Model Answers

Paper Code - AS-2116

M. Sc. (First Semester) Examinations - 2013

Subject - Physics

Paper - Third

(Quantum Mechanics - I)

Maximum Marks - 60

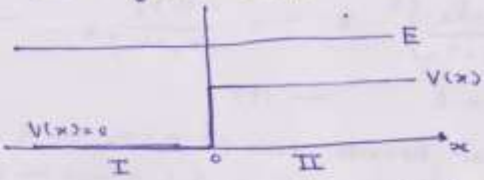
Section - 'A' 10x2 = 20

Q. 1.

Part No.	Answer Option
(i)	(d)
(ii)	(c)
(iii)	(b)
(iv)	(c)
(v)	(a)
(vi)	(a)
(vii)	(a)
(viii)	(c)
(ix)	(a)
(x)	(a)

SECTION - 'B' $5 \times 8 = 40$

Q. 2. The problem can be schematically represented as given below

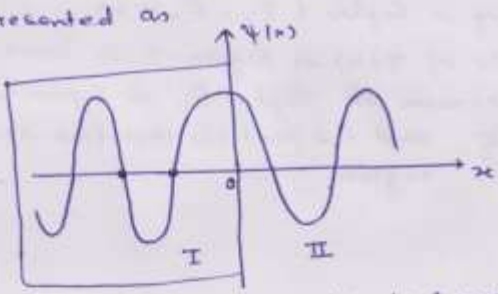


Accordingly, to the left of the barrier (Region-I) - $V(x)=0$

Solutions $\psi(x)$ are free particle plane waves

$$\psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad -(1) \quad \left| k_1 = \sqrt{\frac{2mE}{\hbar^2}} \right.$$

The wave function $\psi(x)$ can be qualitatively represented as

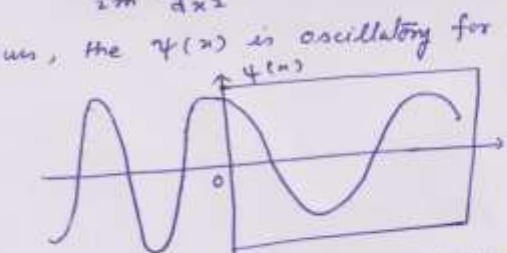


Whereas, Inside step potential region (Region-II) - $V(x)=V_0$

The Schrodinger equation becomes

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

Thus, the $\psi(x)$ is oscillatory for $E>V_0$ in region-II.



As $|\psi(x)|^2$ represent the probability density, it must be finite everywhere. Consequently, $\psi(x)$ is also finite. Moreover, E and V_0 are presumed finite, $\frac{d^2\psi}{dx^2}$ is also finite. This implies $\psi(x)$, $\frac{d\psi}{dx}$ must be continuous, even if $V(x)$ has discontinuity. The wave function as solution of eqn (2) then

$$\psi(x) = Ce^{ik_2 x} \quad -(3) \quad \left| k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar} \right.$$

For this situation, Reflection (R) and Transmission can be obtained as

$$R = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \quad \& \quad T = \frac{4k_1k_2}{(k_1+k_2)^2} \qquad -(4)$$

with $$R + T = 1 \qquad -(5)$$

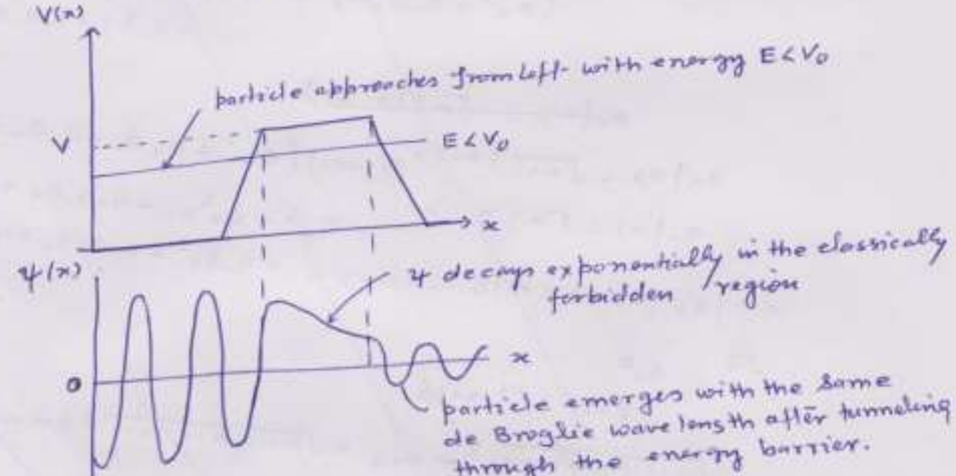
This gives $R \neq 0$ at barrier even if $E > V_0$ as R depends on the wave vector difference (k_1-k_2) but not on which one is larger. Whereas classically $R=0$ for $E > V_0$

Thus, for a particle with $E > V(x)$, $\psi(x)$ oscillates inside the potential step region. However, the frequency of $\psi(x)$ is higher in Region I in comparision to Region-II because the kinetic energy is higher ($E_k = E - V(x)$

The amplitude of $\psi(x)$ is Region-I is lower than in region-II because its higher E_k in Region-I gives a higher velocity, and the particle therefore spends less time in that region.

Q-8 ~~Whenever a quantum particle~~

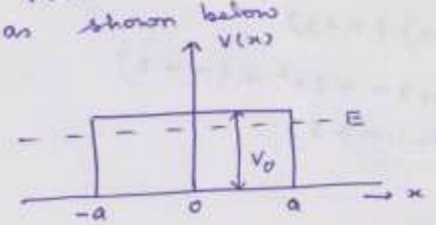
Q.3. Behaviour of a quantum particle approaching a potential barrier is different than its classical counterpart. If a quantum particle has energy E less than the potential energy barrier V, there is still a non-zero probability of finding the particle in classically forbidden region. This phenomena is called "tunneling". The phenomena is sketched is Fig-1.



In order to obtain the conditions that must be fullfilled for the occurrence of tunneling, we use model rectangular barrier defined as

$V(x) = 0$ for $x < -a$; $= V_0$ for $-a < x < a$; and $= 0$ for $x > a$

as shown below



Inside the barrier, Schrodinger eqn

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi(x) = E\psi(x) \quad -(1)$$

which can be recasted as

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

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

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \quad -(3)$$

with the solution $\psi(x) = Ae^{\alpha x} + Be^{-\alpha x} \quad |x| < a \quad -(4)$

Outside the barrier, the Schrodinger is the free particle equation, the solution for $x<-a$ is

$$\psi(x) = e^{ikx} + R e^{-ikx} \quad \Big| \begin{array}{l} x<-a \\ k^2 = 2mE/\hbar^2 \end{array} \quad -(5)$$

The flux from the left incident on the barrier is then

$$J = \frac{\hbar}{2im}\left[(e^{-ikx}+R^* e^{ikx})(ike^{ikx} - ike^{-ikx}) - c.c. \right]$$

$$= \frac{\hbar k}{m}(1-|R|^2) \quad -(6)$$

The first term giving flux $\left(\frac{\hbar k}{m}\right)$ of incident wave e^{ikx} and second term $\hbar k|R|^2/m$ is the flux due to reflected wave.

For $x>a$, the solution takes the form

$$\psi(x) = T e^{ikx} \quad -(7) \quad \Big| x>a$$

where $J = \frac{\hbar k}{m}|T|^2 \quad -(8)$

Imposing boundary conditions as required by continuity of wave function and its derivatives at potential barriers at $x=-a$ and $x=a$; one gets

$$\left.\begin{array}{l} e^{-ika} + R e^{ika} = A e^{-\alpha a} + B e^{\alpha a} \\ ik(e^{-ika} - R e^{ika}) = \alpha(A e^{-\alpha a} - B e^{\alpha a}) \\ A e^{\alpha a} + B e^{-\alpha a} = T e^{ika} \\ \alpha(A e^{\alpha a} - B e^{-\alpha a}) = ikT e^{ika} \end{array}\right\} \quad -(9)$$

From which, the expression for T is obtained as

$$T = e^{-2ika}\left[\frac{2k\alpha}{2k\alpha\cosh 2\alpha a - i(k^2-\alpha^2)\sinh 2\alpha a}\right] \quad -(10)$$

consequently, $|T|^2$, the ratio of transmitted current to incident current, is given by

$$|T|^2 = \frac{(2k\alpha)^2}{(k^2+\alpha^2)^2 \sinh^2 2\alpha a + (2k\alpha)^2} \quad -(11)$$

The finite probability for the transmission of particle is thus obtained even though $E < V_0$.

When $\alpha a >> 0$, the $|T|^2$ becomes

$$\left(\frac{4k\alpha}{k^2+\alpha^2}\right)^2 e^{-4\alpha a} \simeq e^{-4\alpha a} \quad -(12)$$

consequently, the probability of barrier transmission is extremely sensitive to a, the range of barrier, and to $\alpha \equiv V_0 - E$ the barrier height that the object has to jump.

Q.4. From the commutator algebra, three components of J i.e. J_x, J_y, J_z do not commute and have commutation relation

$$[J_x, J_y] = i\hbar J_z \;;\; [J_y, J_z] = i\hbar J_x \;;\; [J_z, J_x] = i\hbar J_y \quad -(1)$$

Also from the generalized uncertainty principle

$$\sigma_{J_x}\sigma_{J_y} \geq \frac{\hbar}{2} |\langle J_z\rangle| \quad -(2)$$

$J^2 = J_x^2 + J_y^2 + J_z^2$ however commutes with J_x, J_y, J_z

$$[J^2, J_x] = [J^2, J_y] = [J^2, J_z] = 0 \quad -(3)$$

This means that one can find simultaneous eigenstates of J^2 and and one of the component of angular momentum, J_z. Let us consider such an state $|jm\rangle$, Then

$$J^2|jm\rangle = \lambda|jm\rangle \;;\; J_z|jm\rangle = \mu|jm\rangle \quad -(4)$$

By using the ladder operators $J_\pm = J_x \pm iJ_y$, the eigenvalues λ and μ are obtained as discussed below.

The commutator of J^2 and J_z with $J_\pm$ can be calculated and are

$$[J_z, J_\pm] = \pm\hbar J_\pm \;;\; [J^2, J_\pm] = 0 \quad -(5)$$

Thus, if $|jm\rangle$ is the eigenstate of both J^2 and J_z, then $J_\pm|jm\rangle$ is also an eigenstate.

$$J^2(J_\pm|jm\rangle) = J_\pm(J^2|jm\rangle) = J_\pm(\lambda|jm\rangle)$$
$$= \lambda(J_\pm|jm\rangle) \quad -(6)$$

$$J_z(J_\pm|jm\rangle) = (J_zJ_\pm - J_\pm J_z)|jm\rangle + J_\pm J_z|jm\rangle$$
$$= \pm\hbar J_\pm|jm\rangle + J_\pm(\mu|jm\rangle)$$
$$= (\mu \pm \hbar)(J_\pm|jm\rangle) \quad -(7)$$

From eqns (6,7), it is clear that the ladder operator $J_\pm$ raise and lower the eigenvalue of J_z by $\hbar$ while leaving the eigenvalue of J^2 unchanged. For each value of λ, we get ladder of states with values of μ separated by $\hbar$. If state $|jm\rangle$ is ~~the~~ simultaneously an eigenfunction of J^2 and $J_\pm$, then $\mu \leq \lambda$. Denoting the state with the largest value of μ as the top of the ladder $|jm_{max}\rangle$

$$J_z|jm_{max}\rangle = \hbar l|jm_{max}\rangle, \text{ where } l \text{ is the maximum}$$

eigenvalue of L_z. Similarly operating from the bottom of the ladder

$$L_z |j\, m_{min}\rangle = -\hbar l\, |j\, m_{min}\rangle$$

Thus L_z has eigenvalues $m\hbar$ where m varies from $-l$ to l in integer steps. Therefore,

$$J_z |j m\rangle = m\hbar\, |j m\rangle$$

Q.5. Energy eigen value of Hydrogen atom are obtained by solving the time independent Schrodinger equation in spherical polar coordinates.

In spherical polar coordinates (r, θ, ϕ) the Laplacian is

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right) \quad -(1)$$

Then, the time-independent Schrodinger equation for potential $V(r)$ becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right] + V\psi = E\psi \quad -(2)$$

Where $\psi(r,\theta,\phi)$ is the associated wave function and E represents the energy of the state.

Firstly, we look for solutions that are separable into products

$$\psi(r,\theta,\phi) = R(r)\cdot Y(\theta,\phi) \quad -(3)$$

Putting ψ from eqn(3) into eqn(2), one gets

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] + VRY = ERY \quad -(4)$$

After dividing by YR and multiplying by $-2mr^2/\hbar^2$ eqn(4) is recasted as

$$\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left([V(r) - E]\right)\right\} + \frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = 0 \quad -(5)$$

The term under first curly bracket depends on r only whereas the remainder depends on θ & ϕ. Thus, both can separately written equal to some constant $l(l+1)$. leading to two equations

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}[V(r) - E] = l(l+1) \quad -(6)$$

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -l(l+1) \quad -(7)$$

Multiplying eqn(7) by $Y\sin^2\theta$ gives

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{\partial^2 Y}{\partial\phi^2}=-l(l+1)\sin^2\theta\, Y \quad -(8)$$

using again separation of variables and writing

$$Y(\theta,\phi)=\Theta(\theta)\Phi(\phi) \quad -(9)$$

After substituting eqn(9) in eqn(8) and diving by $\Theta\Phi$, one gets

$$\left\{\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+l(l+1)\sin^2\theta\right\}+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=0 \quad (10)$$

The first term in eqn(10) is a function of θ, and the second is a function of ϕ only. Therefore, each must be equal to a constant $\equiv m^2$. Thus,

$$\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]+l(l+1)\sin^2\theta=m^2 \quad -(11)$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-m^2 \quad -(12)$$

The solution of eqn (12) gives $\Phi(\phi)=e^{im\phi}$ with $m=0,\pm1,\pm2$, etc. Whereas, th θ eqn

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+[l(l+1)\sin^2\theta-m^2]\Theta=0$$

has solution

$$\Theta(\theta)=A\,P_l^m(\cos\theta)$$

Where P_l^m is the Associated Legendre function, defined as

$$P_l^m(x)=(1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|}P_l(x) \quad -(13)$$

Where $P_l(x)$ is lth Legendre polynomial defined by Rodrigues formula

$$P_l(x)\equiv\frac{1}{2^l\lfloor l}\left(\frac{d}{dx}\right)^l(x^2-1)^l \quad -(14)$$

Where l must be non-negative integers. Further, for any given value of l, then, there are $(2l+1)$ values of m. Thus, $l=0,1,2\cdots$; $m=-l,-l+1,\cdots-1,0,1,\cdots l-1,l$

Further, $R(r)$ and $Y(\theta,\phi)$ must be normalized giving

$$\int_0^\infty R(r)\,r^2dr=1 \quad \text{and} \quad \int_0^{2\pi}\int_0^{\pi}|Y^2|\sin\theta\, d\theta\, d\phi=1$$

using volume element in spherical coordinates as

$$d^3r=r^2\sin\theta\cdot dr\,d\theta\,d\phi$$

The normalized angular wave function $Y(\theta, \phi)$ is called spherical harmonics and is same for all spherically symmetric potentials. $R(r)$, the radial part of the wave function depends on the actual shape of $V(r)$.

Thus, for hydrogen atom, one can find the energy eigen value by putting $V(r)$ in the radial equation

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r)-E\right]R = l(l+1)R \quad -(15)$$

This can be simplified further by substituting $u(r) = rR(r)$ as

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \quad -(16)$$

The hydrogen atom consists of a heavy, essentially rest ~~po~~ proton of charge e, and a much lighter electron of charge $-e$ moving around it. The coloumb potential energy

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\cdot\frac{1}{r} \quad (\text{SI units}) \quad -(17)$$

Thus, the radial equation for hydrogen atom

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \quad (18)$$

Thus, the problem remains is to solve this equation for $u(r)$ and determine the allowed electron energy E for discrete bound states representing hydrogen atom ($E<0$).

The equation gets simplified by substituting $k = \sqrt{-2mE}/\hbar$, $\rho = kr$ and $\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2 k}$ giving

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u \quad -(19)$$

which can be solved ~~for~~ asymptotically for $\rho \to \infty$ & $\rho \to 0$ giving solutions $u(\rho) \sim Ae^{-\rho}$ and $u(\rho) \sim C\rho^{l+1}$ respectively. The general solution thus becomes,

$$u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)$$

where $v(\rho)$ is an arbitrary function and coeffi A & C are merged in $v(\rho)$.

The radial eqn. in terms of $v(\rho)$ becomes

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0 \qquad -(20)$$

and the solution is attempted by expressing

$$v(\rho) = \sum_{j=0}^{\infty} a_j \rho^j \text{ giving } v(\rho) = Ae^{2\rho}$$

Which finally gives $u(\rho) = A\rho^{l+1}e^{\rho}$ and thus not acceptable. The final solution is thus obtained by terminating the series such that the coefficient of expansion $a_{j_{max}+1} = 0$. Putting this condition in the the recursion relation obtained from series solution

$$a_{j+1} = \left\{\frac{2(j+l+1)-\rho_0}{(j+1)(j+2l+2)}\right\}a_j \text{ gives}$$

$$2(j_{max}+l+1) - \rho_0 = 0; \text{ putting } n = j_{max}+l+1$$

$\rho_0 = 2n$, But ρ_0 determines E. Thus

$$E = -\frac{\hbar^2 k^2}{2m} = -\frac{me^4}{8\pi^2 \epsilon_0^2 \hbar^2 \rho_0^2} \qquad -(21)$$

Therefore, the allowed energy values are

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}; \; n = 1, 2, 3, \dots$$

Note : solving of $Y(\theta, \phi)$ is not essential in this problem.

Q. 6 The angular momentum of a particle is defined as $L = r \times p$ classically.

The components $L_x = y p_z - z p_y$. The corresponding quantum mechanical operator for L_x is

$$L_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \quad -(1)$$ (By putting operator form of p_z & p_y)

Similarly $$L_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad -(2)$$

The ladder operator $L_+ = L_x + iL_y$ -(3) (By definition)

The commutator $[L_x, L_+]$ is thus

$$[L_x, L_+] = [L_x, L_x] + i[L_x, L_y] = 0 + i[L_x, L_y] \quad -(4)$$

as $[L_x, L_x] = 0$.

The commutator $[L_x, L_y]$ can be obtained

$$[L_x, L_y]f = \left(\frac{\hbar}{i}\right)^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)f - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)f\right] \quad -(5)$$

where $f(x,y,z)$ is any test function.

$$[L_x, L_y]f = \left(\frac{\hbar}{i}\right)^2\left[y\frac{\partial}{\partial z}\left(z\frac{\partial f}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial f}{\partial z}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial f}{\partial x}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial f}{\partial z}\right) - z\frac{\partial}{\partial x}\left(y\frac{\partial f}{\partial z}\right) + x\frac{\partial}{\partial z}\left(y\frac{\partial f}{\partial z}\right) + z\frac{\partial}{\partial x}\left(z\frac{\partial f}{\partial y}\right) - x\frac{\partial}{\partial z}\left(z\frac{\partial f}{\partial y}\right)\right] \quad -(6)$$

$$= \left(\frac{\hbar}{i}\right)^2\left[y\frac{\partial f}{\partial x} + yz\frac{\partial^2 f}{\partial z\partial x} - yx\frac{\partial^2 f}{\partial z^2} - z^2\frac{\partial^2 f}{\partial y\partial x} + zx\frac{\partial^2 f}{\partial y\partial z} - zy\frac{\partial^2 f}{\partial x\partial z} + xy\frac{\partial^2 f}{\partial z^2} + z^2\frac{\partial^2 f}{\partial x\partial y} - x\frac{\partial f}{\partial y} - xz\frac{\partial^2 f}{\partial z\partial y}\right] \quad -(7)$$

$$= \left(\frac{\hbar}{i}\right)^2\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right]f = i\hbar L_z f \quad -(8)$$

Thus, $[L_x, L_y] = i\hbar L_z$ — (9)

Putting the value in eqn (4), one gets

$$[L_x, L_+] = i(i\hbar L_z) = -\hbar L_z$$

Proved

Q.7. For the harmonic oscillator perturbed by H_1, the Hamiltonian H is given by

$$H = H_0 + H_1 \quad —(1)$$

where $H_0 = p^2/_{2m} + \frac{1}{2}kx^2$ - unperturbed Hamiltonian and $H_1 = bx^3$ is perturbation potential. If the unperturbed ground state is represented by $|\psi_0\rangle$ and corresponding eigenvalue by E_0, then the problem is to calculate $E_0^{(2)}$ - the second order correction

$$E_0^{(2)} = \sum_{m\neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{(E_n^0 - E_m^0)} \quad -(2)$$

The main task is therefore to calculate the off-diagonal matrix elements $\langle \psi_k | bx^3 | \psi_0 \rangle$. This can be easily achieved using the relations

$$\langle \psi_{n+1} | x | \psi_n \rangle = \langle n+1 | x | n \rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \langle n-1 | a_+ | n \rangle$$
$$= (n+1)^{1/2} \left(\hbar/_{2m\omega}\right)^{1/2}$$

$$\langle n-1 | x | n \rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \langle n-1 | a_- | n \rangle = n^{1/2}\left(\frac{\hbar}{2m\omega}\right)^{1/2} \quad —(3)$$

using the identity that $x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a_+ + a_-) \quad -(4)$

where a_+ and a_- are creation and anihilation operators.

Thus, $\langle n' | bx^3 | n \rangle = b \sum_{m,k} \langle n' | x | m \rangle \langle m | x | k \rangle \langle k | x | n \rangle \quad -(5)$

Substituting the matrix elements of x from eqn (3) gives,

$$\langle n' | bx^3 | n \rangle = b\left(\frac{\hbar}{2m\omega}\right)^{3/2} \Big[\{(n+1)(n+2)(n+3)\}^{1/2} \delta_{n',n+3}$$
$$+ \{n(n-1)(n-2)\}^{1/2} \delta_{n',n-3}$$
$$+ 3(n+1)(n+1)^{1/2} \delta_{n',n+1}$$
$$+ 3\, n\, n^{1/2} \delta_{n',n-1} \Big] \quad -(6)$$

For the ground state $|\psi_0\rangle \equiv |0\rangle$, only two states $|1\rangle$ and $|3\rangle$ share matrix elements of the perturbation bx^3 with $|\psi_0\rangle$; these matrix elements are

$$\langle \psi_1 | H' | \psi_0 \rangle = 3b(n+1)(n+1)^{1/2} \delta_{n',n+1} \left(\frac{\hbar}{2m\omega}\right)^{3/2}$$
$$= 3b\left(\frac{\hbar}{2m\omega}\right)^{3/2}(7) \Big| \text{putting } n = 0 = n'$$

and
$$\langle \psi_3 | H' | \psi_0 \rangle = b\left(\frac{\hbar}{2m\omega}\right)^{3/2} \{(n+1)(n+2)(n+3)\}^{1/2} \delta_{n',n+3}$$
$$= \sqrt{6}\, b \left(\frac{\hbar}{2m\omega}\right)^{3/2} \quad -(8)$$

Putting the value in eqn (2)

$$E_0^{(2)} = \frac{\left[3b\left(\frac{\hbar}{2m\omega}\right)^{3/2}\right]^2}{E_0 - E_1} + \frac{\left(\sqrt{6}\, b\left(\hbar/_{2m\omega}\right)^{3/2}\right)^2}{E_0 - E_3} \quad -(9)$$

The unperturbed energy states for harmonic oscillator are given by

$$E_n^0 = (n + \tfrac{1}{2})\hbar\omega \quad \text{with } \omega = \sqrt{k/m}$$

Thus, by putting the values of E_0, E_1 and E_3 in eqn (9)

$$E_0^{(2)} = \frac{9b^2\left(\frac{\hbar}{2m\omega}\right)^3}{\frac{1}{2}\hbar\omega - \frac{3}{2}\hbar\omega} + \frac{6b^2\left(\hbar/2m\omega\right)^3}{\frac{1}{2}\hbar\omega - \frac{5}{2}\hbar\omega}$$

$$= \left(\frac{\hbar}{2m\omega}\right)^3 \left[-\frac{9b^2}{\hbar\omega} - \frac{2b^2}{\hbar\omega}\right] = \frac{\hbar^2}{8m^3\omega^4}\left(-11b^2\right)$$

$$\boxed{E_0^{(2)} = -11b^2\hbar^2/8m^3\omega^4}$$

This is the second order correction to the energy of the ground state of harmonic oscillator.

Q.8 ~~Whenever~~ If a system, ~~was~~ for which the eigenstate $|\psi_n^0\rangle$ and eigenvalues E_n^0 are exactly ~~solvable by~~ the known i.e.

$$H_0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle \quad —(1)$$

is exactly solved; ~~undergoes~~ moves in a potential represented by Hamiltonian H_1 such that the time-independent perturbation, H_1, is small in comparison to unperturbed Hamiltonian H_0, the total Hamiltonian of the system can be written as

$$H = H_0 + \lambda H_1 \quad —(2)$$

where λ is perturbation parameter (varies between 0 and 1). When $\lambda = 0$, $H \equiv H_0$. However, as $\lambda \to 1$, H_0 goes over to H for the system under consideration.

The time-independent perturbation theory is a method to approximate the eigenvalues and eigenstates of H in terms of eigenvalues and eigenfunctions of H_0 using the matrix elements of the perturbation H_1. The correction to the unperturbed eigenstates and eigenvalues of the system are obtained by making power series expansion in powers of λ. If we consider the eigenstates of H as $|\psi_n\rangle$ and eigenvalues as E_n, we have

$$(H_0 + \lambda H_1)|\psi_n\rangle = E_n|\psi_n\rangle \quad —(3)$$

The basic idea of perturbation theory is to develop power series expansions of $|\psi_n\rangle$ and E_n under the constraint that there exist one-to-one correspondence between the set of states $|\psi_n\rangle$ and $|\psi_n^0\rangle$ i.e. $\lambda \to 0$ $|\psi_n\rangle \to |\psi_n^0\rangle$ and $E_n \to E_n^0$.

Since the eigenstates $|\psi_n^0\rangle$ forms a complete set, $|\psi_n\rangle$ is expanded as

$$|\psi_n\rangle = |\psi_n^0\rangle + \sum_{k \neq n} c_{nk}(\lambda)|\psi_k\rangle \quad —(4)$$

where coefficient c_{nk} represents the amount of mixing of k^{th} unperturbed state in the state $|\psi_n\rangle$. | $c_{nk}(0) = 0$ $\lambda \to 0$

Further $c_{nk} = \langle\psi_k^0|\psi_n\rangle$

The power series expansion is then,

$$c_{nk}(\lambda) = \lambda c_{nk}^{(1)} + \lambda^2 c_{nk}^{(2)} + \cdots \quad -(5)$$

and

$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \quad -(6)$$

Substituting these expansions in schrodinger equation

$$(H_0 + \lambda H_1)\left[|\psi_n^0\rangle + \sum_{k\neq n} \lambda c_{nk}^{(1)} |\psi_k^0\rangle + \sum_{k\neq n} \lambda^2 c_{nk}^{(2)} |\psi_k^0\rangle + \cdots \right]$$

$$= (E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots) \times \left[|\psi_n^0\rangle + \sum_{k\neq n} \lambda c_{nk}^{(1)} |\psi_k^0\rangle + \sum_{k\neq n} \lambda^2 c_{nk}^{(2)} |\psi_k^0\rangle + \cdots \right] \quad -(7)$$

Equating the terms of same power of λ, gives series of equations representing various orders of perturbation corrections

Equating terms proportional to λ gives

$$H_0 \sum_{k\neq n} c_{nk}^{(1)} |\psi_k^0\rangle + H_1 |\psi_n^0\rangle = E_n^0 \sum_{k\neq n} c_{nk}^{(1)} |\psi_k^0\rangle + E_n^{(1)} |\psi_n\rangle \quad -(8)$$

using unperturbed eqn. $H_0|\psi_k^0\rangle = E_k^0|\psi_k^0\rangle$, the first order correction $E_n^{(1)}$ to the energy is obtained.

$$E_n^{(1)} |\psi_n^0\rangle = H_1 |\psi_n^0\rangle + \sum_{k\neq n} (E_k^0 - E_n^0) c_{nk}^{(1)} |\psi_k^0\rangle \quad -(9)$$

multiplying with $\langle \psi_n^0|$ and $\langle \psi_n^0|\psi_k^0\rangle = \delta_{nk}$

$$E_n^{(1)} = \langle \psi_n^0 | H_1 | \psi_n^0 \rangle \quad -(10)$$

On the other hand, multiplying eqn (9) with $\langle \psi_m^0|$ $(m \neq n)$

$$\langle \psi_m^0 | H_1 | \psi_n^0 \rangle + (E_m^0 - E_n^0) c_{nm}^{(1)} = 0$$

which gives first order mixing coefficient

$$c_{nk}^{(1)} = \frac{\langle \psi_k^0 | H_1 | \psi_n^0 \rangle}{(E_n^0 - E_k^0)} \quad -(11)$$

Thus, the first order perturbed eigenstate becomes

$$|\psi_n\rangle = |\psi_n^0\rangle + \sum_{k\neq n} \frac{\langle \psi_k^0 | H_1 | \psi_n^0 \rangle}{(E_n^0 - E_k^0)} |\psi_k^0\rangle \quad -(12)$$

In the similar manner, the higher ordered perturbed eigenstates and eigenvalues can be obtained.