0$$

$$\psi_2(x) = ce^{\beta x} + de^{-\beta x}$$

$$\alpha^2 + \beta^2 = 0$$

$$\alpha = \pm \beta$$

$$J_I = V_I \psi_I^* \psi_I \Rightarrow \frac{k\hbar}{m} (A e^{ikx})^* (A e^{ikx}) \Rightarrow \frac{k\hbar}{m} |A|^2$$

$$J_T = V_T \psi_T^* \psi_T \Rightarrow \frac{k\hbar}{m} (B e^{ikx})^* (B e^{ikx}) \Rightarrow \frac{k\hbar}{m} |B|^2$$

$$J_T = V_T \psi_T^* \psi_T \Rightarrow \frac{k\hbar}{m} (c e^{\beta x})^* (c e^{\beta x}) \Rightarrow \frac{k\hbar}{m} |C|^2$$

Boundary condition,

$x = \pm \infty$, finite everywhere
at $x = 0$, $\psi_1 = \psi_2$

$$\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x} \quad A + B = 0$$

$$R = \frac{V_1}{V_2} \cdot \frac{|B|^2}{|A|^2} = \frac{|B|^2}{|A|^2}, \quad T = \frac{V_2}{V_1} \cdot \frac{|C|^2}{|A|^2} = \frac{|C|^2}{|A|^2} \quad A - B = \frac{i\beta D}{K}$$

$$R = \left(\frac{iK - \beta}{iK + \beta} \right)^2$$

$$\psi_1(x) = A e^{ikx} + A \left(\frac{iK - \beta}{iK + \beta} \right) \cdot e^{-ikx}$$

$$\psi_2(x) = A \left(\frac{2ik}{iK + \beta} \right) \cdot e^{-\beta x}$$

$$T = \frac{4K\beta}{(iK + \beta)^2}$$

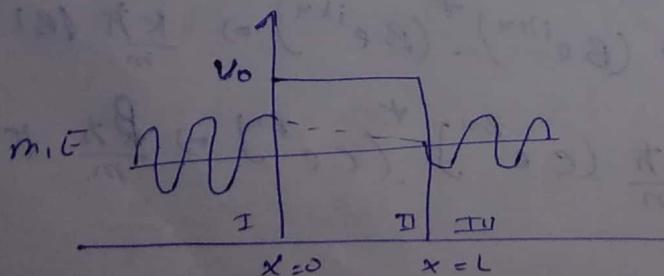
Penetration depth:

$$\psi_2(\text{at } x = \Delta x) = \frac{1}{e} \psi_2(x = 0)$$

$$C e^{-\beta \Delta x} = \frac{1}{e} \cdot C$$

$$\Delta x = \frac{1}{\beta} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

* Rectangular Barrier: Quantum Mechanical Tunneling



$$V(x) = 0 \quad x < 0, x > L$$

$$\approx V_0 \quad 0 \leq x \leq L$$

$$\frac{d^2\psi_1}{dx^2} + \frac{2m(E-0)}{\hbar^2} \psi_1 = 0 \Rightarrow \frac{d^2\psi_1}{dx^2} + \alpha^2 \psi_1 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \frac{2m(\nu_0 - E)}{\hbar^2} \psi_2 = 0 \Rightarrow \frac{d^2\psi_2}{dx^2} + \beta^2 \psi_2 = 0$$

$$\frac{d^2\psi_3}{dx^2} + \frac{2m(E-0)}{\hbar^2} \psi_3 = 0 \Rightarrow \frac{d^2\psi_3}{dx^2} + \alpha^2 \psi_3 = 0$$

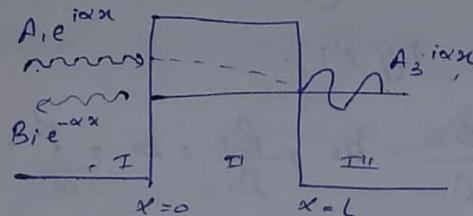
$$\psi_1(x) = A_1 e^{i\alpha x} + B_1 e^{-i\alpha x}$$

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

$$\begin{aligned}\psi_3(x) &= A_3 e^{i\alpha x} + B_3 e^{-i\alpha x} \\ &= A_3 e^{i\alpha x}\end{aligned}$$

$$B_3 e^{-i\alpha x} = 0$$

because, in III region, there is no boundary



$$T = \frac{|A_3|^2}{|A_1|^2} \quad (\text{Find out})$$

Boundary $x = \pm \infty$, finite everywhere
at $x = 0$ $\psi_1(x) = \psi_2(x)$ $A_1 + B_1 = A_2 + B_2$
 $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ $i\alpha(A_1 - B_1) = \beta(A_2 - B_2)$

at $x = L$

$$\begin{aligned}\psi_2(x) &= \psi_3(x) \\ \frac{d\psi_2}{dx} &= \frac{d\psi_3}{dx}\end{aligned}$$

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

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$\frac{d(A_1 e^{i\alpha x} + B_1 e^{-i\alpha x})}{dx} = \frac{d}{dx}(A_2 e^{\beta x} + B_2 e^{-\beta x})$$

at $x = 0$

~~boundary conditions~~

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$$A_1 \cdot e^{inx} \cdot i\alpha - B_1 e^{-inx} \cdot i\alpha = A_2 e^{bx} \cdot \beta - B_2 e^{-bx} \cdot \beta$$

$$i\alpha (A_1 e^{inx} - B_1 e^{-inx}) = \beta (A_2 e^{bx} - B_2 e^{-bx})$$

~~at $n=0$~~ , $i\alpha (A_1 - B_1) = \beta (A_2 - B_2)$ — (1) (Putting $n=0$)

at $n=L$

$$\frac{d \psi_2}{dx} = \frac{d \psi_3}{dx}$$

$$\frac{d}{dx} (A_2 e^{bx} + B_2 e^{-bx}) = \frac{d}{dx} (A_3 e^{inx})$$

$$A_2 \cdot e^{bx} \cdot \beta - B_2 e^{-bx} \cdot \beta = A_3 \cdot e^{inx} \cdot i\alpha$$

$$\beta (A_2 e^{bx} - B_2 e^{-bx}) = A_3 \cdot e^{inx} \cdot i\alpha$$

$$\beta (A_2 e^{bx} - B_2 e^{-bx}) = i\alpha A_3 \cdot e^{inx} - (2) \text{ (Putting } n=L)$$

Dividing by ~~A~~ eq. (1) & (2) by A_1

$$\frac{A_2}{A_1} = a_2, \frac{A_3}{A_1} = a_3, \frac{B_2}{A_1} = b_2, \frac{B_1}{A_1} = b_1, \frac{\beta}{\alpha} = \omega n$$

Putting values of a_2, a_3, b_1, b_2 & ωn in eq. (1) & (2)

$$1 + b_1 = a_2 + b_2 \quad (3)$$

$$1 - b_1 = i\omega n (a_2 - b_2) \quad (4)$$

$$a_2 e^{bx} + b_2 \cdot e^{-bx} = a_3 e^{inx}$$

$$a_2 e^{bx} - b_2 \cdot e^{-bx} = \frac{i}{n} a_3 e^{inx} \quad (4)$$

By solving (3) & (4)

$$a_3 = \frac{4n i e^{inx}}{(n+i)^2 e^{-bx} - (n-i)^2 e^{-bx}}$$

$$\because \beta \gg 1 \\ \therefore e^{-bx} \ll e^{bx}$$

$$\therefore a_3 = \frac{-4n i e^{inx}}{(n-i)^2} \cdot e^{-bx}$$

$$T = \alpha_3^* \alpha_3 = | \alpha_3 |^2$$

$$\alpha_3 = \frac{4n i e^{-i\alpha L} \cdot e^{-\beta L}}{(n+i)^2}$$

$$T = \frac{4n i e^{-i\alpha L} \cdot e^{-\beta L}}{(n+i)^2} \propto \frac{-4n i e^{i\alpha L} \cdot e^{-\beta L}}{(n-i)^2}$$

$$T = \frac{16n^2 e^{-2\beta L}}{(n^2 + 1)^2} \text{, order of } 1$$

$$T \approx e^{-2\beta L} \\ \approx \text{const} \left[-2 \left(\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \right) t \right]$$

The wider the length, transmitting probability is reduce.

* Orthogonality and orthonormality conditions

Schrodinger eq. for free Particle

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m(E)}{\hbar^2} \psi(x) = 0$$

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

$$\textcircled{1} \int_{-\infty}^{+\infty} \psi_m^*(x, t) \psi_n(x, t) dx = 0 \quad (\text{orthogonality})$$

$$\int_{-\infty}^{+\infty} \psi_n^*(x, t) \psi_n(x, t) dx = 1 \quad \boxed{\text{orthonormality}}$$

$$\int_{-\infty}^{+\infty} \psi_m^*(x, t) \psi_m(x, t) dx = 1$$

Orthogonality condition for wave function:

If $\psi_m(n, t)$ and $\psi_n(n, t)$ represents two different quantum states of a system then, the integral of the product of wave fun. and complex conjugate of the other wave fun. over a common domain is equal zero.

$$\int_{-\infty}^{+\infty} \psi_m^* \psi_n = 0$$

Orthogonality condition for stationary state:

Or for Time dependent eq.

$$\psi_n(n, t) = \psi_n(n) e^{-iE_n t}$$

$$\psi_m(n, t) = \psi_m(n) e^{iE_m t}$$

$$\int_{-\infty}^{+\infty} \psi_m^*(n) e^{iE_m t} \psi_n(n) e^{-iE_n t} \frac{dn}{h} = 0$$

$$e^{i(E_m - E_n)t} \int_{-\infty}^{+\infty} \psi_m^*(n) \psi_n(n) dn = 0$$

as $E_m \neq E_n$

$$\therefore \int_{-\infty}^{+\infty} \psi_m^*(n) \psi_n(n) dn = 0$$

Orthonormality condition

$$\int_{-\infty}^{+\infty} \psi_m^*(n, t) \psi_n(n, t) dn = \delta_{mn}$$

Kronecker delta fun. $\delta_{mn} = 0 \quad m \neq n$
 $\delta_{mn} = 1 \quad m = n$

Prove that $\int_{-\infty}^{+\infty} \psi_m^* \psi_n dn = 0$, where ψ_m, ψ_n are the sol. of 1D Time independent Schrödinger eq. for energy values $E_m \neq E_n$.

OR

Q Prove the orthogonal properties of energy eigen fun. for 1D case.

Def Time independent Schrodinger eq.

$$\text{LHS } i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi \quad (\psi = \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}) \\ = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_m^*(x)}{\partial x^2} + V(x) \psi_m^*(x) = E_m \psi_m^*(x) \quad \text{--- (1)}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x) \psi_n(x) = E_n \psi_n(x) \quad \text{--- (2)}$$

Multiply eq. (1) by ψ_n & eq (2) by ψ_m^*

$$-\frac{\hbar^2}{2m} \psi_n \frac{\partial^2 \psi_m^*(x)}{\partial x^2} + V(x) \psi_m^*(x) \psi_n = E_m \psi_m^* \psi_n \quad \text{--- (3)}$$

$$-\frac{\hbar^2}{2m} \psi_m^* \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x) \psi_n(x) \psi_m^* = E_n \psi_n(x) \psi_m^* \quad \text{--- (4)}$$

Sub. (4) from (3)

$$\frac{\hbar^2}{2m} \left(\psi_m^* \frac{\partial^2 \psi_n}{\partial x^2} - \psi_n \frac{\partial^2 \psi_m^*}{\partial x^2} \right) = (E_m - E_n) \psi_m^* \psi_n$$

$$\psi_m^* \frac{\partial^2 \psi_n}{\partial x^2} - \psi_n \frac{\partial^2 \psi_m^*}{\partial x^2} = \frac{2m}{\hbar^2} (E_m - E_n) \psi_m^* \psi_n$$

$$\frac{\partial}{\partial x} \left[\psi_m^* \frac{\partial \psi_n}{\partial x} - \psi_n \frac{\partial \psi_m^*}{\partial x} \right] = \frac{2m}{\hbar^2} (E_m - E_n) \psi_m^* \psi_n$$

$$\int_{-\infty}^{+\infty} \frac{\partial}{\partial x} \left(\psi_m^* \frac{\partial \psi_n}{\partial x} - \psi_n \frac{\partial \psi_m^*}{\partial x} \right) dx = \frac{2m}{\hbar^2} (E_m - E_n) \int_{-\infty}^{+\infty} \psi_m^* \psi_n dx$$

$$\left[\Psi_m^* \frac{\partial \Psi_n}{\partial n} - \Psi_n \frac{\partial \Psi_m}{\partial n} \right]_{-\infty}^{+\infty} = \frac{2m(E_m - E_n)}{\hbar^2} \int_{-\infty}^{+\infty} \Psi_m^* \Psi_n d_n$$

$\stackrel{L=0}{\cancel{=0}}$

$$\frac{2m(E_m - E_n)}{\hbar^2} \int_{-\infty}^{+\infty} \Psi_m^* \Psi_n d_n = 0$$

$\cancel{\text{bcos } E_m \neq E_n}$

∴ $\left[\int_{-\infty}^{+\infty} \Psi_m^* \Psi_n d_n = 0 \right]$ Hence Proved

Q If $\Psi_1(n, t)$ & $\Psi_2(n, t)$ are both sol. of the Schrodinger wave eq. for a given potential $v(n)$
 Show that $\Psi(n, t) = a_1 \Psi_1(n, t) + a_2 \Psi_2(n, t)$

Sol

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1}{\partial n^2} + v(n) \Psi_1(n, t) = i\hbar \frac{\partial \Psi_1}{\partial t} \quad (\Psi \rightarrow \text{Total wave fun.})$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2}{\partial n^2} + v(n) \Psi_2(n, t) = i\hbar \frac{\partial \Psi_2}{\partial t} \quad \times a_2 \Psi_2$$

Superposition Principle says that the linear combination/vector sum of all the wave fun. representing a system multiply by a constant c will result in a wave fun. which also represent the same system.

$$\Psi(x) = \sum c_i \Psi_i(x)$$

Commutation operators & Hermitian operators

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (\text{commutation operators})$$

$$\int_{-\infty}^{+\infty} f(\hat{A}g) dx = \int_{-\infty}^{+\infty} (\hat{A}^* f)^* g dx \quad (\text{Hermitian operators})$$

$$\text{eg (1)} [\hat{x}, \hat{p}_x] \Psi(x) = -i\hbar \left[x \frac{\partial \Psi}{\partial x} - \frac{\partial (x\Psi)}{\partial x} \right] =$$

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

$$[\hat{x}, \hat{p}_x] \Psi(x) = i\hbar \Psi(x)$$

$$[\hat{p}_x = -i\hbar \frac{\partial}{\partial x}]$$

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

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

$$(2) [\hat{y}, \hat{p}_x] = (y\hat{p}_x - \hat{p}_x y)$$

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

$$[\hat{y}, \hat{p}_x] \Psi(x) = -i\hbar \left[y \frac{\partial \Psi}{\partial x} - y \frac{\partial \Psi}{\partial x} - 0 \right]$$

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

(becoz, wave fun is defined on x not on y)

$$(3) [\hat{t}, \hat{E}] = (t\hat{E} - \hat{E}t) = -i\hbar \quad (E = i\hbar \frac{\partial}{\partial t})$$

$$(4) \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial t} \right]$$

Commutation Rel's:

$$(1) [\hat{x}, \hat{p}_x] = i\hbar$$

$$(2) [\hat{t}, \hat{E}] = -i\hbar \quad [\hat{t}, \hat{\psi}] + [\hat{t}, i\hbar \frac{\partial}{\partial t}] \psi = 0$$

$$(3) \left[\frac{\partial^2}{\partial x^2}, \frac{\partial}{\partial t} \right] = \left[\frac{\partial}{\partial t} \frac{\partial}{\partial x} - \frac{\partial^2}{\partial x^2} \frac{\partial}{\partial x} \right] \psi = 0 \quad (4)$$

$$(4) \left[\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial t^2} \right] = \left[\frac{\partial}{\partial x} \cdot \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial t^2} \right] \psi = \left[\frac{\partial^3}{\partial x^2} - \frac{\partial^3}{\partial t^2} \right] \psi = 0$$

$$(5) \left[\hat{n}, [\hat{x}, \hat{H}] \right] = \left(-\frac{\hbar^2}{m} \right), \quad \hat{H} = \frac{\hat{p}_x^2}{2m} + V(x)$$

$$(6) \left[\hat{n}, \hat{p}_{n^2} \right]$$

$$(7) \left[\frac{\partial}{\partial x}, \hat{f}(x) \right] = \begin{cases} [\hat{x}, \hat{f}] = x \cdot -\frac{i\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi + \frac{i\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V(x) \psi \\ = -\frac{i\hbar}{2m} \end{cases}$$

* Properties of a linear operator:

$$1. \hat{A}(\alpha g) = \alpha \hat{A}g, \quad \alpha = \text{constant}$$

$g = \text{function } g(x)$

$$2. \hat{A}(f+g) = \hat{A}f + \hat{A}g$$

$$3. [\hat{A} + \hat{B}, \hat{c}] = [\hat{A}, \hat{c}] + [\hat{B}, \hat{c}]$$

$$4. [\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$5. [\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$

$$6. [\hat{A}, \hat{B} \hat{C}] = [\hat{A}, \hat{B}] \hat{C} + \hat{B} [\hat{A}, \hat{C}]$$

$$7. [\hat{A}, [\hat{B}, \hat{C}]] + [\hat{C}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{C}, \hat{A}]] = 0$$

commutation rel's

$$(6) [\hat{x}, \hat{p}_n^2] = [\hat{x}, \hat{p}_n \hat{p}_n] = [\hat{x}, \hat{p}_n] \hat{p}_n + \hat{p}_n [\hat{x}, \hat{p}_n]$$

$$\hat{x}\hat{p}_n + \hat{p}_n\hat{x} = -i\hbar \left[n \cdot \frac{\partial \Psi}{\partial x} - \frac{\partial (\Psi \cdot \Phi)}{\partial n} \right] \hat{p}_n + \hat{p}_n \left[n \cdot \frac{\partial \Psi}{\partial n} - \frac{\partial (\Psi \cdot \Phi)}{\partial x} \right]$$

$$= -i\hbar \left[n \cdot \frac{\partial \Psi}{\partial x} - n \frac{\partial \Psi}{\partial n} - \Phi \right] \hat{p}_n + \hat{p}_n \left[n \cdot \frac{\partial \Psi}{\partial n} - \frac{n \partial \Psi - \Phi}{\partial x} \right]$$

$$= -i\hbar \left[[-\Psi] \hat{p}_n + \hat{p}_n [-\Psi] \right]$$

$$[\hat{x}, \hat{p}_n^2] \Psi = -i\hbar [$$

$$(5) [\hat{x}, [\hat{x}, \hat{H}]] + [\hat{x} [\hat{x}, \hat{x}]] + [\hat{x}, [\hat{H}, \hat{x}]] = 0$$

$$\left[[\hat{x}, [\hat{x}, \hat{H} - \hat{H} \hat{x}]] \right] + \left[[\hat{x} [\hat{x}, \hat{x}]] \right] + \left[[\hat{x}, [\hat{H}, \hat{x}]] \right] = 0$$

$$[\hat{x}, \hat{H}] = \hat{x} \hat{H} - \hat{H} \hat{x}$$

$$= \hat{x} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + v \right) \Psi - \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + v \right) \hat{x} \Psi$$

$$+ v \Psi - v \Psi = \hat{x} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + v \right) \Psi - \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \hat{x} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} (\hat{x} \Psi) \right)$$

$$= -\hat{x} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \left(\frac{\hbar^2}{2m} \right)^2 \hat{x} \frac{\partial^2}{\partial x^2} \left(n \frac{\partial \Psi}{\partial x} + v \right)$$

$$= -v \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \frac{\hbar^2}{2m} \left[n \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial \Psi}{\partial x} \right] = -\frac{v \hbar^2 \frac{\partial^2 \Psi}{\partial x^2}}{2m} + \frac{n \hbar^2 \frac{\partial^2 \Psi}{\partial x^2}}{2m} + \frac{\hbar^2 \frac{\partial \Psi}{\partial x}}{m \partial x}$$

Ques find the condition in order that $\Psi(x, t)$ be a simultaneous eigenfunction of the operators A & B
 calculate the product $A \& B$ $(\hat{A} \hat{B} \Psi(x, t) - \hat{B} \hat{A} \Psi(x, t)) = \alpha A \Psi(x, t) + \beta B \Psi(x, t)$

$$\hat{A} \Psi(x, t) = \alpha \Psi(x, t)$$

$$\hat{B} \Psi(x, t) = \beta \Psi(x, t)$$

$$\text{calculate } \hat{B} \hat{A} \Psi(x, t) = \beta \alpha \Psi(x, t)$$

$$(\hat{A} \hat{B} - \hat{B} \hat{A}) \Psi(x, t) = (\alpha \beta - \beta \alpha) \Psi(x, t)$$

$[\hat{A}, \hat{B}] = 0$ [Necessary condition so Ψ be a simultaneous function of both operators
 if Ψ is a simultaneous function of two operators then this condition should be necessary for it.]

* Hermitian operators :-

$$[\hat{x}, (\hat{n}, \hat{\psi})] + [\hat{n}, (\hat{\psi}, \hat{x})] + [\hat{\psi}, (\hat{x}, \hat{n})] = 0$$

$$\hat{A}^2 - \hat{B}^2$$

$$\Rightarrow \left[x \left(-\frac{\hat{n} \hbar^2}{2m} \cdot \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) \right] + \left[\frac{\hat{p}_n}{2m} + i \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \cdot \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) \right] = 0$$

$$\Rightarrow \left[n \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) - \left(\frac{\hat{n} \cdot \hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) n \right]$$

$$+ \left[\frac{\hat{p}}{2m} + i \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \cdot \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) - \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) \left(\frac{\hat{p}}{2m} + i \right) \right]$$

$$+ \left[n \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \cdot \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) - \left(-\frac{\hat{n} \cdot \hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \hat{n} + \frac{\hbar^2}{2m} \right) n \right] .$$

$$\Rightarrow -\frac{\hat{n}^3 \hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial n^2} + \frac{\hat{n}^3 \hbar^2}{2m} \frac{\partial^2 \psi}{\partial n^2} + \underbrace{\frac{\hbar^2 \psi}{2m}}_{+}$$

$$[\hat{n}, \hat{H}] \Psi = -\frac{n \hbar^2}{2m} \frac{\partial^2 \psi}{\partial n^2} + \frac{\hbar^2}{2m} \left(2 \frac{\partial \psi}{\partial n} + \frac{\partial^2 \psi}{\partial n^2} \right)$$

$$= -\frac{n \hbar^2}{2m} \cancel{\frac{\partial^2 \psi}{\partial n^2}} + \frac{n \hbar^2}{2m} \cancel{\frac{\partial^2 \psi}{\partial n^2}} + \frac{\hbar^2}{2m} \frac{\partial \psi}{\partial n}$$

$$[\hat{n}, \hat{H}] = \frac{\hbar^2}{m} \frac{\partial}{\partial n} \rightarrow (\hat{n}, \hat{H})$$

$$[\hat{n}, [\hat{n}, \hat{H}]] \Psi = [\hat{n}, \frac{\hbar^2}{m} \frac{\partial}{\partial n}] \Psi$$

$$= n \left[\frac{-\hbar^2 \partial \psi}{m} \right] + \cancel{\frac{-\hbar^2}{m} \frac{\partial}{\partial n} (n \cdot \psi)}$$

$$[\hat{n}, [\hat{n}, \hat{H}]] \Psi = n \frac{\hbar^2}{m} \cancel{\frac{\partial \psi}{\partial n}} - \cancel{n \frac{\hbar^2}{m} \frac{\partial \psi}{\partial n}} - \frac{\hbar^2}{m} \psi = -\frac{\hbar^2}{m} \psi$$

$$[\hat{n}, [\hat{n}, \hat{H}]] = -\frac{\hbar^2}{m}$$

* Hermitian operator.

- The expectation of a dynamical quantity represented by Hermitian operator \hat{A} is always real.
- The two eigen fun. of a Hermitian operator belonging to diff. eigen states are always orthogonal.

Condition for Hermitian operator \hat{A}

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

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

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

$$\hat{A} \psi(n) = \lambda \psi(n)$$

$$(\psi, \hat{A} \psi) = \lambda (\psi, \psi) \quad \text{--- (1)}$$

$$(\hat{A} \psi, \psi) = \lambda^* (\psi, \psi) \quad \text{--- (2)}$$

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

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

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

$$(1) = (2)$$

$$\text{it means } \lambda = \lambda^*$$

ψ_m and ψ_n

$$\hat{A} \psi_m = \lambda_m \psi_m$$

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

To Prove $\int_{-\infty}^{+\infty} \psi_m^* \psi_n dx = 0$

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

If \hat{A} is hermitian then

$$(\psi_m, \hat{A} \psi_n) = (\hat{A} \psi_m, \psi_n) \quad \text{--- (1)}$$

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

∴ eigenvalues of Hermitian operator

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

$$(\lambda_n - \lambda_m)(\Psi_m, \Psi_n) = 0$$

$$\therefore \lambda_n \neq \lambda_m$$

$$\therefore (\Psi_m, \Psi_n) = 0$$

Test
Appiques
Just show that the average motion of a wave packet

satisfy the term condition (1) $\frac{d}{dt} \langle n \rangle = \frac{\langle p_n \rangle}{m}$

(2) $\frac{d}{dt} \langle p_n \rangle = \langle f_n \rangle = - \frac{d \langle v \rangle}{dn}$

Ehrenfest Theorem

→ It states that the quantum mechanics gives the same result as classical mechanics for motion of a wave pack associated with a moving particle if we use the expectation value or average value of dynamical related quantities involved.

$$(1) \quad -\frac{d}{dt} \langle n \rangle = \frac{d}{dt} \int_{-\infty}^{+\infty} \Psi^*(n, t) \underbrace{\Psi(n, t)}_{\text{independent of time}} dn$$

$$= \int_{-\infty}^{+\infty} \frac{\partial \Psi^*}{\partial t} n \Psi dn + \int_{-\infty}^{+\infty} \Psi^* n \frac{\partial \Psi}{\partial t} dn$$

$$\text{TDSE} \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(n, t)}{\partial n^2} + v(n) \Psi(n, t) = i \frac{\hbar}{\partial t} \frac{\partial \Psi}{\partial t}(n, t)$$

$$\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{1}{i\hbar} \frac{\partial^2 \Psi}{\partial n^2} - \frac{i}{\hbar} v \Psi$$

Book → Gupta Kumar Sharma
gold stream

Classical Mechanics

* Constrained Motion: It is a motion which can't proceed arbitrary in any manner.

* Forces of constraint: with the strained by virtue of which they ~~can~~ restrict, the motion of system of particle.

$$f = f(x_1, x_2, \dots, x_{3n}, t)$$

$$f = (x, y, z \ i \ x_2 \ y_2 \ z_2 \ j \ \dots \ i \ x_n \ y_n \ z_n, t)$$

k constraints have forces, dist., 3D

$$f_1 = f_1(x, y, z, \dots, z_n) = a_1$$

$$f_2 = f_2(x, y, z, \dots, z_n) = a_2$$

:

$$f_k = f_k(x, y, z, \dots, z_n) = a_k$$

$3n \cdot k \rightarrow$ Degree of freedom

* Degree of freedom: It is the no. of independent ways in which the mechanical system can move without violating forces of constrained acting on the system

Generalised Coordinates: The set of independent coordinate which describe the configuration of the system.

(q_i 's)

$$H_i = H_i(q_1, q_2, \dots, q_{3N})$$

$$q_i = q_i(\tau_1, \tau_2, \dots, \tau_{3N})$$

of Generalised coordinates

constraints:

- ① Holonomic $f = f(x_1, x_2, \dots, x_{3N}, t) = 0$ (simply the S.G.D.)
 - ② non-Holonomic $f(x_1, x_2, \dots, x_{3N}, t) \geq 0$
 - ③ Unilateral [in the form of inequalities] $f(\vec{x}, \vec{v}, t) \geq 0$] (if it have displacement, Time derivatives velocity and then, it is unilateral or
 - ④ Bilateral [in the form of equation] $f(\vec{x}, \vec{v}, t) = 0$] Bilateral constraints
 - ⑤ Differential or kinematic constraints $f(\vec{x}, \vec{v}, t) \geq 0$
 - ⑥ Geometric constraints $f(\vec{x}, t) = 0$
 $f(\vec{r}) = 0$
 - ⑦ Rheonomous constraints : explicit Time Dependence
 - ⑧ Scleronomous " : No explicit Time "
- e.g. ① $x^2 - a^2 \geq 0$ — ②, ④, ⑤, ⑥ Type

? ② simple Pendulum

$$x^2 = x^2 + y^2 + z^2 = l^2 \rightarrow ②, ⑤, ⑧$$

? ③ A spherical container of fixed radius r with a gas
The constraints eq in this case $|x_i|^2 \leq r^2$
Type of constraints $\rightarrow ②, ⑤, ⑥$

Generalised Displacement

Configuration Space

" Velocity

" Acceleration

" K.E

" Potential

" Momentum

* Generalised Displacement

($i \rightarrow$ real index)
 $i \rightarrow 1 \text{ to } N$)

$$\vec{q}_i = q_i (q_1, q_2, \dots, q_{3N}; t)$$

\vec{s}_{qi} = Arbitrary displacement

We can consider a small displacement of N particles \vec{s}_{qi} = Arbitrary displacement

$$\vec{s}_{qi} = \sum_{j=1}^{3N} \frac{\partial \vec{q}_i}{\partial q_j} \vec{s}_j$$

$\vec{s}_j \rightarrow$ Arbitrary generalised displacement

* Generalised Velocity $v = \frac{D}{T}$

$$\vec{v}_i = \frac{d(\vec{q}_i)}{dt} = \sum_j \frac{\partial \vec{q}_i}{\partial q_j} v_j$$

$$= \sum_j \frac{\partial \vec{q}_i}{\partial q_j} v_j + \vec{a}$$

Time is taken 0, because b/w transitioning stage all state are equilibrium so we assume there is no time change

* Generalised Acceleration

$$\vec{a}_i = \frac{d(\vec{v}_i)}{dt}$$

$$= \frac{d}{dt} \left[\sum_{j=1}^{3N} \frac{\partial \vec{q}_i}{\partial q_j} v_j + \frac{\partial \vec{q}_i}{\partial t} \right]$$

$$= \sum_{j=1}^{3N} \left[\frac{d}{dt} \left(\frac{\partial \vec{q}_i}{\partial q_j} \right) v_j + \frac{\partial \vec{q}_i}{\partial q_j} \frac{d(v_j)}{dt} + \frac{\partial}{\partial t} \left(\frac{\partial \vec{q}_i}{\partial t} \right) \right]$$

$a = \text{Velocity} \times \text{Time}$

$$\ddot{q}_i = \sum_j \left[\frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{\partial \dot{q}_i}{\partial t} \right] \left[\frac{1}{\partial t} \rightarrow \cdot \right]$$

$$\ddot{q}_i = \sum_j \frac{\partial}{\partial q_j} \left(\frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{\partial \dot{q}_i}{\partial t} \right) \dot{q}_j + \sum_j \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \sum_j \left[\sum_{k=1}^N \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{\partial \dot{q}_i}{\partial t} \right]$$

$$\ddot{q}_i = \sum_j \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \sum_j \frac{\partial^2 \dot{q}_i}{\partial q_j^2} \dot{q}_j \dot{q}_k + 2 \sum_j \frac{\partial^2 \dot{q}_i}{\partial q_j \partial t} \dot{q}_j + \frac{\partial^2 \dot{q}_i}{\partial t^2}$$

quadratic terms in generalised acceleration.

* Generalised K.E.

$$T = \frac{1}{2} \sum_{j=1}^N m_j (\dot{q}_j)^2 = \frac{1}{2} \sum_{i=1}^N m_i (\dot{q}_i)^2$$

$$\dot{q}_i \dot{q}_i = \left[\sum_{j=1}^N \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{\partial \dot{q}_i}{\partial t} \right] \left[\sum_{k=1}^N \frac{\partial \dot{q}_i}{\partial q_k} \dot{q}_k + \frac{\partial \dot{q}_i}{\partial t} \right]$$

$$= \sum_{k=1}^N \sum_j \frac{\partial \dot{q}_i}{\partial q_j} \cdot \frac{\partial \dot{q}_i}{\partial q_k} \dot{q}_j \dot{q}_k + 2 \sum_k \frac{\partial^2 \dot{q}_i}{\partial t \partial q_k} \cdot \dot{q}_{jk} + \left(\frac{\partial \dot{q}_i}{\partial t} \right)^2$$

$$T = \sum_{i=1}^N \left[\frac{1}{2} \sum_{j,k} \left(\frac{\partial \dot{q}_i}{\partial q_j} \right) \left(\frac{\partial \dot{q}_i}{\partial q_k} \right) \dot{q}_j \dot{q}_k + \sum_k \frac{\partial^2 \dot{q}_i}{\partial t \partial q_k} \dot{q}_{jk} + \frac{1}{2} \left(\frac{\partial \dot{q}_i}{\partial t} \right)^2 \right]$$

$$T^{(1)} + T^{(2)} + T^{(3)}$$

if these are $\neq 0$ Time dependent

$$\therefore T = \sum_{i=1}^N \left[\frac{1}{2} \sum_{j,k} \left(\frac{\partial \dot{q}_i}{\partial q_j} \right) \left(\frac{\partial \dot{q}_i}{\partial q_k} \right) \dot{q}_j \dot{q}_k \right]$$

$$\left[\frac{m_1}{48} + \frac{m_2}{48} + \frac{m_3}{48} \right] \frac{t}{t_0} + \left[\frac{m_1}{48} \frac{t}{t_0} + \frac{m_2}{48} \frac{t}{t_0} + \frac{m_3}{48} \frac{t}{t_0} \right] \frac{t^2}{t_0^2}$$

* Generalised Kinetic Energy

$$T = \sum_{i=1}^N \frac{1}{2} m_i (\dot{q}_i^2) = \sum_i m_i \left[\frac{1}{2} \sum_{j,k} \left(\frac{\partial \dot{q}_i}{\partial q_j} \right) \left(\frac{\partial \dot{q}_i}{\partial q_k} \right) \dot{q}_j \dot{q}_k + \sum_j \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{1}{2} \frac{\partial \dot{q}_i}{\partial t} \right]$$

& justify the statement generalised energy of a system is a quadratic fun. of generalised velocity

$$\vec{q}_i \cdot \vec{q}_i$$

$$\vec{q}_i \cdot \vec{q}_i = \left(\sum_{j=1}^{3N} \frac{\partial \dot{q}_i}{\partial q_j} \dot{q}_j + \frac{\partial \dot{q}_i}{\partial t} \right) \left(\sum_{k=1}^{3N} \frac{\partial \dot{q}_i}{\partial q_k} \dot{q}_k + \frac{\partial \dot{q}_i}{\partial t} \right)$$

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

if no explicit time dependence $T = \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k$, $a_{jk} = \sum_i \frac{1}{2} m_i \left(\frac{\partial \dot{q}_i}{\partial q_j} \right) \left(\frac{\partial \dot{q}_i}{\partial q_k} \right)$

$$\left(\frac{\partial \dot{q}_i}{\partial q_j} \right) \left(\frac{\partial \dot{q}_i}{\partial q_k} \right) = 0 \quad (j \neq k)$$

Then it is orthogonal system.

long

circular

q u, v

$$\vec{r} = \vec{x} + \vec{y}$$

$$x = r \cos \theta \Rightarrow \frac{\partial x}{\partial \theta} = -r \sin \theta$$

$$y = r \sin \theta \Rightarrow \frac{\partial y}{\partial \theta} = r \cos \theta$$

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

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

$$\frac{\partial x}{\partial \theta} = -r \sin \theta$$

$$\frac{\partial y}{\partial \theta} = r \cos \theta$$

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

$$T = \sum_{i,j,k} \frac{1}{2} m_i \left(\frac{\partial \vec{r}_i}{\partial q_j} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial q_k} \right) \dot{q}_j \dot{q}_k$$

$$T = \frac{1}{2} m \sum_{j=1}^2 \sum_{k=1}^2 \left(\frac{\partial \vec{r}_i}{\partial q_j} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial q_k} \right) \dot{q}_j \dot{q}_k$$

$$= \frac{1}{2} m \left[\left(\frac{\partial \vec{r}_i}{\partial x_i} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial x_i} \right) + \left(\frac{\partial \vec{r}_i}{\partial \theta} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial \theta} \right) \dot{\theta}^2 + 2 \left(\frac{\partial \vec{r}_i}{\partial x_i} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial \theta} \right) \dot{x}_i \dot{\theta} \right]$$

1st term = $\left(\frac{\partial \vec{r}_i}{\partial x_i} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial x_i} \right) \dot{x}_i^2$

$$= \left(\frac{\partial (x_i + y_i)}{\partial x_i} \right) \cdot \left(\frac{\partial (x_i + y_i)}{\partial x_i} \right) \dot{x}_i^2$$

$$= \left(\frac{\partial x_i}{\partial x_i} + \frac{\partial y_i}{\partial x_i} \right) \left(\frac{\partial x_i}{\partial x_i} + \frac{\partial y_i}{\partial x_i} \right) \dot{x}_i^2$$

$$= (\cos^2 \theta + \sin^2 \theta) \dot{x}_i^2$$

$$= \dot{x}_i^2$$

2nd term = $\left(\frac{\partial \vec{r}_i}{\partial \theta} \right) \cdot \left(\frac{\partial \vec{r}_i}{\partial \theta} \right) \dot{\theta}^2$

$$= \left(\frac{\partial (x_i + y_i)}{\partial \theta} \right) \cdot \left(\frac{\partial (x_i + y_i)}{\partial \theta} \right) \dot{\theta}^2$$

$$= \left(\frac{\partial x_i}{\partial \theta} + \frac{\partial y_i}{\partial \theta} \right) \cdot \left(\frac{\partial x_i}{\partial \theta} + \frac{\partial y_i}{\partial \theta} \right) \dot{\theta}^2$$

$$= \cancel{\dot{\theta}^2 \sin^2 \theta + \dot{\theta}^2 \cos^2 \theta}$$

$$= (-\dot{x}_i \sin \theta + \dot{y}_i \cos \theta) \cdot (-\dot{x}_i \sin \theta + \dot{y}_i \cos \theta) \dot{\theta}^2$$

$$= (\dot{x}_i^2)$$

$$= (\dot{y}_i^2)$$

$$\underbrace{(\cos^2 \theta + \sin^2 \theta)}_{\text{3rd Term}} = 1$$

$$\boxed{T}$$

* Gener

$$\begin{aligned}
 &= (\omega^2 r^2 \sin^2 \theta - g r \sin \theta \cos \theta - g^2 r^2 \sin^2 \theta + g^2 r^2 \cos^2 \theta) \dot{\theta}^2 \\
 &= (g r^2 - 2 g r^2 \sin^2 \theta) \dot{\theta}^2 = g r^2 \dot{\theta}^2 \\
 &(r \sin^2 \theta + \sin^2 \theta) r^2 + (-r \sin \theta \cos \theta + r \cos^2 \theta) r^2 \\
 3^{rd} \text{ Term: same as } &+ (r \sin \theta \cos \theta) r^2 \dot{\theta}^2 \\
 T &= \frac{1}{2} m (r^2 + r^2 \dot{\theta}^2)
 \end{aligned}$$

* Generalised Momentum :

$$p_{x_i} = \frac{\partial T}{\partial \dot{x}_i} \quad (P = \text{mass} \times \text{velocity})$$

$$T = \frac{1}{2} m_i \dot{x}_i^2$$

$$p_{x_i} = \frac{\partial T}{\partial \dot{x}_i} = m_i \dot{x}_i$$

$$p_k = \frac{\partial T}{\partial \dot{q}_{k_i}}$$

$$p_j = \sum_{i,j,k} \frac{1}{2} m_i \left(\frac{\partial \dot{x}_i}{\partial q_j} \right) \cdot \left(\frac{\partial \dot{x}_i}{\partial q_k} \right) q_{jk} + \sum_i m_i \left(\frac{\partial \dot{x}_i}{\partial t} \right)$$

* Generalised force :

If \vec{F}_i is the external force acting on the system and causes an arbitrary displacement $\vec{d}\dot{x}_i$ of a system then acc. to work energy theorem, the work done by the system will be equal to

$$S_{W1} = \sum_{i=1}^N \vec{F}_i \cdot \vec{d}\dot{x}_i$$

$$= \sum_{i=1}^N \vec{F}_i \cdot \sum_j \frac{\partial \dot{x}_i}{\partial q_j} d\dot{q}_j$$

$$= \sum_{j=1}^M Q_j \cdot d\dot{q}_j \quad \left[\text{where } Q_j = \sum_{i=1}^N \vec{F}_i \frac{\partial \dot{x}_i}{\partial q_j} \right]$$

Ques What will be the expression for generalised force in circular polar combination.

$$\vec{F}_i = -\nabla_i u_i$$

$$u_i = \left(i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z} \right)$$

$$Q_j = \sum_{i=1}^N -\nabla_i u_i \left(\frac{\partial \vec{r}_i}{\partial q_j} \right)$$

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

$$\vec{d}\vec{r}_i = dx_i \hat{i} + dy_i \hat{j} + dz_i \hat{k}$$

D'Alembert's Principle

- Virtual displacement (\vec{dr}_i)
- Work done by forces of constraints (f_i)
- Work done in equil. on i^{th} particle (sw) in static & dynamic equilibrium.

Virtual Displacement :-

it is an imaginary displacement which a system of L particle undergoes in configuration space consisting with the forces of constraint acting on a system at any instant (without changing the time or time is constant).

virtual displacement
at fixed time

$\vec{F}_i = \vec{f}_i^{(o)}$ external app. forces (- frictional forces)

+

f_i forces of constraint

$$\delta W = \sum_i \vec{f}_i^{(o)} \cdot \underbrace{\delta r_i}_{\text{virtual displacement}} + \sum_i f_i \cdot \underbrace{\delta r_i}_{0} = 0$$

The virtual work done by the applied forces ($\vec{f}_i^{(o)}$) acting on the system consisting under the condition of static equilibrium will be zero provided no frequent for frictional forces are present

$$\vec{f}_i^{(o)} = \vec{p}_i$$

$$\Rightarrow \vec{f}_i^{(o)} - \underbrace{\vec{p}_i}_{\substack{\text{effective force} \\ \text{or} \\ \text{kinetic reaction}}} = 0$$

$$\boxed{\delta W = \sum_i (\vec{f}_i^{(o)} - \vec{p}_i) \delta r_i = 0}$$

D'Alembert's No. in dynamic equilibrium

Lagrange's Equation by D'Alembert's Principle

$$\delta W = \sum_i (F_i^{(a)} - \vec{p}_i) \cdot \delta \vec{r}_i = 0 \quad \text{Total work done}$$

$$\Rightarrow \sum_i (F_i^{(a)} - \vec{p}_i) \cdot \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \cdot \delta q_j = 0 \quad \text{--- (1)}$$

$$\begin{aligned} \text{1st term} &= \sum_i \left(F_i^{(a)} \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \right) \delta q_j = 0 \\ &= \sum_j Q_j \delta q_j \quad \text{--- (A)} \end{aligned}$$

$$\begin{aligned} \text{2nd term} &= \sum_i \vec{p}_i \cdot \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \cdot \delta q_j \\ &= \sum_i m_i \vec{v}_i \cdot \sum_j \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j \end{aligned}$$

$$\begin{aligned} (\text{Rewrite}) \rightarrow &= \sum_i \sum_j m_i \frac{d}{dt} \left[\vec{r}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right] \delta q_j - \sum_{i,j} m_i \vec{v}_i \frac{d}{dt} \left(\frac{\partial \vec{r}_i}{\partial q_j} \right) \delta q_j \\ &= \sum_i \sum_j m_i \frac{d}{dt} \left[\vec{r}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right] \delta q_j - \sum_{i,j} m_i \vec{v}_i \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j \\ &= \sum_i \sum_j \left[m_i \frac{d}{dt} \left[\frac{\partial}{\partial q_j} \left(\frac{1}{2} \vec{r}_i \cdot \vec{r}_i \right) \right] - m_i \frac{\partial}{\partial q_j} \left(\frac{1}{2} \vec{r}_i \cdot \vec{r}_i \right) \right] \delta q_j \end{aligned}$$

$$\begin{aligned} \left(\begin{aligned} \frac{\partial}{\partial q_j} (\vec{r}_i \cdot \vec{r}_i) &= \frac{\partial \vec{r}_i}{\partial q_j} \cdot \vec{r}_i + \vec{r}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \\ &= 2 \left(\frac{\partial \vec{r}_i}{\partial q_j} \cdot \vec{r}_i \right) \end{aligned} \right)$$

$$= \sum_j \left[\frac{d}{dt} \left(\frac{\partial}{\partial q_j} T \right) - \frac{\partial}{\partial q_j} T \right] \delta q_j \quad \text{--- (B)}$$

Put the values eq. (A) & (B) in eq (1)

$$S_W = \sum_i f_i^{(a)} \frac{\partial \vec{q}_i}{\partial v_j} \cdot \vec{s} v_j = \sum_i \frac{\partial \vec{q}_i}{\partial v_j} \cdot \vec{s} v_j$$

$$\Rightarrow \dot{q}_j \vec{s} v_j = \left[\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \frac{\partial T}{\partial v_j} \right] \vec{s} v_j$$

$$\Rightarrow \dot{q}_j = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial v_j} \quad \boxed{L = T - V}$$

\rightarrow calculate lagrange's eq. for conservative system

$$\dot{q}_j = - \frac{\partial V}{\partial q_j}$$

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

$$L = T - V$$

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

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

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

$\left(\because \frac{\partial V}{\partial q_j} = 0 \text{ in conservative forces} \right)$

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

\rightarrow for non-conservative system

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

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

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

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

* Lagrangian formulation

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

Q3
B/T

(3/5)²

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

① Particle moving in space ; $\vec{F} = f_x \hat{i} + f_y \hat{j} + f_z \hat{k}$

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

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{x}} \right) - \frac{\partial T}{\partial x} = f_x \Rightarrow m \ddot{x} \Rightarrow f_x = \frac{d p_x}{dt}$$

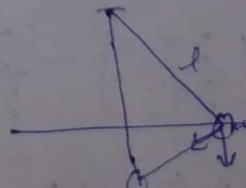
$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{y}} \right) - \frac{\partial T}{\partial y} = f_y \Rightarrow m \ddot{y} \Rightarrow f_y = \frac{d p_y}{dt}$$

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{z}} \right) - \frac{\partial T}{\partial z} = f_z \Rightarrow m \ddot{z} \Rightarrow f_z = \frac{d p_z}{dt}$$

② Simple Pendulum

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

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = \frac{1}{l} m l^2 \ddot{\theta} = m l^2 \ddot{\theta}$$



$$\frac{\partial L}{\partial \dot{\theta}} = m g l \sin \theta \quad T = \frac{1}{2} m (l \dot{\theta})^2$$

$$V = m g l (1 - \cos \theta)$$

$$L = T - V \Rightarrow L = \frac{1}{2} m l^2 \dot{\theta}^2 - m g l (1 - \cos \theta)$$

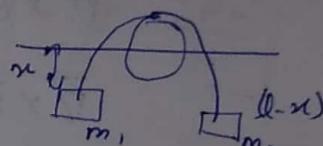
$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0 \Rightarrow \frac{d}{dt}(ml^2\ddot{\theta}) + mgl\sin\theta \Rightarrow ml^2\ddot{\theta} + mgl\sin\theta = 0$$

$$\ddot{\theta} + \left(\frac{g}{l}\right)\sin\theta = 0 \quad \text{or} \quad \ddot{\theta} = -\frac{g}{l}\sin\theta$$

$\sin\theta = 0$ for small θ

Q Consider a consider a frictional pulley device.

Q Derive the eq. of sys. using Lagrangian formulation.



Q A Particle of mass m moves on a Plane in the given forces by $\vec{F} = -\hat{r}_1 \cdot gk \cos\theta$, where k is a constant and \hat{r}_1 is the radial unit vector. obtain the differential eq. of the orbit of the Particle.

Q A beam slide on the ^{wire} in the shape of cycloid describe by the eq's $x = a(\theta - \sin\theta)$, $y = a(1 + \cos\theta)$, $0 \leq \theta \leq \pi$. find the lagrangian L(a, l) & find

Q find the lagrangia eq. for the electric circuit with inductance l and capistance c. The conductor is charge ~~to~~ q of colums & the circuit current following in the circuit is i Amh.

$$ME = \frac{1}{2}li^2 = \frac{1}{2}L\dot{q}^2$$

$$EE = \frac{1}{2} \frac{q^2}{C}$$

$$L = T - V \Rightarrow L = ME + EE$$

* Lagrangian of a charged particle in Electromagnetic field :

$$\vec{F} = q \vec{v} (\vec{E} + \vec{v} \times \vec{B}) \quad (\text{Lorentz force eq})$$

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

$$\vec{\nabla} \cdot \vec{B} = 0$$

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

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

$$\vec{\nabla} \cdot \vec{B} = 0 \Rightarrow B = -(\vec{\nabla} \times \vec{A}) \quad \text{--- (A)}$$

where $A \rightarrow$ magnetic vector Potential

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

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

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

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

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

$$\vec{E} = - \vec{\nabla} \phi - \frac{\partial \vec{A}}{\partial t} \quad \text{--- (B)}$$

Put (A) & (B) in Lorentz eq force eq.

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

x component of this eq.

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

$$\begin{aligned} \vec{\nabla} \times \vec{A} &= \begin{vmatrix} i & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} \\ &= \hat{i} \left[\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right] - \hat{j} \left[\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right] + \hat{k} \left[\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right] \end{aligned}$$

$$\begin{aligned} (\vec{v} \times \vec{\nabla} \times \vec{A})_x &= \begin{pmatrix} i & j & k \\ v_x & v_y & v_z \\ \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) & \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) & \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \end{pmatrix} \\ &= i \left[v_y \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) - v_z \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \right] \end{aligned}$$

$$\Rightarrow v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} - v_y \frac{\partial A_x}{\partial y} - v_z \frac{\partial A_x}{\partial z}$$

add and subtract, $v_x \frac{\partial A_x}{\partial x}$

$$\begin{aligned} \vec{v} \times (\vec{\nabla} \times \vec{A})_x &= v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_y}{\partial x} + v_z \frac{\partial A_z}{\partial x} - v_x \frac{\partial A_x}{\partial x} - v_y \frac{\partial A_x}{\partial y} \\ &\quad - v_z \frac{\partial A_x}{\partial z} \end{aligned}$$

$$\frac{\partial (\vec{v} \cdot \vec{A})}{\partial x}$$

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

$$\frac{dA_n}{dt} = \frac{\partial A_n}{\partial t} + \left[\frac{\partial A_n}{\partial x} v_x + \frac{\partial A_n}{\partial y} v_y + \frac{\partial A_n}{\partial z} v_z \right]$$

$$\frac{dA_n}{dt} - \frac{\partial A_n}{\partial t} = \frac{\partial A_n}{\partial x} v_x + \frac{\partial A_n}{\partial y} v_y + \frac{\partial A_n}{\partial z} v_z$$

$$f_n = q \left[-\frac{\partial \phi}{\partial x} - \frac{\partial A_n}{\partial t} + \frac{\partial (\vec{v} \cdot \vec{A})}{\partial x} - \frac{\partial A_n}{\partial t} + \frac{\partial A_n}{\partial t} \right]$$

$$= q \left[-\frac{\partial \phi}{\partial x} + \frac{\partial (\vec{v} \cdot \vec{A})}{\partial x} - \frac{\partial A_n}{\partial t} \right]$$

$$= q \left[-\frac{\partial(\phi - \vec{v} \cdot \vec{A})}{\partial x} - \frac{\partial A_n}{\partial t} \right]$$

$$= q \left[-\frac{\partial(\phi - \vec{v} \cdot \vec{A})}{\partial x} - \frac{d}{dt} \left(\frac{\partial(\vec{v} \cdot \vec{A})}{\partial v_n} \right) \right], \quad \text{where, } A_n = \frac{\partial(\vec{v} \cdot \vec{A})}{\partial v_n}$$

if $\frac{d}{dt} \left(\frac{\partial \phi}{\partial v_n} \right) = 0$

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

$$\text{Put } q(\phi - \vec{v} \cdot \vec{A}) = u$$

$$f_n = -\frac{\partial u}{\partial x} + \frac{d}{dt} \left(\frac{\partial u}{\partial v_n} \right)$$

write this eq. in the form of lagrangian eq

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

Rewrite this, if there is non conservation; then it is equal \ddot{q}_j , otherwise it is equal 0.

Rewrite above eq.

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

$$L = T - V$$

$$L = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - g(z)$$

For friction force,

$$f_{fx} = -k_x v_x$$

$$\vec{F}_f = -[k_x v_x \hat{i} + k_y v_y \hat{j} + k_z v_z \hat{k}]$$

* Rayleigh's dissipation function (F)

$$F = \frac{1}{2} \sum_i [k_x v_{xi} + k_y v_{yi} + k_z v_{zi}]$$

$$\vec{F}_f = -\nabla_v F$$

$\vec{\nabla}_v$ = velocity dependent differential

$$= \hat{i} \frac{\partial}{\partial v_x} + \hat{j} \frac{\partial}{\partial v_y} + \hat{k} \frac{\partial}{\partial v_z}$$

Work energy done $dW = \vec{F}_f \cdot d\vec{r}$

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

$$= -(k_x v_x^2 + k_y v_y^2 + k_z v_z^2) dt$$

$$dW = 2F dt$$

The work done by the non conservative frictional force is twice of Rayleigh's dissipation function.

Generalized force for Rayleigh's eq.

$$\phi_j = \sum_i \vec{F}_i \frac{\partial \vec{r}_i}{\partial q_j}$$

$$\begin{aligned}\phi_j &= - \sum_i \vec{\nabla}_{q_j} F_i \frac{\partial \vec{r}_i}{\partial q_j} \\ &= - \frac{\partial \vec{F}}{\partial q_j}\end{aligned}$$

$$\left(\frac{\partial \vec{r}_i}{\partial q_j} = \frac{\partial \vec{r}_i}{\partial q_j} \right)$$

(Cyclic \rightarrow if coordinate is not present in lagrangian eq.)

$$\left[\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right] = \phi_j$$

If q_j is absent

$$\frac{\partial L}{\partial q_j} = 0$$

$$\therefore \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = 0 \quad \Rightarrow \quad \frac{\partial L}{\partial \dot{q}_j} = \text{constant} = p_j$$

$$\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i} - \frac{\partial U}{\partial \dot{q}_i}$$

$$T = \frac{1}{2} m \dot{q}^2$$

* Conservation laws :-

- ① Conservation of linear momentum
- ② Conservation of Angular momentum
- ③ Conservation of Energy

① if a coordinate corresponding to a displacement is cyclic, then the translation of the sys. has no effect i.e., the description of motion of such system remains if the time does not invariant and the corresponding momentum is conserved.

if q_j is cyclic

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

$$L = T - V$$

$$\text{as } T \neq T(q_j)$$

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

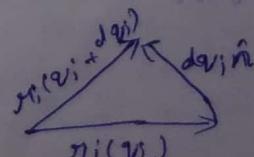
$$\boxed{\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) = -\frac{\partial V}{\partial q_j} = \phi_j} \quad - \textcircled{A} \quad \left(\phi_j = \sum_i \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \right)$$

if ϕ_j is in $(\text{dim}^n \times \text{dim}^n)$

$$\frac{\partial \vec{r}_i}{\partial q_j} = \vec{v}_j \hat{n}$$

$$\frac{\partial \vec{r}_i}{\partial q_j} = \hat{n}$$

$$\therefore \phi_j = \sum_i \vec{F}_i \cdot \hat{n} \quad \text{--- ①}$$



$$T = \frac{1}{2} m_i \dot{\vec{r}_i}^2$$

$$\frac{\partial T}{\partial q_j} = m_i \dot{\vec{r}_i} \cdot \frac{\partial \vec{r}_i}{\partial q_j}$$

$$= m_i \dot{\vec{r}_i} \cdot \hat{n}$$

$$\frac{\partial T}{\partial q_j} = p_j \cdot \hat{n} \quad \text{--- (2)}$$

Put eq. (1) & (2) in eq. (A)

$$\frac{d}{dt}(p_j) = -\frac{\partial v}{\partial q_j} = \dot{q}_j = \vec{F}_i \cdot \hat{n}$$

q_j cyclic, $\frac{\partial v}{\partial q_j} = 0$ so $\vec{F}_i \cdot \hat{n} = 0$ so $p_j = \text{const.}$

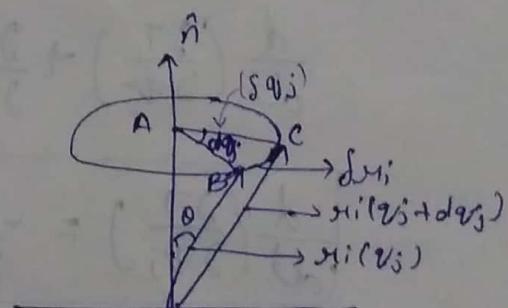
Case II

(2) if the system is not in the dir. of the generalized force.

$$\vec{s}_{ri} = AB dq_j$$

$$\vec{s}_{ri} = r_i \sin \theta \vec{v}_j$$

$$\frac{\vec{s}_{ri}}{\vec{s}_{v_j}} = \vec{g}_i \times \hat{n}$$



$$T = \sum_i \frac{1}{2} m_i \dot{r}_i^2$$

$$\frac{\partial T}{\partial q_j} = m_i \dot{r}_i \frac{\partial \dot{r}_i}{\partial q_j}$$

$$\frac{\partial T}{\partial q_j} = m_i \cancel{\dot{r}_i^2} \dot{r}_i \vec{n}$$

$$\frac{\partial T}{\partial q_j} = m_i \dot{r}_i^2 \cdot (\dot{r}_i \times \vec{n}) \Rightarrow p_j \cdot \dot{r}_i^2 \times \vec{n}$$

$$\theta_j = \sum_i \vec{f}_i \cdot \frac{\partial \dot{r}_i}{\partial q_j}$$

$$\theta_j = \sum_i \vec{f}_i \cdot (\dot{r}_i \times \vec{n})$$

$$\theta_j = \vec{n} \cdot (\dot{r}_i \times \vec{f}_i)$$

$$\theta_j = \vec{n} \cdot \vec{N}_i$$

($\dot{r}_i \times \vec{F}_i$ represents
Torque acting on a sys.)

$$\frac{d}{dt} \left(\frac{\partial T}{\partial q_j} \right) = \frac{d}{dt} (p_j \cdot \dot{r}_i \times \vec{n})$$

$$= \frac{d}{dt} (\vec{n} \cdot \dot{r}_i \times \vec{p}_i)$$

$$= \frac{d}{dt} (\vec{n} \cdot \vec{l})$$

($\dot{r}_i \times \vec{p}_i$) represents
Angular momentum
associated with particle)

if q_j is cyclic

$$\vec{n} \cdot \vec{l} = \text{const.}$$

if a coordinate corresponds to a rotational is
cyclic, then the rotational of the sys. has no effect
i.e., description of motion of such system remains
invariant and corresponding angular momentum is constant.

Lagrangian for central force

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

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

$$V = V(r)$$

$$L = T - V$$

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

θ = cyclic

(angular mom. in
dis. of θ is conserved)

Conservation of energy

- ① The Lagrange of a sys. is given by $T - V$
where, T is a fun. of \dot{q}_j and V is a fun. of (q_j)
- ② The constraints of a sys. does not change with time i.e., the transformation eq. does not depend upon the time explicitly.

$$L(q_j, \dot{q}_j) = T(\dot{q}_j) - V(q_j)$$

$$\frac{dL}{dt} = \frac{\partial L}{\partial \dot{q}_j} \frac{d\dot{q}_j}{dt} + \frac{\partial L}{\partial q_j} \frac{dq_j}{dt}$$

Lagrangian eq. of motion

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

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

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

$$\frac{dL}{dt} = \frac{d}{dt} (q_i; p_j)$$

$$\frac{d}{dt} (T - q_i p_j) = 0$$

$$\frac{d}{dt} (T - v - q_i p_j) = 0$$

Euler's theorem state that there is function f which is a homogenous fun. of order n depending upon variable q_i , then Euler's theorem states

$$\sum_j q_i \frac{\partial f}{\partial q_i} = n f$$

$$T = \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k$$

$$\sum_j \dot{q}_j \frac{\partial T}{\partial \dot{q}_j} = n T$$

$$\sum_j \dot{q}_j \frac{\partial T}{\partial \dot{q}_j} = 2T$$

$$\sum_j q_i p_j = 2T$$

$$\frac{d}{dt} (T - v - q_j p_j) = 0$$

$$\frac{d}{dt} (T - v - 2T) = 0$$

$$T + v = \text{const} = \text{Hamiltonian } (H)$$

if coordinates corresponding to time is cyclic,

$$H = (L - q_j p_j) = T + v$$

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

Phase space (6-D)

Hamilton eq.

Advantage

①

② \ddot{q}_j is 1st diff. order.

$$T_R = \frac{16}{386} \cdot 10^3$$

$$T_B = \frac{16}{386} \cdot 10^3$$

$$T_S = 18 \cdot 10^3$$

Hamiltonian formulation :- Hamilton's EOM

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

$$dH = \frac{\partial H}{\partial q_j} dq_j + \frac{\partial H}{\partial p_j} dp_j + \frac{\partial H}{\partial t} dt$$

$$dL = \frac{\partial L}{\partial q_j} dq_j + \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j + \frac{\partial L}{\partial t} dt$$

$$d \in q_j p_j = \sum_j dq_j p_j + \sum_j q_j dp_j$$

$$\left(\frac{\partial L}{\partial q_j} = p_j, \frac{\partial L}{\partial \dot{q}_j} = p_j \right)$$

$$\frac{\partial H}{\partial q_j} = -p_j, \quad \frac{\partial H}{\partial p_j} = q_j, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$$

Cylindrical coordinates

$$(r, \phi, z)$$

$$x = r \cos \phi$$

$$y = r \sin \phi$$

$$z = z$$

$$L = T - V$$

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

Momentum cons. with \$(r, \phi, z)\$

$$p_r = \frac{\partial L}{\partial \dot{r}} \quad p_\phi = \frac{\partial L}{\partial \dot{\phi}}$$

$$P_{\dot{r}} = \frac{\partial L}{\partial \dot{r}} = m \dot{r} \quad [\ddot{r} = \frac{P_{\dot{r}}}{m} \Rightarrow \dot{r}^2 = \frac{P_{\dot{r}}^2}{m^2}]$$

$$P_{\dot{\phi}} = \frac{\partial L}{\partial \dot{\phi}} = m \omega^2 \dot{\phi} \quad [\dot{r}^2 \dot{\phi} = \frac{P_{\dot{\phi}}}{m} \Rightarrow \dot{r}^4 \dot{\phi}^2 = \frac{P_{\dot{\phi}}^2}{m^2} \Rightarrow r^2 \dot{\phi}^2 = \frac{P_{\dot{\phi}}^2}{m^2}]$$

$$P_z = \frac{\partial L}{\partial \dot{z}} = m \dot{z} \quad [z = \frac{P_z}{m} \Rightarrow \dot{z}^2 = \frac{P_z^2}{m^2}]$$

$$L = \frac{1}{2m} \left[P_{\dot{r}}^2 + \frac{P_{\dot{\phi}}^2}{\omega^2} + P_z^2 \right] - V$$

$$H = \frac{1}{2m} \left[P_{\dot{r}}^2 + \frac{P_{\dot{\phi}}^2}{\omega^2} + P_z^2 \right] + V$$

$$\frac{\partial H}{\partial \dot{r}} = \frac{P_{\dot{r}}}{m} - \frac{P_{\dot{\phi}}^2}{m \omega^2}$$

$$\frac{\partial H}{\partial P_{\dot{r}}} = \frac{1}{m}$$

$$\frac{\partial H}{\partial \dot{\phi}} = \frac{P_{\dot{\phi}}}{m \omega^2}$$

$$\frac{\partial H}{\partial P_{\dot{\phi}}} = \frac{P_{\dot{\phi}}}{m \omega^2}$$

$$\frac{\partial H}{\partial z} = \frac{P_z}{m}$$

$$\frac{\partial H}{\partial z} = \frac{P_z}{m}$$

* Central forces

$$F(r) = \frac{k}{r^{n+1}}, \text{ e.g. } \rightarrow \text{General form}$$

$k = \text{constant}$

$$\text{if } n = -1 \quad F = k/r \quad (\text{Simple forces})$$

$$n = 2$$

Properties of central forces

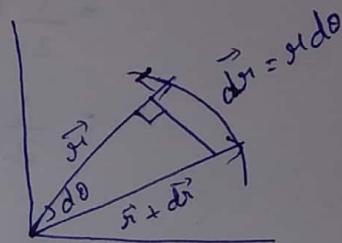
- (1) conservation of energy
- (2) conser. of angular momentum
- (3) conser. of radial velocities.

* Central forces

- (1) conservation of angular momentum

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

$$= \vec{r} \times m\vec{v}$$



using, $\vec{v} = \frac{d\vec{r}}{dt} \hat{e}_r + r \frac{d\theta}{dt} \hat{e}_\theta$

$$\Rightarrow \vec{r} \times m(r \hat{e}_r + r\dot{\theta}\hat{e}_\theta)$$

$$= r\hat{e}_r \times m(r\hat{e}_r + r\dot{\theta}\hat{e}_\theta)$$

$$= mr\dot{\theta}[\hat{e}_r \times \hat{e}_\theta] \quad \text{as } \hat{e}_r \times \hat{e}_\theta$$

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

\hat{n} → unit vector which is \perp to plane containing \hat{e}_r & \hat{e}_θ
respectively

Torque, $\vec{\tau} = \vec{r} \times \vec{F} = \frac{d\vec{L}}{dt} \Rightarrow \vec{L} = \text{const.} = mr^2\dot{\theta}\hat{n}$

$$= r\hat{e}_r \times f_r \hat{e}_r \frac{d\theta}{dt}$$

$$= 0$$

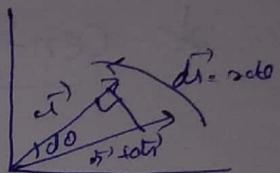
② conservation of areal velocity

Areal velocity is a term used to denote the surface area swept out by the radial vector \vec{r} per unit time during the planar motion of particle under the influence of a central force.

$$\text{Surface Area } d\vec{A} = \frac{1}{2} (\vec{r} \times d\vec{r}) \quad (\Delta \text{ law})$$

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

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



$$d\vec{A} = \frac{1}{2} r^2 d\theta \hat{n}$$

$$\frac{d\vec{A}}{dt} = \frac{1}{2} r^2 \frac{d\theta}{dt} \hat{n}$$

$$\frac{d\vec{A}}{dt} = \frac{\vec{l}}{2m} \quad \text{or} \quad \frac{dA}{dt} = \frac{l}{2m} = \text{constant}$$

& Lagrange eq. for central force

$$L = T - V$$

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

$$\left(\frac{\partial L}{\partial \dot{r}} = \frac{1}{2} m \cdot 2\dot{r} = m\dot{r}, \frac{\partial L}{\partial r} = \frac{1}{2} m \cdot 2r\dot{\theta}^2 = mr\dot{\theta}^2 \right)$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} = 0 \quad \left(\frac{\partial L}{\partial \dot{r}} = \frac{1}{2} m \cdot 2\dot{r} = m\dot{r}, \frac{\partial L}{\partial r} = \frac{1}{2} m \cdot 2r\dot{\theta}^2 = mr\dot{\theta}^2 \right)$$

$$\Rightarrow \frac{d}{dt} (m\dot{r}) - m\dot{r}\dot{\theta}^2 + \frac{\partial V}{\partial r} = 0$$

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

$\therefore mr^2\dot{\theta} = \text{constant}$ (which is angular momentum)

$r(t)$ and $\theta(t)$

$$L = mr^2\dot{\theta} \quad (\text{in terms of } \theta)$$

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

$$\int_{\theta_0}^{\theta} d\theta = \int_0^t \frac{L}{mr^2(t)} dt \quad \text{--- (A)}$$

\rightarrow in terms of r

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

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

$$mr\dot{\theta}^2 = \frac{L}{r^2}$$

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

$$mr\dot{\theta} = \frac{L}{r^2}$$

$$m\ddot{r} = -\frac{\partial V}{\partial r} + \frac{L^2}{mr^3} \quad \text{--- (B)}$$

$$m\ddot{r} = -\frac{\partial}{\partial r} \left[V + \frac{L^2}{2mr^2} \right] \frac{\partial r}{\partial t}$$

$$\frac{d}{dt} \left(\frac{1}{2} m\dot{r}^2 \right) = -\frac{\partial}{\partial t} \left[V + \frac{L^2}{2mr^2} \right]$$

$$\text{or} \quad \frac{\partial}{\partial t} \left[\frac{1}{2} m\dot{r}^2 + V + \frac{L^2}{2mr^2} \right] = 0$$

$$= \frac{1}{2} m\dot{r}^2 + v + \left(\frac{l^2}{2mr^2} \right) \xrightarrow{\text{acceleration produced in the particle}} \text{const.} = E$$

$$\Rightarrow \frac{1}{2} m\dot{r}^2 + v' = E$$

$$\dot{r}^2 = \frac{2(E-v')}{m}$$

$$\int_{r_0}^{r_1} dr = \pm \sqrt{\frac{2}{m}(E-v')} dt$$

$$\text{Force } \frac{l^2}{mr^3} = \frac{(mr^2\dot{\theta})^2}{mr^3}$$

$$= \frac{m^2 r^4 \dot{\theta}^2}{mr^3}$$

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

$$= \frac{m v_\theta^2}{r}$$

- if $E > v'$, motion is possible
- but if $E < v'$, then motion is not poss.
- $E = v'$, it is in equilibrium

in classical equilibrium mechanics, points \rightarrow Turning Points

Radial or tangential forces
then eq in terms of $r(t)$ & $\dot{r}(t)$

A particle of mass m which is moving in the influence of a spherically symmetrically inverse square force is given by

$$f_r = -\frac{C}{r^2} \left(\frac{v}{r} \right)^2 + v' \quad \dots$$

$$m a_r = f_r = -\frac{C}{r^2} \left[\frac{v}{r} + v' \right] \frac{1}{r} = \left(\frac{v}{r} + v' \right) \frac{C}{r^3}$$

from Lagrange's Radial eqn,

$$m\ddot{r} - mr\dot{\theta}^2 = -\frac{C}{r^2} \left[\frac{v}{r} + v' \right] \frac{C}{r^3} = -\frac{C^2}{r^5} \quad \dots \text{①}$$

$$m\ddot{r} - \frac{l^2}{mr^3} = -\frac{c}{r^2} \quad (2^{\text{nd}} \text{ order diff. eq})$$

$$\text{Replace } r = \frac{1}{u}$$

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

$$\dot{\theta} = \frac{L}{mr^2} = \frac{Lu^2}{m} = Ku^2 \quad (K = \frac{L}{m} = \text{const.})$$

$$\begin{aligned} \frac{dr}{dt} &= \frac{d}{dt}\left(\frac{1}{u}\right) = -\frac{1}{u^2} \frac{du}{dt} = -\frac{1}{u^2} \frac{du}{d\theta} \cdot \frac{d\theta}{dt} \\ &= -\frac{1}{u^2} Ku^2 \frac{du}{d\theta} \Rightarrow -K \frac{du}{d\theta} \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\left(\frac{dr}{dt}\right) &= \frac{d}{dt}\left(-K \frac{du}{d\theta}\right) \\ &= \frac{d}{d\theta}\left(-K \frac{du}{d\theta}\right) \frac{d\theta}{dt} \\ &= -K \frac{d^2u}{d\theta^2} + Ku^2 \\ &= -K^2 u^2 \frac{d^2u}{d\theta^2} \end{aligned}$$

Put values of $m\ddot{r}$ in eq. ①

$$-mK^2 u^2 \frac{d^2u}{d\theta^2} - \frac{m(Ku^2)^2}{u} = -cu^2$$

$$-mK^2 u^2 \frac{d^2u}{d\theta^2} - mK^2 u^3 = -cu^2$$

divided by $m \kappa^2 u^2$

$$\frac{d^2 u}{d\theta^2} + u = \frac{cu^2}{m \kappa^2 u^2} = \frac{c}{m \kappa^2} = A \text{ (say)}$$

$$\left(\begin{array}{l} A = \frac{c}{m \kappa^2} \\ f_{rc} = -\frac{c}{r^2} \end{array} \right)$$

$$\frac{d^2 u}{d\theta^2} + u = A$$

$$c = GM_S m$$

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

or

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

$$\text{as } \frac{d^2 A}{d\theta^2} = 0$$

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

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

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

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

$$\boxed{\frac{1}{r} = 1 + e \cos(\theta - \theta_0)} \quad \left(\frac{1}{A} = p, \frac{B}{A} = e \right)$$

$e = 0$	circle	Bounded motion
$e < 1$	elliptical	
$e = 1$	parabola	
$e > 1$	hyperbola	unbounded motion

Perigee \rightarrow Distance of closest approach

$$\text{Perigee} : \frac{P}{\delta_{\min}} = 1 + e \cos(\theta - \theta_0)$$

$$\theta = 0$$

$$\boxed{\frac{P}{\delta_{\min}} = 1 + e}$$

$$\boxed{\frac{P}{\delta_{\max}} = 1 - e}$$

$$\boxed{P = \frac{\delta_{\max} - \delta_{\min}}{\delta_{\max} + \delta_{\min}}}$$

$$\boxed{e = \frac{2\delta_{\max}\delta_{\min}}{\delta_{\max} + \delta_{\min}}}$$

Poisson bracket in quantum mech. with its commutation relation in classical mech.

Approximation Techniques.

* Hilbert space $\rightarrow |\psi\rangle |\psi^+\rangle$

Any wave fun. & Particle vector is represented by

BRA vector - KET vector

KET vector $\rightarrow |\psi\rangle \rightarrow \psi(n, t) / \psi(n)$

BRA vector $\rightarrow \langle\psi| \rightarrow \psi^*(n, t) / \psi^*(n)$

$$P = \int_{-\infty}^{+\infty} \psi^* \psi dx = (\psi, \psi)$$

$= \langle\psi|\psi\rangle$ (in hilbert space)

$$\langle n | = \int_{-\infty}^{\infty} \psi_n^* \psi dx = (\psi, n \psi)$$

$= \langle\psi|n|\psi\rangle$ (in hilbert space)

$H_0 + H'$
 ↓ ↓
 Hamiltonian
of exactly
Solved sys.
slight
deviation

Perturbation
Theory Time dep.
Time independent

* Time dependent Perturbation Theory

$$H_0 \Psi = E_0 \Psi$$

H is taken
only as
single order
(not order
derivative)

, $H_0 \rightarrow$ unperturbed hamiltonian

$$H = H_0 + \lambda H' + \lambda^2 H'' + \dots$$

$\lambda \rightarrow$ degeneracy parameter, which vary from 0 to 1

Hamiltonian eq. for the system

$$H \Psi = E \Psi$$

$$\Psi = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \dots$$

$$E = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

$$H \Psi = E \Psi$$

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

$$\lambda^0 \Rightarrow H_0 \Psi_n^{(0)} = E_n^{(0)} \Psi_n^{(0)}$$

(unperturbed hamiltonian eq.)

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

$$\lambda^2 \Rightarrow H_0 \Psi_n^{(2)} + H' \Psi_n^{(1)} = E_n^{(0)} \Psi_n^{(2)} + E_n^{(1)} \Psi_n^{(1)} + E^{(2)} \Psi_n^{(0)}$$

In General

$$\lambda^j \Rightarrow H_0 \Psi_n^j + H' \Psi_n^{j-1} = E_n^{(0)} \Psi_n^j + E_n^{(1)} \Psi_n^{j-1} + \dots + E_n^{(j)} \Psi_n^{(0)}$$

Correction in the energies \rightarrow Permutably by $\psi_n^{(0)*}$
and integrating over space

$$\text{for } \lambda', \int_{-\infty}^{+\infty} \psi_n^{(0)} H_0 \psi_n^{(0)} dx = E_n \int_{-\infty}^{+\infty} \psi_n^{(0)*} \psi_n^{(0)} dx$$

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

in Bra - Ket Notation, $\int_{-\infty}^{+\infty} \psi_n^{(0)} H_0 \psi_n^{(0)} dx = \langle \psi_n^{(0)} | H_0 | \psi_n^{(0)} \rangle$

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

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

as H_0 is Hermitian,

$$\therefore 1^{\text{st}} \text{ term} \rightarrow \langle \psi_n^{(1)} | H_0 - E_n^{(0)} | \psi_n^{(0)} \rangle^* = \langle \psi_n^{(1)} | E_n^{(0)} - E_n^{(0)} | \psi_n^{(0)} \rangle = 0$$

$$2^{\text{nd}} \text{ term} \rightarrow \langle \psi_n^{(0)} | H' - E_n^{(1)} | \psi_n^{(0)} \rangle$$

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

$$H'_{nn} = \int_{-\infty}^{+\infty} \psi_n^{(0)*} H' \psi_n^{(0)} dx$$

$$\int_{-\infty}^{+\infty} \psi_n^{(0)*} E_n^{(1)} \psi_n^{(0)} dx = E_n^{(0)} \int_{-\infty}^{+\infty} \psi_n^{(0)*} \psi_n^{(0)} dx$$

$$\therefore H'_{nn} - E_n^{(0)} \int_{nm} = 0$$

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

in Partical in box ,

1st order correction , $E_n^{(1)} = \int_{-\infty}^{+\infty} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \cdot v_0 \sqrt{\frac{2}{L}} \sin \frac{m\pi x}{L} dx$

$$E_n = E_n^{(0)} + E_n^{(1)}$$

* Time Independent Perturbation Theory

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

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

$$\int_{-\infty}^{+\infty} \Psi_n^{(0)*} H' \Psi_n^{(0)} dx$$

2nd order Perturbation eq.,

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

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

$$H = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 + bx^3$$

↓
H.O

$$H'_{nn} = \int_{-\infty}^{+\infty} \Psi_n^{(0)*} b x^3 \Psi_n^{(0)} dx$$

↓
stdand integral

$$+\Psi_n^{(0)*} \text{ and } \int_{-\infty}^{+\infty} (\cdot) dn$$

$$\underbrace{\langle \Psi_n^{(0)} | H_0 - E_n^{(0)} | \Psi_2^{(2)} \rangle}_{\vdots} + \langle \Psi_n | H^1 - E_n^{(1)} | \Psi_n^{(1)} \rangle = E_n^{(2)} \underbrace{\langle \Psi_n^{(0)} | \Psi_n^{(0)} \rangle}_{\vdots}$$

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

⇒ Third order energy eigen value

To find Correction in wave fun. we will used nearly Schrodinger Lagrange's techniques in which the Perturb wave fun. is expanded as a basis set of the unperturb wave function.

$$\Psi_n^{(1)} = \sum_k a_{nk}^{(1)} \Psi_k^{(0)}$$

1st order
wave fun. → $H_0 \Psi_n^{(0)} + H^1 \Psi_n^{(0)} = E_n^{(0)} \Psi_n^{(0)} + E_n^{(1)} \Psi_n^{(0)}$
Perturbation eq. $(H_0 - E_n^{(0)}) \Psi_n^{(0)} + (H^1 - E_n^{(0)}) \Psi_n^{(0)} = 0$

* Permutability by $\Psi_l^{(0)*}$ and $\int_{-\infty}^{+\infty} (\cdot) dn$

$$\Rightarrow \langle \Psi_l^{(0)} | H_0 - E_n^{(0)} | \Psi_n^{(1)} \rangle + \langle \Psi_l^{(0)*} | H^1 - E_n^{(1)} | \Psi_n^{(0)} \rangle = 0$$

$$\langle \Psi_l^{(0)} | H_0 | \Psi_n^{(1)} \rangle - \langle \Psi_l^{(0)} | E_n^{(0)} | \Psi_n^{(1)} \rangle$$

$$\Rightarrow \langle \Psi_{\ell}^{(0)} | H_0 | \sum_k a_{nk}^{(1)} \Psi_k^{(0)} \rangle - \langle \Psi_{\ell}^{(0)} | E_n^{(0)} | \sum_k a_{nk}^{(1)} \Psi_k^{(0)} \rangle = 0$$

$$H_0 |\Psi_k^{(0)}\rangle = E_k^{(0)}$$

$$\int_{-\infty}^{+\infty} \Psi_{\ell}^{(0)} H_0 a_{nk}^{(1)} \Psi_k^{(0)} dn = \int \Psi_{\ell}^{(0)} \Psi_k^{(0)} dn = \delta_{\ell k} = 1 \quad \ell = k \\ = 0 \quad \ell \neq k$$

$$\therefore = E_{\ell}^{(0)} a_{nk}^{(1)}$$

1st term

$$\langle \Psi_{\ell}^{(0)} | H_0 - E_n^{(0)} | \Psi_n^{(1)} \rangle = (E_{\ell}^{(0)} - E_n^{(0)}) a_{nl}^{(1)}$$

2nd term.

$$\langle \Psi_{\ell}^{(0)} | H' - E_n^{(1)} | \Psi_n^{(0)} \rangle = 0 \Rightarrow E_n^{(1)} \delta_{ln} = 0$$

$$\boxed{(E_{\ell}^{(0)} - E_n^{(0)}) a_{nl}^{(1)} + H'_{ln} - E_n^{(1)} \delta_{ln} = 0}$$

$$\boxed{\int_{-\infty}^{+\infty} \Psi_{\ell}^{(0)} H' \Psi_n^{(0)} dn}$$

$$\text{if } \delta_{ln} = 1, \quad \ell = n$$

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

$$\text{if } \ell \neq n, \quad \delta_{ln} = 0$$

$$(E_{\ell}^{(0)} - E_n^{(0)}) a_{nl}^{(1)} \rightarrow 0 = - H'_{ln}$$

$$a_{nl}^{(1)} = \frac{- H'_{ln}}{E_{\ell}^{(0)} - E_n^{(0)}} = \frac{H'_{ln}}{E_n^{(0)} - E_{\ell}^{(0)}}$$

1st order
correction,

$$\begin{aligned} \Psi_n &= \Psi_n^{(0)} + \lambda \Psi_n^{(1)} \\ &= \Psi_n^{(0)} + \lambda \frac{H'_{ln}}{E_n^{(0)} - E_{\ell}^{(0)}} \cdot \Psi_{\ell}^{(0)} \end{aligned}$$

$$\boxed{\Psi_n^{(1)} = \sum_k a_{nk}^{(1)} \Psi_k^{(0)}} \quad \text{using}$$

if $\lambda = 1$

$$\Psi_n = \Psi_n^{(0)} + \sum_k \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} \cdot \Psi_k^{(0)}$$

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

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

$$\langle \Psi_l^{(0)} | H_0 - E_n^{(0)} | \Psi_n^{(2)} \rangle + \langle \Psi_l^{(0)} | H' - E_n^{(1)} | \Psi_n^{(1)} \rangle = E_n^{(2)} \langle \Psi_l^{(0)} | \Psi_n^{(0)} \rangle$$
$$= E_n^{(2)} \delta_{ln}$$

$$\Psi_n^{(2)} = \sum_k a_{nk}^{(2)} \Psi_k^{(0)} ; \quad \Psi_n^{(1)} = \sum_k a_{nk}^{(1)} \Psi_k^{(0)}$$

$$\langle \Psi_l^{(0)} | H_0 - E_n^{(0)} | \sum_k a_{nk}^{(2)} \Psi_k^{(0)} \rangle + \langle \Psi_l^{(0)} | H' - E_n^{(1)} | \sum_k a_{nk}^{(1)} \Psi_k^{(0)} \rangle$$
$$= E_n^{(2)} \delta_{ln}$$

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

if $n = l$

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

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

using:

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

$$\Psi_n^{(1)} = \sum_k a_{nk}^{(1)} \Psi_k^{(0)}$$

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

Case II if $n \neq l$

$$[E_j^{(0)} - E_n^{(0)}] a_{nl}^{(2)} + H'_{jk} a_{nk}^{(1)} - E_n^{(0)} a_{nl}^{(1)} = 0$$

$$\begin{aligned} [E_j^{(0)} - E_n^{(0)}] a_{nl}^{(2)} &= H'_{nn} a_{nl}^{(1)} - H'_{jk} a_{nk}^{(1)} \quad (E_n^{(1)} = H'_{nn}) \\ &= H'_{nn} \cdot \frac{H'_{ln}}{E_n^{(0)} - E_l^{(0)}} - H'_{jk} \sum_k \frac{H'_{nk}}{E_n^{(0)} - E_k^{(0)}} \end{aligned}$$

$$a_{nl}^{(2)} = \frac{1}{E_j^{(0)} - E_n^{(0)}} \left(\dots \right) - \frac{H'_{jk} H'_{nk}}{(E_n^{(0)} - E_k^{(0)})(E_j^{(0)} - E_n^{(0)})}$$

$$\Psi_n = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)}$$

$$\Psi_n = \Psi_n^{(0)} + \lambda \sum_k a_{nk}^{(1)} \Psi_k^{(0)} + \lambda^2 \sum_k a_{nk}^{(2)} \Psi_k^{(0)}$$

$$H' - E_n^{(0)} / \sum_k a_{nk}^{(1)} \Psi_k^{(0)} = E_n^{(2)} \delta_{nl}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} \quad \text{if } \lambda = 1$$

$$E_0 \leq \langle H_0 \rangle$$

$$H_0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V(r)$$

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

$$\Phi(u) = e^{-\alpha u^2}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0$$

$$\langle H \rangle_{\min} = E_0$$