Tribhuvan University - 2074

Subject: Quantum Mechanics

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1. List the issues examplaining inadequacy of classical mechanics. How Quantum mechanics became useful to give better solution. How Davisson - Germer experiment supported quantum mechanics? Explain.

⇒ 1st part.

classical mechanics is based upon the Newton's three laws of motion (i) Law of Inertia (ii) Law of Force (iii) Law of action and reaction, totally germinated on the ground of absolute mass, absolute space and absolute time that could explain the motion of the body with non-relativistic speed. (i.e. $v << c$)

One of the major differences between the quantum theory and classical theory is that quantum theory describes energy and matter both as waves and particles where as classical physics treats matter strictly as particles. In the view of such discripe-ncies between the two theories, the inadequacies of classical mechanics can be stated as:

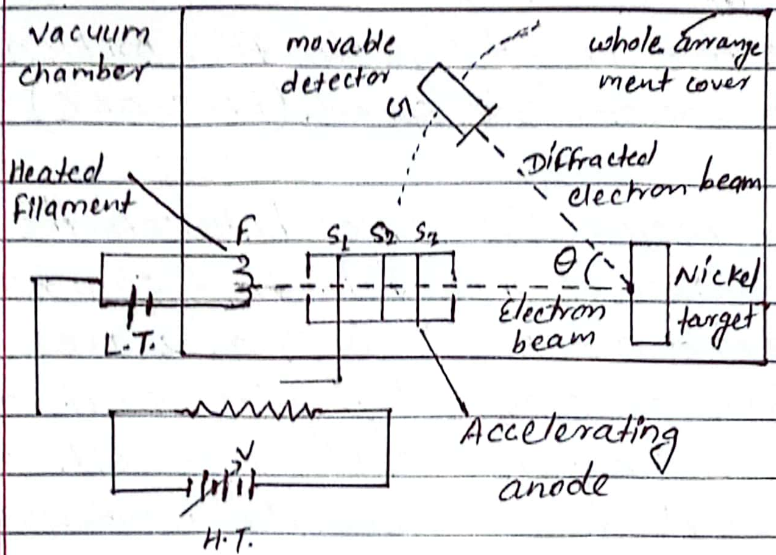
1. Classical mechanics could not explain the stability of atoms.
2. It couldn't explain the black body radiation.
3. It couldn't explain the observed variation of specific heat of solid.
4. It couldn't explain the origin of discrete spectrum of the atom.
5. It couldn't explain the non-relativistic motion of atoms, electrons, protons etc.
6. It could not explain a large number of phenomenon like photoelectric ~~effect classical mechanics lead to the development~~ effect, compton effect,

Raman effect etc.

The Inadequacies of classical mechanics lead to the development of quantum mechanics.

2nd part

The Davisson of Germer proposed the wave nature of electrons which was given by de-Broglie.



Experimental Arrangement:

The experimental arrangement of Davisson-Germer experiment is shown in the fig. above. The experiment filament 'F', under the heating by a low tension battery (L.T), produces the electrons. Then the electrons are collimated by a systems of slit S_1, S_2 and S_3 and are accelerated by anode provided with small hole. The scattered electrons are collected by a collectors, which can move along a graduated circular scale S_1 so that it is able to receive the reflected electrons at all angles between 20°

and 90°. The collecter is connected with the galvanometer 'G' and can be moved along a graduated circular scale 'S' then it is able to receive the electrons which are reflected at angles between 0° to 90°. There are two walls in the collecter i.e. C & D, they are insulated from each other. A potential is applied between two walls collecter so that only electrons having the incident velocity but not the slow electrons, which are excited by collision with atoms enter the collecter.

Explanation of experiments:

The beam of electron falls normally on the crystal surface the we can see a diffraction effect from the surface layer of the crystal. We move the collector to different position of galvanometer deflection, which gives a measure of the intensity of the diffracted beam of electrons. The graph is plotted between the galvanometer deflection and the incident beam, the beam which are entering the collecter. These observations are repeated for a different accelerating voltages and the number of curves are drawn as shown in fig. below. It is observed that the polar graphs are smooth up to 40V high tension potential, when a spur appears on the curves. As the accelerating voltage is increased, the length of the spur increases, then it reaches to 54 V at angle 50°. When are further decrease the length it finally disappears at 68 V.

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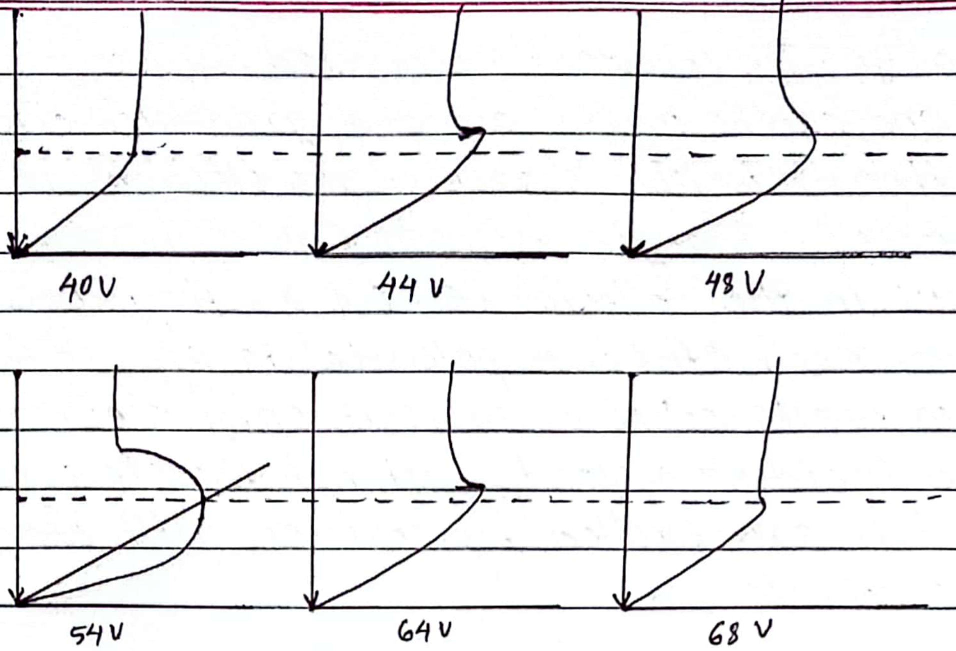

Fig: Results of Davisson - Germer Experiment

According to de-Broglie's theory, the wave length of electrons accelerated through p.d. of 54V is given by,

$$\lambda = \frac{12.27}{\sqrt{54}} A^\circ = 1.66 A^\circ$$

According to experiment, we have a different beam at an angle of 50 for the p.df 54V.

For nickel target, reflecting plane $d = 2.15 A^\circ$

$d \sin\theta = n\lambda$

where, $n = 1$ for the 1st order

$$2.15 \times \sin 50^\circ = \lambda$$

$$\lambda = 1.65 A^\circ$$

Thus, the experiment value is almost close to the theoretical value. This shows that the beams of electrons behave like x-rays, suffer diffraction at reflecting surfaces and has more like characteristics.

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OR

Develop time - independent schrodinger wave equation and describe the nature of its solution

⇒ A particle is equivalent to wave packet. The size of packet is large as compare to size of particle to locate the particle within the wave packet, schrodinger gave an equation called guiding wave equation.

consider a system of stationary waves to be associated with the particle. Let $\psi(\vec{r},t)$ be the wave displacement for De-broglie waves at any location.

$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \text{ at time 't'}$$

Then from the wave equation.

$$\Delta^2\psi = \frac{1}{\psi^2}\frac{\partial^2\psi}{\partial t^2}(\vec{r},t) \text{ ——— (1)}$$

where, u = wave velocity

Let the solution of eqⁿ (1)

$$\psi(\vec{r},t) = \psi_0(\vec{r})e^{-i\omega t} \text{ ——— (2)}$$

where ψ_0 is the amplitude at the point consider.

It is a function of position or (x,y,z).

Then $\frac{\partial\psi}{\partial t}(\vec{r},t) = \psi_0(\vec{r})\cdot(-i\omega)e^{-i\omega t}$

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$$\frac{\partial^2 \psi}{\partial t^2} = \psi_0(\vec{r}) \cdot (-i\omega) \cdot (-i\omega) e^{-i\omega t}$$

$$= \psi_0(\vec{r}) \cdot i^2 \omega^2 \cdot e^{-i\omega t}$$

$$= -\omega^2 \psi_0(r) e^{-i\omega t}$$

$$= -\omega^2 \psi(\vec{r}, t)$$

putting values in eqn ①, we get,

$$\nabla^2 \psi = \frac{1}{u^2}(-\omega^2 \psi)$$

$$\nabla^2 \psi = -\left(\frac{\omega}{u}\right)^2 \psi$$

$$\nabla^2 \psi = -\left(\frac{2\pi f}{u}\right)^2 \psi$$

$$\nabla^2 \psi = -\left(\frac{2\pi}{\lambda}\right)^2 \psi$$

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0$$

$$\nabla^2 \psi + \frac{4\pi^2}{h^2} m^2 v^2 \psi = 0 \quad \text{——} ④$$

$$\left[\because \lambda = \frac{h}{p} = \frac{h}{mv}\right]$$

If E = total energy
V = potential energy
$K.E. = \frac{1}{2} mv^2$

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

$$\frac{mv^2}{2} = E - V$$

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multiplying on both sides by m

$$m^2v^2 = 2m(E-V)$$

putting this value in eqn (4)

$$\nabla^2\psi + \frac{4\pi^2}{h^2} 2m(E-V)\psi = 0$$

$$\nabla^2\psi + \frac{2m}{\left(\frac{h}{2\pi}\right)^2}(E-V)\psi = 0$$

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

which is schrodinger time independent equation for free particle, V=0

$$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0}$$

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2. Find the expression for the energy levels of a finite square potential well, described by the potential $V(x)$ for a beam of quantum particles having energy $E < V_0$,

$V(x) = 0$ for $x < a$
$= -V_0$ for $a \le x < a$
$= 0$ for $x \ge a$

⇒ soln:-

Consider, a beam of particles of average energy E being incident towards a square potential well of depth $|V_0|$ as shown in figure. Quantum mechanically, when the particle strikes the sides of the wall, it bounces back and forth and has a certain probability of penetrating into the regions II and III even though $E < V_0$. Then, the potential is defined as.

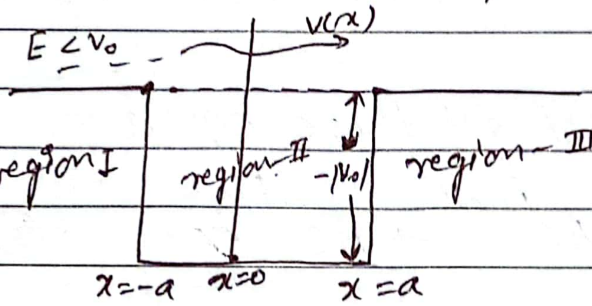

Fig:- Square potential well of finite depth.

The Schrodinger wave eqn in region I

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

$$\frac{d^2\psi_1(x)}{dx^2} + K_0^2\psi_1(x) = 0 \quad \text{——— ①}$$

where, $K_0^2 = \dfrac{2mE}{\hbar^2}$

Schrodinger wave equation in region II

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

$$\frac{d^2\psi_2(x)}{dx^2} + k^2\psi_2(x) = 0 \quad \text{—— (2)}$$

where, $k^2 = \frac{2m}{\hbar^2}[E-V]$

Schrodinger wave eqn in region III

$$\frac{d^2\psi_3(x)}{dx^2} + \frac{2m}{\hbar^2}E\,\psi_3(x) = 0$$

$$\frac{d^2\psi_3(x)}{dx^2} + k_0^2\psi_3(x) = 0 \quad \text{—— (3)}$$

where, $k_0^2 = \frac{2m}{\hbar^2}E$

The solution of all these eqn are,

$$\psi_1(x) = Ae^{ik_0x} + Be^{-ik_0x} \quad \text{—— (4)}$$

$$\psi_2(x) = Ce^{ikx} + De^{-ikx} \quad \text{—— (5)}$$

$$\psi_3(x) = A'e^{ik_0x} \quad \text{—— (6)}$$

No wave reflacted in region III so, $B' = 0$

Applying boundary condition.

$$\psi_1(x)\big|_{x=-a} = \psi_2(x)\big|_{x=+a}$$

$$\psi_1'(x)\big|_{x=-a} = \psi_2'(x)\big|_{x=+a}$$

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Eqn (4) and (5) becomes

$$Ae^{-ik_0a} + Be^{ik_0a} = Ce^{-ika} + De^{ika} \quad \text{——— (7)}$$

and, $ik_0Ae^{-ika} - ik_0Be^{ik_0a} = ikCe^{-ika} - ikDe^{ika}$

or, $$Ae^{-ik_0a} - Be^{ik_0a} = \frac{k}{k_0}(Ce^{-ika} - De^{ika}) \quad \text{——— (8)}$$

Adding eqn (7) & (8)

$$2Ae^{-ik_0a} = \left(1+\frac{k}{k_0}\right)Ce^{-ika} + \left(1-\frac{k}{k_0}\right)De^{ika}$$

$$A = \frac{C}{2}\left(1+\frac{k}{k_0}\right)e^{-ika}\cdot e^{ik_0a} + \frac{D}{2}\left(1-\frac{k}{k_0}\right)e^{ika}\cdot e^{ik_0a} \quad \text{——— (9)}$$

Similarly, equation (8) from (7), we get,

$$B = \frac{C}{2}\left(1-\frac{k}{k_0}\right)e^{-ika}\cdot e^{ik_0a} + \frac{D}{2}\left(1+\frac{k}{k_0}\right)e^{ika}\cdot e^{-ik_0a} \quad \text{——— (10)}$$

Again, using boundary condition,

$$\psi_2(x)|_{x=a} = \psi_3(x)|_{x=a}$$
$$\psi_2'(x)|_{x=a} = \psi_3'(x)|_{x=a}$$

Then, eqn (5) and (6) becomes,

$$Ce^{ika} + De^{-ika} = A'e^{ik_0a} \quad \text{——— (11)}$$

and $ikCe^{ika} - ikDe^{-ika} = ik_0A'e^{ik_0a}$

$$Ce^{ika} - De^{-ika} = \frac{k_0}{k}A'e^{ik_0a} \quad \text{——— (12)}$$

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Adding eqⁿ (11) & (12), we get,

$$2Ce^{ika} = \left(1+\frac{k_0}{k}\right)A'e^{ik_0a}$$

$$C = \frac{A'}{2}\left(1+\frac{k_0}{k}\right)e^{ik_0a}\cdot e^{-ik_0a} \quad \text{—— (13)}$$

Substracting eqⁿ (12) from (11), we get,

$$D = \frac{A'}{2}\left(1-\frac{k_0}{k}\right)e^{ik_0a}\cdot e^{ika} \quad \text{—— (14)}$$

Using the values of C and D from eqⁿ (13) & (14) in eqⁿ (9), we get,

$$A = \frac{A'}{4}\left(1+\frac{k}{k_0}\right)\left(1+\frac{k_0}{k}\right)e^{2ik_0a}\cdot e^{-2ika} +$$

$$\frac{A'}{4}\left(1-\frac{k}{k_0}\right)\left(1-\frac{k_0}{k}\right)e^{2ik_0a}\cdot e^{2ika}$$

$$\text{or, } A = \frac{A'}{4}e^{2ik_0a}\left[\frac{(k_0+k)^2\cdot e^{-2ika} - (k-k_0)^2 e^{2ika}}{k_0k}\right]$$

$$\text{or, } \frac{A'}{A} = \frac{4k_0ke^{-2ik_0a}}{(k_0^2+k^2)(e^{-2ika}-e^{2ika}) + 2k_0k(e^{-2ika}+e^{2ika})}$$

$$\text{or, } \frac{A'}{A} = \frac{4k_0ke^{-2ika}}{-2i(k_0^2+k^2)\left(\frac{e^{2ika}-e^{-2ika}}{2i}\right) + 4k_0k\left(\frac{e^{2ika}+e^{-2ika}}{2}\right)}$$

$$\text{or, } \frac{A'}{A} = \frac{4k_0ke^{-2ik_0a}}{4k_0k\cos 2ka - 2i(k_0^2+k^2)\sin 2ka} \quad \text{—— (15)}$$

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Then the transmission coefficient is given by

$$T = \left(\frac{A'}{A}\right)^2 = \left(\frac{A'}{A}\right)^{*} \times \left(\frac{A'}{A}\right)$$

$$T = \frac{(4K_0Ke^{-iK_0l})^2}{(4K_0K\cos 2Ka - 2i(K_0^2+K^2)\sin 2Ka)^2}$$

$$T = \frac{16K_0^2K^2}{16K_0^2K^2\cos^2 2Ka + 4(K_0^2+K^2)^2\sin^2 2Ka}$$

$$T = \frac{1}{\cos^2 2Ka + \frac{(K_0^2+K^2)^2}{4K_0^2K^2}\cdot\sin^2 2Ka}$$

since, $\cos^2 2Ka = 1 - \sin^2 2Ka$

$$T = \frac{1}{1 + \left[\frac{(K_0^2+K^2)^2}{2K_0K} - 1\right]\sin^2 2Ka}$$

$$T = \frac{1}{1 + \left(\frac{K_0^2-K^2}{2K_0K}\right)^2\sin^2 2Ka} \qquad (16)$$

$$K_0^2 = \frac{2mE}{\hbar^2}, \quad K^2 = \frac{2m}{\hbar^2}(E+|V_0|)$$

So, $$\frac{K^2-K^2}{2K_0K} = \frac{\frac{2mE}{\hbar^2} - \frac{2m}{\hbar^2}(E+|V_0|)}{2\sqrt{\frac{2mE}{\hbar^2}}\cdot\sqrt{\frac{2m(E+|V_0|)}{\hbar^2}}}$$

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$$\left(\frac{K_0^2 - K^2}{2K_0 K}\right) = \frac{-|V_0|}{2\sqrt{E}\cdot\sqrt{E+|V_0|}}$$

$$\left(\frac{K_0^2 - K^2}{2K_0 K}\right)^2 = \frac{V_0^2}{4E(E+|V_0|)}$$

Eqn (16) becomes,

$$T_E = \frac{1}{1 + \frac{V_0^2}{4E(E+|V_0|)\sin^2 2Ka}}$$

$$T_E = \frac{4E(E+|V_0|)}{4E(E+|V_0| + V_0^2 \sin^2 2Ka}$$

This give transmission coefficient of the partical in potential well of finite depth. when $E < V_0$

Again, Reflection Coefficient,

$$R_E = 1 - T_E$$

$$R_E = \frac{V_0^2 \sin 2Ka}{4E(E+|V_0|) + V_0^2 \sin^2 2Ka}$$

which is required reflaction coefficient.

OR

Separate radial part of Schrodinger equation using method of separation of variables and find it's solution for Hydrogen atom.

⇒ The schrodinger's equation in spherical polar co-ordinates for the problem of hydrogen atom is that in the form it may be separated into three independent equations, each involving only a single co-ordinate.

Let us first separate the wave function $\psi(r,\theta,\phi)$ into a radial and angular parts.
Here,

$$\psi(r,\theta,\phi) = R(r)\cdot\psi(\theta,\phi) \quad \text{——— (i)}$$

In which $R(r)$ is independent of angles and $Y(\theta,\phi)$ is independent for r.
The Schrodinger's equation is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta\,\partial\theta}\partial\left(\sin\theta\frac{\theta\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\psi^2}+\frac{2\mu}{\hbar^2}$$

$$[E-V(r)]\,\psi=0 \quad \text{——— (ii)}$$

Equation (i) substituting in equation (ii)

$$\frac{Y}{r^2}\cdot\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\,\partial Y}{\partial\theta}\right)+\left[\frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2 Y}{\partial\phi^2}\right]R$$

$$+\frac{2\mu}{\hbar^2}[E-V(r)]RY=0$$

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Dividing by RY and multiplying by r^2 on both sides,

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{1}{Y}\left[\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\cdot\frac{\partial^2 Y}{\partial\phi^2}\right]$$

$$+\frac{2\mu r^2}{\hbar^2}\left[E-V(r)\right]=0$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2\mu r^2}{\hbar^2}\left[E-V(r)\right]=-\frac{1}{Y}\left[\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)\right.$$

$$\left.+\frac{1}{\sin^2\theta}\cdot\frac{\partial^2 Y}{\partial\theta^2}\right]=\lambda \text{ (say)}$$

Thus, the above equation gives the radial equation of the form.

$$\frac{1}{\partial^2}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\left\{\frac{2\mu}{\hbar^2}\left((E-V)-\frac{\lambda}{r^2}\right)\right\}R=0$$

3. Show that Newton's law of motion can be derived from Ehrenfest theorem. State and explain this theorem.

⟹ Sol^n:

Statement: classical mechanics reduces to quantum mechanics on the basis of Schrodinger equation when expectation value of dynamical variables are taken into account.

Proof: The Hamilton of a particle in one dimension is

$$H = \frac{P_x^2}{2m} + V(x) \text{ ——— } ①$$

We know, that the equation of motion for an observable F is given by,

$$\frac{d\langle F\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{F}, \hat{H}]\rangle \text{ ——— } ②$$

Here, F does not contain time explicitly here $\hat{F}$ is a hermition operator. Let us suppose, the observable is simply 'x', then.

$$\frac{d\langle x\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{x}, \hat{H}]\rangle$$

$$= \frac{1}{i\hbar}\langle[x, \frac{P_x^2}{2m} + V(x)]\rangle$$

$$= \frac{1}{2i\hbar m}\langle[\hat{x}, \hat{P}_x \hat{P}_x] + [\hat{x}, V(x)]\rangle$$

Since both are time independent this term variables to zero.

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$$\frac{d\langle x\rangle}{dt} = \frac{1}{2i\hbar m}\langle\{[\hat{x},\hat{P_x}]\hat{P_x} + \hat{P_x}[\hat{x},\hat{P_x}]\}\rangle$$

$$= \frac{1}{2i\hbar m}\langle i\hbar P_x + i\hbar P_x\rangle$$

$$= \frac{2i\hbar}{2i\hbar m}\langle P_x\rangle$$

$$\frac{d\langle x\rangle}{dt} = \frac{\langle P_x\rangle}{m} \text{ ——— } (3)$$

Differentiating eqⁿ (1) w.r.to P_x

$$\frac{\partial H}{\partial P_x} = \frac{P_x}{m}$$

$$\left\langle\frac{\partial H}{\partial P_x}\right\rangle = \frac{\langle P_x\rangle}{m} \text{ ——— } (4)$$

Comparing (3) & (4) we get,

$$\frac{d\langle x\rangle}{dt} = \frac{\langle P_x\rangle}{m}$$

$$= \left\langle\frac{\partial H}{\partial P_x}\right\rangle \text{ ——— } (5)$$

For a system of particles, this equation is analogues to,

$$\frac{d\langle q_j\rangle}{dt} = \frac{\langle P_j\rangle}{m}$$

$$= \left\langle\frac{\partial H}{\partial P_j}\right\rangle$$

$$\therefore \boxed{q_j = \frac{\partial H}{\partial P_j}} \text{ ——— } (6)$$

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Similarly, taking P_x as an observable eq^n(6) can be written as,

$$\frac{d\langle P_x\rangle}{dt} = \frac{1}{i\hbar}\langle[P_x, H]\rangle$$

$$= \frac{1}{i\hbar}\langle\left[P_x, \frac{P_x^2}{2m} + V(x)\right]\rangle$$

$$= \frac{1}{i\hbar}\langle\{\tfrac{1}{2}m + [P_x, V(x)\}\rangle$$

$$= \frac{1}{i\hbar}\langle\left[-i\hbar\frac{\partial}{\partial x}, V(x)\right]\rangle$$

$$\frac{d}{dt}\langle P_x\rangle = \langle-\frac{\partial V}{\partial x}\rangle \text{ ——— } (7)$$

Differentiating eq^n (1) w.r.t. x',

$$\frac{\partial H}{\partial x} = \frac{\partial V}{\partial x}$$

$$\langle\frac{\partial H}{\partial x}\rangle = \langle\frac{\partial V}{\partial x}\rangle \text{ ——— } (8)$$

comparing (7) & (8) we get,

$$\frac{d}{dt}\langle P_x\rangle = \langle-\frac{\partial H}{\partial x}\rangle$$

$$= \langle-\frac{\partial V}{\partial x}\rangle \text{ ——— } (9)$$

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For a system of particles, we can write;

$$\frac{dp_j}{\partial t} = -\frac{\partial H}{\partial q_j}$$

$$\dot{p}_j = -\frac{\partial H}{\partial q_j} \quad \text{—— (10)}$$

Equations (7) & (10) represent Hamilton's eqn of motion. In 3-D representations. we can write,

$$\frac{d}{dt}\langle \hat{r} \rangle = \frac{\langle \hat{p} \rangle}{m}$$

$$\text{and} \quad \frac{d}{dt}\langle p \rangle = -\langle \nabla V(\vec{r}) \rangle \Big\} \quad \text{—— (11)}$$

These are analogous to Hamilton-Jacobi equation. The second eqn reduces to Newton's 2nd Law.

$$\frac{dp}{dt} = -\nabla V(r)$$
$$= \text{Force}$$
$$= \frac{md^2r}{dt^2}$$

Schrodinger eqn leads to the classical (newton's) laws of motion on average.

4. Find the expression of the spherical harmonics when $l=2$ and $m=\pm 1$ in terms of spherical polar coordinates (θ and ϕ). Make plot of the above spherical harmonics versus θ in any plane through z-axis.

⟹ Here, the spherical harmonics,

$$\boxed{Y_l^m(\theta,\phi) = \varepsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}\, e^{im\phi}\cdot P_l^m(\cos\theta)}$$

where, $\varepsilon = (-1)^m$ for $m \geq 0$ and $\varepsilon = 1$ for $m \leq 0$

we have,

$$\int_0^{2\pi}\int_0^{\pi}[Y_l^m(\theta,\phi)]^*[Y_{l'}^{m'}(\theta,\phi)]\sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'}$$

Here, $l=2$ and $m=+1,-1$

$$\boxed{Y_2^{\pm 1} = \pm\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}}$$

Also, $Y_0^0 = \frac{1}{\sqrt{4\pi}}$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$

$$Y_1^1 = -\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{i\phi}$$

$$Y_1^{-1} = +\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{-i\phi}$$

$$Y_2^0 = \left(\frac{5}{8\pi}\right)^{1/2}(3\cos^2\theta - 1)$$

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$$Y_2^1 = -\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^{-1} = \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{-i\phi}$$

$$Y_2^2 = -\left(\frac{15}{32\pi}\right)^{1/2} \sin\theta\, e^{2i\phi}$$

$$Y_2^{-2} = -\left(\frac{15}{32\pi}\right) \sin^2\theta\, e^{-2i\phi}$$

Y_l^m is Independent of ϕ and there is rotational symmetry about z-axis. It is enough to represent $|Y_l^m|^2$ in any plane that includes the z-axis.

$$Y_0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_{1,\pm 1} = \pm\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{\pm i\phi}$$

$$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_{1,2} = \pm\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_{2,\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{\pm 2i\phi}$$

$$Y_{3,0} = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$$

$$Y_{3,\pm1} = \pm\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta\,(5\cos^2\theta - 1)\, e^{\pm i\phi}$$

$$Y_{3,\pm2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta \cos\theta \, e^{\pm 2i\phi}$$

$$Y_{3,\pm3} = \pm\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta \, e^{\pm 3i\phi}$$

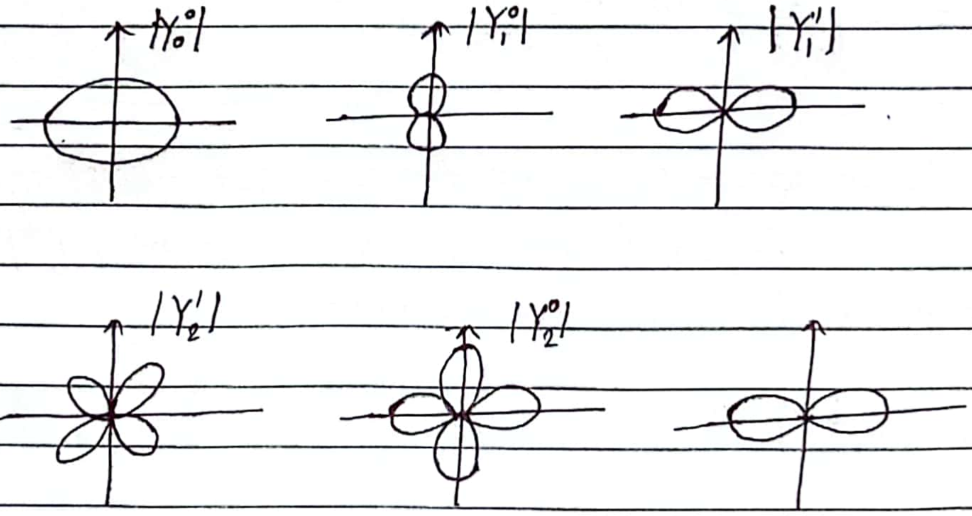

fig: Polar graphs of probability, $|Y_m^l|$ vs θ in any plane through z-axis for $l = 0, 1, 2, --- n$.

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5 Find the expression for energy eigen-values of non-dimensional harmonic oscillator using creation and annihilation operator and their relationships.

⇒ Solⁿ: The Hamiltonian of classical harmonic oscillator is

$$H = \frac{P_x^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad [\because K = m\omega^2]$$

$$= \frac{1}{2} m\omega^2 x^2 + \frac{P_x^2}{2m}$$

$$= \omega \left[\frac{m\omega x^2}{2} + \frac{P_x^2}{2m} \right]$$

$$= \omega \left[\left(\frac{m\omega}{2}\right)^{1/2} . x - \frac{iP_x}{(2m\omega)^{1/2}} \right] \left[\left(\frac{m\omega}{2}\right)^{1/2} . x + \frac{iP_x}{(2m\omega)^{1/2}} \right]$$

$$= \left[\frac{\sqrt{\hbar}}{\sqrt{2}} \left(\frac{m\omega}{\hbar}\right)^{1/2} x - \frac{i\sqrt{\hbar} P_x}{\sqrt{2}(m\omega\hbar)^{1/2}} \right] \times \left[\frac{\sqrt{\hbar}}{2} \left(\frac{m\omega}{\hbar}\right)^{1/2} . x + \frac{i\sqrt{\hbar} P_x}{\sqrt{2}(m\omega\hbar)^{1/2}} \right]$$

$$= \omega\hbar \left[\frac{1}{\sqrt{2}} \left\{ \left(\frac{m\omega}{\hbar}\right)^{1/2} . x - \frac{iP_x}{(m\omega\hbar)^{1/2}} \right\} \right] \left[\frac{1}{\sqrt{2}} \left\{ \left(\frac{m\omega}{\hbar}\right)^{1/2} . x + \frac{iP_x}{(m\omega\hbar)^{1/2}} \right\} \right]$$

Now, Let us consider new parameters,

$$X = \left(\frac{m\omega}{\hbar}\right)^{1/2} x = \alpha x \quad \text{—— (2)}$$

$$P = \frac{P_x}{(m\omega\hbar)^{1/2}} = \frac{P_x}{\alpha} \quad \text{—— (3)} \quad [\because (m\omega\hbar)^{1/2} = \alpha, \text{ from}$$

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Then,

$$[X, P] = \left[\alpha x, \frac{P_x}{\alpha \hbar}\right]$$

$$= \frac{1}{\hbar}[x, P_x]$$

$$= \frac{1}{\hbar} \, i\hbar$$

$$= i \quad \text{———} \quad (4)$$

$\therefore$ Eqn (1) becomes,

$$H = \omega\hbar \left[\frac{X - iP}{\sqrt{2}}\right]\left[\frac{X + iP}{\sqrt{2}}\right]$$

$$\Rightarrow \frac{H}{\omega\hbar} = \left[\frac{X - iP}{\sqrt{2}}\right]\left[\frac{X + iP}{\sqrt{2}}\right]$$

So, the Hamiltonian of classical harmonic oscillator is given by,

$$\mathcal{H} = \frac{H}{\omega\hbar}$$

$$= \left[\frac{X - iP}{\sqrt{2}}\right]\left[\frac{X + iP}{\sqrt{2}}\right]$$

$$= \frac{1}{2}(X^2 + P^2)$$

$$\therefore \mathcal{H} = \frac{1}{2}[X^2 + P^2] - \frac{1}{2} + \frac{1}{2}$$

$$= \frac{1}{2}[X^2 + P^2] + \frac{i \cdot i}{2} + \frac{1}{2}$$

$$= \frac{1}{2}[x^2+p^2] + \frac{i}{2}[x,p] + \frac{1}{2} \quad [\because \text{from } ④]$$

$$= \frac{1}{2}[x^2+p^2+i(xp-px)] + \frac{1}{2}$$

$$= \frac{1}{2}[x^2+ixp+p^2-ipx] + \frac{1}{2}$$

$$= \frac{1}{2}[x(x+ip) - ip(x+ip)] + \frac{1}{2}$$

$$= \frac{1}{2}(x+ip)(x-ip) + \frac{1}{2}$$

$$H = \left\{\frac{1}{\sqrt{2}}(x+ip)\right\}\left\{\frac{1}{\sqrt{2}}(x-ip)\right\} + \frac{1}{2} \quad — ⑤$$

consider two non-Hermitian dimensionsless Operators

$$\hat{a} = \frac{1}{\sqrt{2}}(x+ip) \text{ and } \hat{a}^+ = \frac{1}{\sqrt{2}}(x-ip)$$

where,

$\hat{a}$ = Annihilation Operaters

$\hat{a}^+$ = Creation Operators

Using the value of $\frac{x-ip}{\sqrt{2}} = \hat{a}^+$ and $\frac{x-ip}{\sqrt{2}} = \hat{a}$ in eqⁿ

$$H = \hat{a}^+\hat{a} + \frac{1}{2} \quad — ⑥$$

Again,

$$\hat{a}^+ + \hat{a} = \frac{1}{2}(x-ip) + \frac{1}{\sqrt{2}}(x+ip)$$

$= \sqrt{2}\, X$

$\Rightarrow X = \dfrac{\hat{a}^{+} + \hat{a}}{\sqrt{2}}$ ——— (7)

Again,

$\hat{a}^{+} + \hat{a} = \sqrt{2}(-ip)$

$\Rightarrow p = \dfrac{i}{\sqrt{2}}(\hat{a}^{+} - \hat{a})$ ——— (8)

Now,

$[\hat{a} + \hat{a}^{+}] = \frac{1}{2}[X + ip, X - ip]$

$= \frac{1}{2}\{[X, X] + [ip, X] - [X, ip] - [ip, ip]\}$

$= \frac{1}{2}\{i[p, X] - i[X, p]$

$= \frac{1}{2}\{i(-i) - i(i)\}$ ·[from (4)]

$= 1$

$\Rightarrow \hat{a} + \hat{a}^{+} - \hat{a}^{+} + \hat{a} = 1$ ——— (9)

So, from eq^n (6) and (9)

$H = \hat{a}\hat{a}^{+} - 1 + \frac{1}{2}$

$H = \hat{a}\hat{a}^{+} - \frac{1}{2}$ ——— (10)

Adding (6) & (10),

$2H = \hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}$

$\therefore \boxed{H = \dfrac{\hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}}{2}}$ which is required expression of Harmonic oscillator in terms of creation and Annihilation operators.

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6. Separate radial part of schrodinger equation using method of separation of variables and find its solution for Hydrogen atom.

⇒ Solⁿ: The Hydrogen atom consists of a proton around which the electron revolves. The proton is assumed at rest at the origin and electron is orbiting around a fixed at a distance 'r' under the influence of the attractive coulomb field.

The potential energy function due to coulomb field is,

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

Let m_p and m_e be the mass of proton and mass of electron respectively. Then the reduced mass of the system will be.

$$\mu = \frac{m_e m_p}{m_e + m_p} \quad \text{——— (2)}$$

We know that, radial wave eqⁿ of hydrogen atom problem is,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \left[\frac{2\mu}{\hbar^2}(E-V) - \frac{\lambda}{r^2}\right]R = 0 \quad \text{——— (3)}$$

Let us introduced a variables (ρ) such that,

$$\rho = \alpha r . \Rightarrow r = \frac{\rho}{\alpha}$$

$$\frac{d\rho}{dr} = \alpha$$

$$\frac{d}{dr} = \alpha \frac{d}{d\rho}.$$

Also,

$$V = \frac{-Ze^2}{r}$$

Then above eqn becomes.

$$\frac{\alpha^2}{\rho^2}\alpha\frac{d}{d\rho}\left(\frac{\rho^2}{\alpha^2}\cdot\alpha\frac{d}{d\rho}\right)+\frac{2\mu}{\hbar^2}\left(E-\frac{Ze^2}{r}\right)$$

$$-\left(\frac{l(l+1)\alpha^2}{\rho^2}\right)R=0$$

$$\frac{\alpha^2}{\rho^2}\cdot\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\left[\frac{2\mu}{\hbar^2}\left(E+\frac{Ze^2\alpha}{\rho}\right)-\frac{l(l+1)\alpha^2}{\rho^2}\right]R=0$$

Dividing both side by α^2

$$\frac{1}{\rho^2}\frac{d}{\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\left[\left(\frac{2\mu E}{\hbar\alpha^2}+\frac{2\mu Ze^2}{\hbar^2\rho\alpha}\right)\right.$$

$$\left.-\frac{l(l+1)}{\rho^2}\right]R=0$$

For bound state.

$$E_n=-|E_n|$$

Also, let,

$$\frac{2\mu Ze^2}{\hbar^2\alpha}=\lambda'$$

$$\frac{2\mu E}{\hbar^2\alpha^2}=-\frac{1}{4}$$

Then,

$$\Rightarrow \frac{1}{\rho^2}\cdot\frac{d}{d\rho}\cdot\left(\rho^2\frac{dR}{d\rho}\right)+\left[-\frac{1}{4}+\frac{\lambda'}{\rho}-\frac{l(l+1)}{\rho^2}\right]R=0$$

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$$\Rightarrow \frac{1}{\rho^2}\cdot\frac{\rho^2 d^2R}{d\rho^2}+\frac{1}{\rho^2}\,2\rho\cdot\frac{dR}{d\rho}+\left[-\frac{1}{4}+\frac{\lambda'}{\rho}-\frac{l(l+1)}{\rho^2}\right]R=0$$

$$\Rightarrow \frac{d^2R}{d\rho^2}+\frac{2}{\rho}\frac{dR}{d\rho}+\left[-\frac{1}{4}+\frac{\lambda'}{\rho}-\frac{l(l+1)}{\rho^2}\right]R=0 \longrightarrow (4)$$

The asymmetric solution of eqn (4) is,

$$R(\rho)=F(\rho)\,e^{-\rho/2}$$

$$\frac{dR}{d\rho}=F'(\rho)\cdot e^{-\rho/2}-\frac{1}{2}F(\rho)\cdot e^{-\rho/2}$$

$$\frac{dR}{d\rho}=\left[F'(\rho)-\frac{1}{2}F(\rho)\right]e^{-\rho/2}$$

$$\frac{d^2R}{d\rho^2}=\left[F'(\rho)-\frac{1}{2}F(\rho)\right]e^{-\rho/2}$$

$$\frac{d^2R}{d\rho^2}=\left[F'(\rho)-\frac{1}{2}F'(\rho)\right]e^{-\rho/2}-\frac{1}{2}e^{-\rho/2}\left[F'(\rho)-\frac{1}{2}F(\rho)\right]$$

$$\frac{d^2R}{d\rho^2}=e^{-\rho/2}\left[F''(\rho)-\frac{F'(\rho)}{2}-\frac{F'(\rho)}{2}+\frac{F(\rho)}{4}\right]$$

$$\frac{d^2R}{d\rho^2}=e^{-\rho/2}\left[F''(\rho)-F'(\rho)+\frac{F(\rho)}{4}\right]$$

putting those value in eqn (4)

$$e^{-\rho/2}\left[F''(\rho)-F'(\rho)+\frac{F(\rho)}{4}\right]+\frac{2}{\rho}\left[F'(\rho)-\frac{1}{2}F(\rho)\right]e^{-\rho/2}$$
$$+\left[-\frac{1}{4}+\frac{\lambda'}{\rho}-\frac{l(l+1)}{\rho^2}\right]\cdot F(\rho)\,e^{-\rho/2}=0$$

$$e^{-\rho/2}\left[F''(\rho)+\left(\frac{2}{\rho}-1\right)F(\rho)+\left(-\frac{1}{\rho}+\frac{\lambda'}{\rho}\right)-\frac{l(l+1)}{\rho^2}\right)$$
$$F(\rho)\Big]=0$$

$$F''(\rho)+\left(\frac{2}{\rho}-1\right)F'(\rho)+\left(\frac{\lambda'-1}{\rho}-\frac{l(l+1)}{\rho^2}\right)F(\rho)=0 \quad \text{—— (5)}$$

Let solution of eqn (2) is of the form

$$F(\rho)=\rho^{l}L(\rho)$$

$$F'(\rho)=\rho^{l}L'(\rho)+l\rho^{l-1}.L\rho$$

$$F''(\rho)=\rho^{l}L''(\rho)+\rho^{l-1}L'(\rho)+l(l-1)\rho^{l-2}L(\rho)$$

$$F''(\rho)=\rho^{l}L''(\rho)+2l\rho^{l-1}L'(\rho)+l(l-1)\rho^{l-2}.L(\rho)$$

putting those in eqn (5)

$$\rho^{l}L''(\rho)+2l\rho^{l-1}L'(\rho)+l(l-1)\rho^{l-2}L(\rho)+\left(\frac{2}{\rho}-1\right)$$
$$\left(\rho^{l}L'(\rho)+l\rho^{l-1}L(\rho)\right)+\left[\left(\frac{\lambda'-1}{\rho}\right)-\frac{l(l+1)}{\rho^2}\right]\rho^{2}L(\rho)=0$$

Multiplying this with $\frac{\rho^2}{\rho^l}$

$$\rho^{2}L''(\rho)+2l\rho L'(\rho)+l(l-1)L(\rho)+(2-\rho)\rho(L'\rho+l\rho^{-1}$$
$$L(\rho))+$$
$$[(\lambda'-1)\rho-l(l+1)]L(\rho)=0$$

$$\rho^{2}L''(\rho)+\rho L'(\rho)(2l+(2-\rho))+[l(l-1)+(2-\rho)l+(\lambda'-1)\rho$$
$$-l(l+1)]L(\rho)=0$$

put $\lambda' = n$

$$\rho^2 L''(\rho) + [2l+2-\rho]\rho L'(\rho) + [(\lambda'-1)\rho - \rho l]L(\rho) = 0$$

$$\rho^2 L''(\rho) + (2l+2-\rho)\rho L'(\rho) + (n-l-1)\rho \cdot L(\rho) = 0$$

Dividing by 'ρ'

$$\rho L''(\rho) + \{(2l+1)+1-\rho\} L'(\rho) + (n-l-1)L(\rho) = 0$$

This eqn comparable with associated Laguerre polynomial,

$$\rho L''^{p}_{q} + (p+1-q) L'^{p}_{q} + (q-p) L^{p}_{q} = 0$$

we get, $p = 2l+1$; $q = n+2$

This its soln is,

$$L(\rho) = C \cdot L^{2l+1}_{n+l}(\rho)$$

$$R_{nl}(r) = Ce^{-\rho/2} \cdot e^{l} L(\rho)$$

where, C is normalization constant, by using normalization condition. we get,

$$\int_0^\infty R_{nl}(r) \cdot R^*_{nl}(r) r^2 dr = 1$$

$$C = \left[\frac{\alpha^3 (n-l-1)!}{2n(n+1)!^3}\right]^{1/3}$$

$\therefore$ The final solution is.

$$R_{nl}(r) = \left[\frac{\alpha^3 (n-l-1)!}{2n(n+1)!^3}\right]^{1/3} \cdot e^{-\rho/2} \rho^{l} L^{2l+1}_{n+1}(r)$$

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I. Answer all questions.
a) State and explain Heisenberg uncertainty principle.
⇒ Statement:-
It is impossible to specify precisely and simultaneously the values of both members of particular pair of physical variables that describe the behaviour of an atomic system.

The position and momentum of a particle can not be determine simultaneously with the same level of accuracy. If momentum is measured more accurately there will be more error in the determination of position.
Mathematically,
$$\Delta x \cdot \Delta p \geq \frac{h}{2\pi}$$
where, $\Delta x \rightarrow$ Uncertainty in position.
$\Delta p \rightarrow$ Uncertainty in moment.
Likewise,
$$\Delta E \cdot \Delta t \geq \frac{h}{2\pi}$$

$$\Delta \theta \cdot \Delta L \geq \frac{h}{2\pi}$$

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OR,

Find de Broglie wave length of a 10g grass-hopper jumping at the speed of 80km/h in a straight field.

⇒ solution:

Given,

mass(m) = 10g
$= 10 \times 10^{-3}$ kg

velocity (v) = 80 km/hr

wavelength (λ) = ?

have de-Broglie wavelength

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

$$= \frac{6.62 \times 10^{-34}}{10 \times 10^{-3} \times 80}$$

$$= 0.08275 \times 10^{-32} m$$

which is much lesser than the dimensions of the grasshopper, hence, wave like properties can not be observed.

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b) Classical physics could not explain the behaviour of a black body radiator at very short wave lengths. What was the problem? Explain.

⇒ soln:-

According to classical theory of radiation, the exchange of radiation between source of temperature 'T' and enclosure of temperature T_0 takes place continuously i.e. the radiation emits in all possible frequencies grouping from 0 to ∞.

Then the energy exchange relations as given by Rayleigh Jeans law. i.e. Total energy radiated per unit volume belonging to range $d\nu$ is,

$$u(\nu)d\nu = \frac{8T_oSt\nu^2}{c^3} kT_0 d\nu$$

where, $u(\nu)$ = energy radiated per unit frequency range

T_0 = Temperature of enclosure

k = Boltzmann constant

c = velocity of light.

So, the total energy radiated per unit volume 0, $h\nu$, $2h\nu$ i.e. in multiples of some small unit called quantum.

Now, to calculate the average energy of resonators, we use maxwell's Boltzmann's Statistics given by,

$$\mathcal{E} = \frac{\sum_{n=0}^{\infty} f(\mathcal{E}_n)\, \mathcal{E}_n}{\sum_{n=0}^{\infty} f(\mathcal{E}_n)}$$

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OR

Describe the meaning of barrier penetration.

⇒ Solⁿ:

Barrier penetration refers to the phenomenon in quantum mechanics where a particle, such as an electron, is able to pass through a potential energy barrier that it classically shouldn't be able to overcome. This occurs due to the wave-like nature of particles, allowing them to exhibit behaviors such as tunneling through barriers that would be impossible according to classical physics. It's a key concept in understanding various quantum mechanical phenomena, such as nuclear fusion in stars and the operation of semiconducter devices.

8. Answer all Questions.

a) Explain zero-point energy of one-dimensional harmonic oscillator.

⇒ Sol^n:-

we know that, the energy value of Harmonic Oscillater is

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$\text{If } n=0, \; E_0 = \frac{1}{2}\hbar\omega$$

This is called zero point energy. A comparision with the result $E_n = nh\nu$ or $n\hbar\omega$, obtained by using old Quantum theory shows a difference regarding the space of the energy levels. The only difference is that all equally space energy level are shifted upward by an amount equal to half the separation of energy levels. i.e. $\frac{1}{2}\hbar\omega$ equal to zero point energy. Thus. it is clear that in the lowest state, the Harmonic oscillator has energy greater than it would have if it were at rest in its equilibrium position. The existence of zero point energy is in agreement with experiment and is an important features of Quantum mechanics.

(b) What do you mean by the expectation value of a dynamical quantity Quantum mechanics?

⇒ sol^n: The expectation value of a dynamical quantity is defined as its mathematical average for the measurement. The expectation value of any function

$$F(r) = F(x, y, z) \text{ is,}$$

$$\langle F \rangle = \int \psi^* . F . \psi dv$$

If the wave function ψ is not normalized then expectation value of F is,

$$\langle F \rangle = \frac{\int \psi^* F(r) \psi dv}{\int \psi^* \psi dv}$$

For eg:- Expectation value of position

$$\langle x \rangle = \int \psi^* . x . \psi dx$$

For expectation value of momentum,

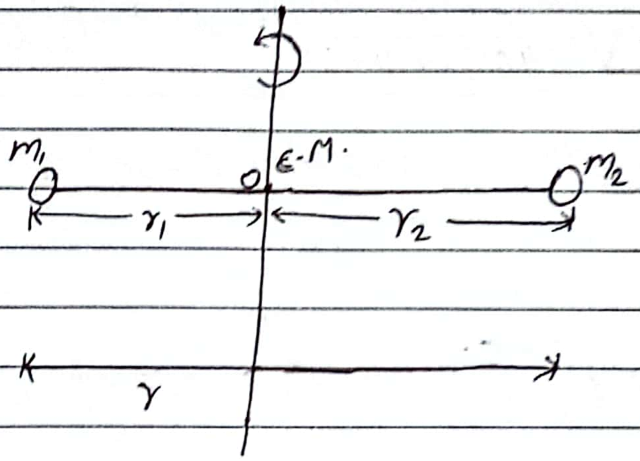
$$\langle p \rangle = \int \psi^* (-i\hbar \nabla) \psi dv$$

For expectation value of energy,

$$\langle E \rangle = \int \psi^* \left(i\hbar \frac{\partial}{\partial t}\right) \psi dv$$

c) What is rigid Rotator?

⇒ A rigid body consist of two particles (point particles) separated by a fixed distance (r). so, its potential is zero. i.e. $V(r) = 0$. i.e. $V(r) = 0$, so that the system rotate about an axis passing through the centre of mass.



As the system is rotating about an axis passing through centre of mass. we can write,

$$m_1 r_1 = m_2 r_2$$

$$m_1 (r - r_2) = m_2 r_2 \quad (\because r_1 + r_2 = r)$$

$$r_2 = \frac{m_1 r}{m_1 + m_2}$$

similarly, $r_1 = \frac{m_2 r}{m_1 + m_2}$

The moment of inertia of a system is,

$$(I) = m_1 r_1^2 + m_2 r_2^2$$

$$(I) = m_1 \frac{m_2^2 r^2}{(m_1+m_2)^2} + m_2 \cdot \frac{m_1^2 r^2}{(m_1+m_2)^2}$$

$$(I) = \frac{m_1 m_2}{m_1 + m_2} \cdot r^2$$

$(I) = \mu r^2$ (where, $\mu = \frac{m_1 m_2}{m_1 + m_2}$ called reduced mass.)

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(d) Discuss the condition under which total parity is conserved.

⇒ soln :-

Parity refers to the behavior of wave function under spatial inversion. The space inversion refers to the reflection of spatial coordinates about the origin.

Let, $|\psi(r)\rangle$ represents the state function then the parity operater can be expressed as,

$$\hat{\pi}|\psi(r)\rangle = |\psi(-r)\rangle$$

$$\hat{\pi}|\psi(-r)\rangle = |\psi(r)\rangle \quad \text{——— (1)}$$

The parity operator inverts the space of the state function $|\psi(r,t)\rangle$ i.e. $\hat{\pi}|\psi(r)\rangle = |\psi(-r)\rangle$

Applying Hamiltonian,

$$\hat{H}\hat{\pi}|\psi(r)\rangle = H|\psi(-r)\rangle$$

or, $\hat{H}\hat{\pi}|\psi(r)\rangle = E|\psi(-r)\rangle$ ——— (2)

$[\because H|\psi\rangle = E|\psi\rangle]$

Again, we can write,

$$\hat{H}|\psi(r)\rangle = E|\psi(r)\rangle$$

Applying parity operator

$$\hat{\pi}\hat{H}|\psi(r)\rangle = \hat{\pi}E|\psi(r)\rangle$$
$$= E\{\hat{\pi}|\psi(r)\rangle\}$$

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9. Find the value of the commulator $[x,(x,H)]$ where H represents Hermitian operator.

⇒ Sol^n,

$$H = \frac{P_x^2 + P_y^2 + P_z^2}{2m}$$

$$[x, P_x] = i\hbar, \quad [x, P_y] = 0, \quad [x, P_z] = 0$$

$$[x, H] = \frac{1}{2m}[x, P_x]$$

$$= \frac{1}{2m} \times 2i\hbar P_x$$

$$= \frac{i\hbar}{m} P_x$$

$$[x,[x,H]] = \left[x, \frac{i\hbar P_x}{m}\right]$$

$$= \frac{i\hbar}{m}[x, P_x]$$

$$= \frac{i\hbar}{m} \times i\hbar$$

$$= -\frac{\hbar^2}{m}$$

10. The wave function of a particle confined in a box of length a is

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right), \quad 0 \le x \le a.$$

Find the probability of finding particle in the region $0 \le x \frac{a}{2}$.

⇒ Solution

we have a given wave function,

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \quad \text{for } 0 \le x \le a.$$

we have to find the probability of finding particle in the region $0 \le x \le \frac{a}{2}$.

The complex conjugate of wave function $\psi(x)$ is $\psi^*(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$.

we know that probability density for region $0 \le x \le \frac{a}{2}$ is.

$$\rho(x) = \int_0^{a/2} \psi^*(x)\, \psi(x)\, dx$$

$$\text{or, } \rho(x) = \int_0^{a/2} \left(\frac{2}{a}\right) \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$\text{or, } \rho(x) = \frac{2}{a} \int_0^{a/2} \left(\frac{1 - \cos\frac{2\pi x}{a}}{2}\right) dx$$

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or, $\rho(x) = \frac{1}{a}\left[x - \frac{a}{2\pi}\sin\frac{2\pi x}{a}\right]_0^{a/2}$

or, $\rho(x) = \frac{1}{a}\left[\frac{a}{2} - 0\right]$.

$= \frac{1}{2}$

$\therefore \rho(x) = \rho\left(0 \leq x \leq \frac{a}{2}\right)$.

$= \frac{1}{2}$.

Therefore, the probability of finding the particle in region $\left(0 \leq x \leq \frac{a}{2}\right)$ is $\rho(x) = \frac{1}{2}$.

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11. If A and B are Hermitian operators, the check whether $i[A,B]$ is Hermitian or not.

⇒ Soln:-

$\cancel{\int \psi_m^*}$

$$\int \psi_m^* \, i[A,B] \psi_n \, dx = i\int \psi_m^* AB \psi_n \, dx - i\int \psi_m^* BA \psi_n \, dx$$

$$= i\int B^* A^* \psi_m^* \psi_n \, dx - i\int A^* B^* \psi_m^* \psi_n \, dx$$

$$= \int \left(i[A,B]\psi_m\right)^* \psi_n \, dx$$

Hence, $i[A,B]$ is Hermitian.

For the product AB to be Hermitian, it is necessary that

$$\int \psi_m^* AB \psi_n \, dx = \int A^* B^* \psi_m^* \psi_n \, dx$$

Since A and B are Hermitian, this equation reduces to

$$\int B^* A^* \psi_m^* \psi_n \, dx = \int A^* B^* \psi_m^* \psi_n \, dx$$

which is possible only if

$$AB = BA$$

This is, ~~possible~~ for AB to be Hermitian, A must commute with B.

12. An electron moves in one-dimensional potential of width 8Å and depth of ev. find the number of bound state present. Interpret the nature of the wave function.

⇒ solⁿ:- Square potential well with finite walls

$$\text{potential } V(x) = \begin{cases} V_0, & x < -a \\ 0, & -a < x < a \\ V_0, & x > a, \end{cases}$$

case 1: $E < V_0$: The wave function inside the wall can either be symmetric or anti symmetric about the origin.

Symmetric case: $ka \tan ka = \alpha a$

Antisymmetric case: $ka \cot ka = -\alpha a$

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

The solutions of above equation gives results regarding the no. of bound states in the well:

one (symmetric) if $0 < V_0 a^2 < \frac{\pi^2 \hbar^2}{8m}$

Two (1- symmetric, 1- antisymmetric)

if $\frac{\pi^2 \hbar^2}{8m} < V_0 a^2 < \frac{4\pi \hbar^2}{8m}$

Three (two symmetric, one anti symmetric,

if $\frac{4\pi \hbar^2}{8m} < V_0 a^2 < \frac{9\pi^2 \hbar^2}{8m}$

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case II : $E > V_0$, in this case, particle is not bound and the wave function is sinusoidal in all three regions.

Here, $V_0 a^2 = (12 \times 1.6 \times 10^{-19})(16 \times 10^{-20})$ $[a = 4\mathring{A}]$

$$= 307.2 \times 10^{-39} \, kg\, m^4 s^2$$

$$\frac{\pi^2 \hbar^2}{8m} = \frac{\pi^2 (1.05 \times 10^{-34})}{8 \times 9.1 \times 10^{-31}}$$

$$= 14.96 \times 10^{-39} \, kg\, m^4 s^{-2}$$

$\therefore$ $V_0 a^2 = 307.2 \times 10^{-39}$ $kg\, m^4 s^{-2}$ lies betn $\frac{16\pi^2\hbar^2}{8m}$ & $\frac{25\pi^2\hbar^2}{8m}$

$\therefore$ The no. of bound states present is 5.

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13. A free particle of mass m is trapped in a one-dimensional box of width a. The wave function is known to be:

$$\psi(x) = \frac{1}{4}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + A\sqrt{\frac{1}{a}}\sin\left(\frac{3\pi x}{a}\right) - \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right)$$

Find A show that $\psi(x)$ is normalized. which state is the most probable state?

$\Rightarrow$ soln:- The basis function for 1-D box a,

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

$$\therefore \psi(x) = \frac{1}{2}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + A\sqrt{\frac{1}{a}}\sin\left(\frac{3\pi x}{a}\right) - \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right)$$

$$= \frac{1}{2}\phi_1(x) + A\phi_3(x) - \phi_4(x)$$

when, $(\psi(x), \psi(x)) = 1$

$$\Rightarrow \cancel{\frac{\phi}{4} + A^2 7},$$

$$\frac{1}{2} + A + 1 = 1$$

$$\Rightarrow A = -\frac{1}{2}$$

$$\therefore \psi(x) = \frac{1}{2}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{1}{a}}\sin\left(\frac{3\pi x}{a}\right) - \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right)$$

$$= \frac{1}{2}\phi_1(x) + \phi_3(x) - \phi_4(x)$$

state	Energy measurements	probability
$\phi_1(x)$	$\frac{\pi^2\hbar^2}{2ma^2}$	$\left(\frac{1}{2}\right) = 0.5$
$\phi_2(x)$	$\frac{4\pi^2\hbar^2}{2ma^2}$	$1 = 1$
$\phi_3(x)$	$\frac{16\pi^2\hbar^2}{2ma^2}$	$\frac{1}{2} = 0.5$

$\therefore$ The most probable state is $\phi_2(x)$ with probable energy.

$$E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$$

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14. For the n^{th} state of the harmonic oscillator, evaluate the uncertainity produce $(\Delta x)(\Delta p)$. Show that the zero-point energy of $\frac{1}{2}\hbar\omega$ of a linear Harmonic oscillator is a manifestation of the uncertainity principle.

⇒ Sol^n:-

According to initial theorem, average values of kinetic and potential energies of a classical harmonic oscillator are equal. Assuming this holds for the expectation values of quantum oscillator,

$$\frac{1}{2m}\langle p_x^2\rangle = \frac{1}{2}K\langle x^2\rangle = \left(n+\frac{1}{2}\right)\frac{\hbar\omega}{2}$$

Hence,

$$\langle p_x^2\rangle = m\hbar\omega\left(n+\frac{1}{2}\right)$$

$$\langle x^2\rangle = \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)$$

Here, $(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle x^2\rangle$

and $(\Delta p_x)^2 = \langle p_x^2\rangle$

$$\therefore (\Delta x)^2(\Delta p_x)^2 = \left(n+\frac{1}{2}\right)\hbar^2$$

$$\therefore \Delta x\cdot\Delta p_x = \left(n+\frac{1}{2}\right)\hbar$$

Here,

$$\langle E\rangle = \frac{1}{2m}\langle p^2\rangle + \frac{1}{2}K\langle x^2\rangle$$

$$= \frac{1}{2m}\langle\Delta p\rangle^2 + \frac{1}{2}K\langle\Delta x\rangle^2$$

we have,

$$\langle \Delta p \rangle^2 \langle \Delta x \rangle^2 = \frac{\hbar^2}{4}$$

$$\langle E \rangle = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2} k (\Delta x)^2$$

For R.H.S. to be minimum,

$$\frac{\partial \langle E \rangle}{\partial \langle \Delta x \rangle^2} = 0,$$

$$\frac{\hbar^2}{8m(\Delta x)^4_{min}} + \frac{1}{2} k - 0,$$

$$(\Delta x)^2_{min} = \frac{\hbar^2}{2m\omega}$$

$$\therefore \langle E \rangle_{min} = \frac{\hbar^2}{8m} \frac{2m\omega}{h} + \frac{1}{2} m\omega^2 \frac{\hbar}{2m\omega}$$

$$= \frac{1}{2} \hbar\omega$$