Name of Paper	**: Quantum Mechanics and Applications**
Name of the Course	**: B.Sc. (Hons.) Physics**
Semester	**: V**
Duration	**: 3 Hours**
Maximum Marks	**: 75**

Nov. / Dec. 2019

Attempt five questions in all Q. 1. and all its parts are compulsory.
Attempt any four questions from the rest. Also, attempt any two parts
out of three from each questions.
Non-programmable calculators are allowed.

Q. 1. (a) Normalize the wave function, $\psi(x) = e^{-|x|/a}$. (3)

Ans.
$$\psi = e^{-|x|/a}, \qquad \psi^* = e^{-|x|/a}$$
$$\psi\psi^* = e^{-|x|/a},$$

For mormalization $\int_{-\infty}^{\infty} \psi \psi^* \, dx = 1$

So,
$$\int_{-\infty}^{0} e^{-2|x|/a} dx = 1$$

$$\Rightarrow \int_{-\infty}^{0} e^{2x/a} dx + \int_{0}^{\infty} e^{-2x/a} = 1$$

$$\Rightarrow \left[\frac{e^{2x/a}}{\alpha/a}\right]_{-\infty}^{0} + \left[\frac{e^{-2x/a}}{-\alpha/a}\right]_{0}^{\infty} = 1$$

$$\left[\frac{a}{a} - 0\right] + \left[0 - \left(\frac{-a}{a}\right)\right] = 1$$

So, $a = 1$

Normalize wave function $= \psi = e^{-|x|}$.

(b) Write the Schrodinger equation for a system of two particles of masses m_1 and m_2 carrying charges e_1 and e_2 respectively in what kind of field ? (2)

Ans. $m_1, e_1 =$ mass and charge of Ist particles
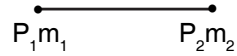
$m_2, e_2 =$ mass and charge of IInd particles

When two charges kept in a system they interact with each othes through ibctrostatic foro.

$$\text{Potential is given by} = V(x) = \frac{1}{4\pi\varepsilon_0} \frac{e_1 \, e_2}{x}$$

$$x = \text{Distance between two charges}$$

There common mass at

$$\text{Centre of mass} = \mu = \frac{m_1 + m_2}{m_1 + m_2}$$

P₁m₁   P₂m₂

General Schrodinger equation is :

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

$$\frac{d^2\psi}{dx^2} - \frac{2\mu}{\hbar^2} V(x)\psi(x) = E\psi(x) \times \left(\frac{-\hbar^2}{2\mu} \right)$$

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2} [E - V(x)]\psi(x) = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2} \left[E - \frac{1}{4\pi\varepsilon} \frac{e_1 \, e_x}{x} \right]\psi = 0$$

(c) Given that the position and momentum operators are Hermitian, verify whether the operator $\hat{x}^2 + \hat{x}\hat{p}_x$, is Hermitian. **(3)**

Ans. $\hat{x} \rightarrow$ Hermitian $\hat{p} \rightarrow$ Hermitian

If operator A is Hermitian then $A^+ = A$

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

Using $(A + B)^+ = A^+ + B^+$

$$= (\hat{x}^+)^2 + \hat{p}_x \, \hat{x}^+$$

$$\hat{x}^+ = \hat{x} \text{ and } \hat{p}_x^+ = \hat{p}_x$$

$$[\hat{x}^2 + \hat{x}\,\hat{p}_x]^+ = \hat{x}^2 + \hat{p}_x \, \hat{x}$$

Since, $\hat{x}$ & $\hat{p}$ do not commute with so given operator is not hermitian.

(d) Write the values of quantum numbers n, l, s, j, m_1 for the following states :
       (i) $2^2S_{1/2}$ **(ii) $5^2F_{5/2}$.** **(3)**

Ans. (*i*) $2^2S_{1/2}$

General notation $\rightarrow n^{2S+1}L_j$

So, $n = 2$, $S = \dfrac{1}{2}$, $L = 0$, $j = \dfrac{1}{2}$ $m_e = 0$

(*ii*) $5^2F_{5/2}$

So, $n = 5$, $S = \dfrac{1}{2}$, $L = 0$, $j = \dfrac{1}{2}$ $L = 3$, $m_e = -3, -3, -1, 0, 1, 2, 3$

(*e*) **Consider the state, $\psi = \sqrt{\dfrac{1}{10}}\phi_1 + \sqrt{\dfrac{3}{5}}\phi_2 + \sqrt{\dfrac{3}{10}}\phi_3$, where ϕ_n are orthonormal eigenstates of an operator $\hat{A}$. Find the expectation value of the operator $\hat{A}$ is the state ϕ, if it satisfies the eigenvalue equation $\hat{A}\phi_n = (2n^2 + 1)\phi_n$.** **(3)**

Ans. $\psi = \sqrt{\dfrac{1}{10}}\phi_1 + \sqrt{\dfrac{3}{5}}\phi_2 + \sqrt{\dfrac{3}{10}}\phi_3$

$$\hat{A}\phi_n = (2n^2 + 1)\phi_n, \quad \langle\psi\psi\rangle = 1$$

Expectation of $\hat{A} = \langle\psi|\hat{A}|\psi\rangle / \langle\psi|\psi\rangle$

$$= \left[\sqrt{\frac{1}{10}} <\phi_1| + \sqrt{\frac{3}{5}} <\phi_2| + \sqrt{\frac{3}{10}} <\phi_3|\right]$$

$$\hat{A}\left[\sqrt{\frac{1}{10}}|\phi_1> + \sqrt{\frac{3}{5}}|\phi_2> + \sqrt{\frac{3}{10}}|\phi_3>\right]$$

$$= \left[\sqrt{\frac{1}{10}} <\phi_1| + \sqrt{\frac{3}{5}} <\phi_2| + \sqrt{\frac{3}{10}} <\phi_3|\right]$$

$$\left[(2(1)^2 + 1)\sqrt{\frac{1}{10}}|\phi_1> + (2(2)^2 + 1)\sqrt{\frac{3}{5}}|\phi_2>\right.$$

$$\left. + (2(3)^2 + 1)\sqrt{\frac{3}{10}}|\phi_3>\right]$$

$$= \frac{3}{10} + \frac{3}{5} \times 9 + \frac{3}{10} \times 19 = \frac{2}{10} + \frac{27}{5} + \frac{57}{10}$$

$$= \frac{3 + 54 + 57}{10} = \frac{114}{10} = 11.4.$$

(f) Write down the wave function for a system of (i) two Bosons and (ii) two fermions indistinguishable. **(2)**

Ans. If $\psi\,(\xi_1, \xi_2)$ is any normalized assymetric wave function.

(i) Two Bosons : Bosons have symmetric wave function

$$\psi_s(\xi_1, \xi_2) = \frac{1}{\sqrt{2}}[\psi(\xi_1, \xi_2) - \psi(\xi_2, \xi_1)]$$

(ii) Fermions : Fermions have anti symmetric wave function

$$\psi_a(\xi_1, \xi_2) = \frac{1}{\sqrt{2}}[\psi(\xi_1, \xi_2) - \psi(\xi_2, \xi_1)]$$

(g) What is the probability that an electron in the state $\psi_{210} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0^{5/2}}\right) re^{-t/2a_0} \cos(\theta)$ of the hydrogen atom, exists between a distance of $3a_0$ to $6a_0$ from the nucleus. **(3)**

Ans. $\psi_{210} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0^{5/2}}\right) re^{-t/2a_0} \cos(\theta)$

$$P = \int_{0}^{2\pi}\int_{0}^{\pi}\int_{3a_0}^{6a_0} \psi_{210} \times \psi_{210}^{*} \; dV$$

$$= \int_{0}^{2\pi}\int_{0}^{\pi}\int_{3a_0}^{6a_0} \frac{1}{\pi} \times \frac{1}{a_0^{s}} r^2 e^{-r/a_0} \cos^2\theta$$

$$= \int_{0}^{2\pi}\int_{0}^{\pi}\int_{3a_0}^{6a_0} \times \frac{1}{\pi} \times \frac{1}{a_0 s} r^2 e^{-r/a_0} \cos^2\theta \times r^2 \sin dr\, d\theta\, d\phi$$

$$= \frac{1}{\pi a_0^{s}} \int_{0}^{2\pi}\int_{0}^{\pi}\int_{3a_0}^{6a_0} r^4 e^{-r/a_0} \; dr \sin\phi\, d\phi \cos^2\theta d\theta$$

$$= \frac{1}{\pi a_0^{s}} \int_{0}^{2\pi} \cos^2\theta\, d\theta \int_{0}^{\pi} \sin\phi\, a\phi \int_{3a_0}^{6a_2} r^4 e^{-r/a_0}$$

$$= \frac{1}{\pi a_0^s} \int_0^{2\pi} \left(\frac{1 + \cos 2\theta}{2} \right) d\theta \times 2 \times \int_{3a_1}^{6a_0} r^4 \, e^{-r/a_0} \, dr$$

$$= \frac{2}{\pi a_a^s} \left[\frac{\theta}{2} \right]_0^{2\pi} \int_{3a_0}^{6a_0} r^4 \, e^{-r/a_0} \, dr$$

$$= \frac{2}{\pi a_0^s} \times \frac{2\pi}{2} \int_{3a_0}^{6a_0} r^4 \, e^{-r/a_0} \, dr$$

$$= \frac{2}{a_a^s} \left[r^4 \frac{e^{-r/a_0}}{(-1/a_0)} - \int 4r^3 \times \frac{e^{-r/a_0}}{-1/a_0} \right]$$

$$= \frac{2}{a_a^s} \left[r^4 a_0 e^{-r/a_0} + 4r^3 a_0 \frac{e^{-r/a_0}}{(-1/a_0)} \right] + 12a_0^2 \int r^2 e^{-r/a_0} \, dr$$

$$= \frac{2}{a_0^s} \left[-r^4 a_0 e^{-r/a_0} - 4r^3 a_0^2 e^{-r/a_0} \right] + 12a_0^2$$

$$r^2 \frac{e^{-r/a_0}}{(-1/a_0)} - 12a_0^2 \int 2r \frac{e^{-r/a_0}}{(-1/a_0)}$$

$$= \frac{2}{a_0^s} \left[-r^4 a_0 e^{-r/a} - 4r^3 a_0^2 e^{-r/a_0} - 12r^2 a_0^3 \right.$$

$$e^{-r/a_0} + 24a_0^3 \int r e^{-r/a_0} \bigg]$$

$$= \frac{2}{a_0^s} \left[-r^4 \, a . e^{-r/a_0} - 4r^3 a_0^2 \, e^{-r/a_0} - 12r^2 a_0^3 \, e^{-r/a_0} \right.$$

$$+ \frac{24a_0^3 \, r \, e^{-r/a_0}}{-1/a_0} - \frac{24a_0^3 \, e^{-r/a_0}}{-1/a_0 \times -1/a_0}$$

$$= \frac{2}{a_0^s} \left\{ e^{-r/1a_0} \left[-r^4 a_0 - 4r^3 a_0^2 - 12r^2 a_0^3 - 6a_0 \; 24 \, r \, a_0^4 - 24a_0^s \right] \right\} 3a_0$$

$$= \frac{2}{a_0^s} \left\{ e^{-6} [-(6)^4 a_0^s - 4(6)^3 a_0^s - 12(6)^2 a_0^s - 24(6) a_0^s - 24 a_0^s] \right.$$

$$+ [(3)^4 a_0^s + 4(3)^3 a_0^s + 12(3)^2 a_0^s + 24(3) a_0^s + 24 a_0^s] e^{-3} \}$$

$$= 2 \left\{ e^{-3} [81 + 108 + 108 + 72 + 24] - e^{-6} \right.$$

$$[1296 + 864 + 432 + 144 + 24] \}$$

$$P = 2[3a3e^{-3} - 2760 e^{-6}].$$

Q. 2. (*a*) (*i*) Set up the time dependent Schrodinger equation and hence derive the time independent Schrodinger equation. **(4)**

(*ii*) Starting with the Schrodinger equation in one dimension and using a de Broglie plane wave as a solution, show that when V = 0 this leads to the correct nonrelativistic relationship between energy and momentum. **(3)**

Ans. (*i*) Find this expression in this text book.

(*ii*) Schrodinger equation in 1 – D

$$\frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\, \psi(x) = E \psi(x) \qquad \qquad ...(1)$$

De Broglie plane wave solution = $\psi(x) = A\ \alpha bi (kx - wj)$

$$\frac{d^2 \psi}{dx^2} = i^2 k^2 A\, exb\ i\ (kx - wt) = i^2 k^2 \psi$$

Put in (1)

$$\frac{-\hbar^2}{2m} (i^2 k^2 \psi) + V\psi = E\psi \qquad \qquad [V = 0 \text{ (given)}]$$

So, $$\frac{-\hbar^2}{2m} i^2 k^2 \psi + V\psi = E\psi$$

$$E = \frac{-\hbar^2 k^2}{2m} \quad \Rightarrow \quad P = \hbar k$$

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

nonrelativistic relationship between energy and momentum.

(*b*) **For a Gaussian wave packet**

$$\psi(x) = A e^{\frac{x^2}{4\alpha^2}} e^{-i(k_0 x - w_0 t)}$$

corresponding to a free particle (*i*) Find the probability current density and (*ii*) Verify the continuity equation. (4 + 3)

Ans. Look at the Schrodinger equation for a free particle.

(*c*) (*i*) **Explain spreading of a Gaussian wave packet for a flee particle in one dimension.** (5)

(*ii*) **Calculate the fractional change in the width of the wave packet in one second if the wave packet corresponds to a particle of mass 6.644 × 10^{-27} Kg. The initial width being of the order of 10^{-19} m.** (2)

Ans. (*i*) This is also in the section dedicated to the Schrodinger of free particle.

(*ii*) $m = 6.644 \times 10^{-27}$ Kg.

If initial width is Δx, then width at time t is

$$\Delta x(t) = \Delta x_0 \sqrt{1 + \left(\frac{\delta x}{\Delta x_0}\right)^2}$$

$$\frac{\delta x}{\Delta x_0} = \frac{\hbar t}{2m(\Delta x_0)^2}$$

$$\frac{\Delta x(t)}{\Delta x_0} = \sqrt{1 + \left(\frac{\delta x}{\Delta x_0}\right)^2}$$

$$\frac{\delta x}{\Delta x_0} = \frac{h}{4\pi m(\Delta x_0)^2} = \frac{6.6 \times 10^{-34}}{4 \times 3.14 \times 6.6 \times 10^{-27} (10^{-10})^2}$$

$$= \frac{10^{13}}{4 \times 3.14} = \frac{10}{4 \times 3.14} \times 10^{12}$$

$$\frac{\Delta x(t)}{\Delta x_0} = \sqrt{1 + \left(\frac{10}{4 \times 3.14} \times 10^{12}\right)^2}$$

Q. 3. (*a*) **Write the Schrodinger equations for a linear Harmonic oscillator and solve it to obtain the energy eigen values.** (7)

Ans. Find its solution in the chapter portion of this textbook.

(b) (i) A Harmonic Oscillator has a wave functions which is a superposition of the ground state and the second excited state eigenfunctions $\psi(x) = \psi_0(x) + 2\psi_2(x)$. Find the expectation value of energy. **(3)**

(ii) Using the Uncertainty Principle show that the ground state energy for a Harmonic Oscillator is non-zero. **(4)**

Ans.
$$\psi(x) = \psi_0(x) + 2\psi_2(x)$$

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

normalize the wave function on

$$\psi(x) = \frac{1}{\sqrt{5}}\psi_0(x) + \frac{2}{\sqrt{5}}\psi_2(x)$$

$$<\psi|E|\psi> = \left\langle \left(\frac{\psi_0(x)}{5} + \frac{2\psi_2}{\sqrt{5}}\right)\middle|E\middle|\left(\frac{\psi_0}{\sqrt{5}} + \frac{2}{\sqrt{5}}\psi_0 1\right)\right\rangle$$

$$= \frac{1}{\sqrt{5}}\left[\psi_0 | + \frac{2}{\sqrt{5}} <\psi_0 |\right]\left[\left(0 + \frac{1}{2}\right)\hbar w \frac{1}{\sqrt{5}}|\psi_0 + \left(2 + \frac{1}{2}\right)\hbar w \frac{2}{\sqrt{5}}|\psi_2 >\right]$$

$$= \frac{1}{5}\times\frac{\hbar w}{2}<\psi_0|\psi_0> + \frac{4}{5}\times\frac{5}{2}\hbar w<\psi_2|\psi_2>$$

$$= \frac{\hbar w}{10} + 2\hbar w$$

$$<\psi|E|\psi> = \frac{21}{10}\hbar w$$

(ii) The ground state energy for the quantum harmonic oscillator can be shown to be shown to be minimum energy allowed by the uncertainty principle.

The energy of the quantum harmonic oscillator must be at least

$$E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Δx = position uncertainty

Δp = momentum uncertainty

Taking the lower limit from the uncertainty principle

$$\Delta x \Delta p = \frac{h}{2}$$

Then the energy expressed in terms of the position uncertainty can be written

$$E = \frac{h^2}{2} + \frac{1}{2}m\omega^2(\Delta x)^2$$

Minimizing this energy by taking the derivative with respect to the position uncertainty and setting it equal to zero gives

$$-\frac{\hbar^2}{4m(\Delta x)^3} + m\omega^2 \Delta x = 0$$

Solving for the position uncertainty gives

$$\Delta x = \sqrt{\frac{h}{2m\omega}}$$

Substituting gives the minimum value of energy allowed.

$$E_0 = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

This is a very significant physical result because it tells us that the energy of a system described by a harmonic oscillator potential cannot have zero energy. Physical system such as atoms in a solid lattice or in polyatomic molecules in a gas cannot have zero energy even at absolute zero temperature. The energy of the ground vibrational state is often referred to as "zero point vibration". The zero point energy is sufficient to prevent liquid helium-4 from freezing at atmospheric pressure, no matter how low the temperature.

(c) (i) An electron is confined in the ground state of a one-dimensional harmonic oscillator such that $\Delta x = 10^{-10}$m. Assuming that the average Kinetic energy is equal to the average Potential energy, find the energy is electron volts required to excite it to the first excited state. (4)

(ii) For a linear harmonic oscillator in its ground state, show that the probability of finding it beyond the classical limits is approximately 0.16. (3)

Ans. (i) Use the above relation and find out the energy difference between excited state according to the statement given in the question.

$$\Delta x = 10^{(-10)}\text{m}$$

$$<\text{K. E}> = <\text{P. E}> \qquad\qquad\text{[Given]}$$

From uncertainity principle

$$\Delta x \ \Delta P = \frac{\hbar}{2}$$

$$\Delta P = \frac{\hbar}{2\Delta x}$$

$$\text{K. E.} = \frac{(\Delta P)^2}{2m} = \frac{\hbar^2}{h\,m(\Delta x)^2} = \frac{h}{8\pi m(\Delta x)^2}$$

$$K.\,E. = \frac{6.60 \times 10^{-34}}{8 \times 3.14 \times 9.10 \times 10^{-31} \times 10^{-20}}$$

$$= \frac{6.6}{228.592} \times 10^{17} \text{ J}$$

$$= 0.02887 \times 10^{17} \text{J}$$

$$= 2.9 \times 10^{15} \text{J}$$

Since, K. E. = P. E.

So,   Total Energy = 2 × K. E

$$= 2 \times 2.9 \times 10^{15} \text{J}$$

$$E = 5.8 \times 10^{15} \text{J}$$

(ii) $\qquad E_0 = \frac{1}{2}\hbar w \qquad\qquad$ If Amplitude = A

$$E_0 = \frac{1}{2}mw^2 A^2$$

$$\frac{1}{2}mw^2 A^2 = \frac{1}{2}\hbar w$$

$$\psi = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}} \exp\left(-\frac{1}{2}\alpha^2 x^2\right)$$

P_{in} = Probability classical limit

$$= \int_{-A}^{A} \psi_0{}^* \psi_0 \, dx$$

$$= \frac{\alpha}{\sqrt{\pi}} \int_{-1/\alpha}^{1/\alpha} e^{-\alpha^2 x^2} dx$$

$$= y = \alpha x, \quad \alpha y = \alpha \, dx$$

$$= \frac{2\alpha}{\sqrt{\pi}} \int_{0}^{1/\alpha} e^{-y^2} dy$$

$$= \frac{2\alpha}{\sqrt{\pi}} \int_{0}^{1/2} \left[1 - y^2 + \frac{y^4}{2!} - \frac{y^6}{3!} + \ldots\ldots\right] dy$$

$$= 0.84$$
$$P_{out} = 1 - P_{in} = 1 - 0.84 = 0.16.$$

Q. 4. (a) (i) Obtain the solution for the Legendre equation

$$(1 - \xi^2)\frac{d^2P(\xi)}{d\xi^2} - 2\xi\frac{dP(\xi)}{d\xi} + \lambda P(\xi) = 0.$$

What are the conditions that need to be imposed so that the solution are well behaved ? What do the conditions imply. **(4)**

(ii) Verify whether the function $Y_{1,1}(\theta, \phi) = -\sqrt{\dfrac{3}{8\pi}} \sin\theta e^{i\theta}$ is an eigenstate of the following angular momentum operator :

$$\hat{L}_x = ih\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$ **(3)**

Ans. (i) First solution of legendre differential equation

$$y_1 = a_0\left[x^n - \frac{n(n-1)}{2(2n-1)}x^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2.4.(2n-1)(2n-3)}x^{n-4} + ...\right]$$

This is a terminating series also called legendre polynomial of nth order *i.e.*, $P_n(x)$

(*ii*) Second solution of lengendre differential equation

$$y_2 = a_1\left[x^{-n-1} + \frac{n(n+1)}{2(2n+3)}x^{-n-3} + ...\right]$$

This is a non-terminating series.

(*ii*) $$y_{1,1}(\theta, \phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\theta}$$

$$\hat{L}_x = ih\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_x\, y_{1,1}(\theta, \phi) = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\theta}\right)$$

$$\left[-\sqrt{\frac{3}{8\pi}}\sin\theta e^{i}\phi\right]$$

$$= i\hbar\left(-\sqrt{\frac{3}{8\pi}}\right)\left[\sin\phi\cos\theta e^{i\phi} + \cot\theta\cos\phi\sin\theta\, e^{i}\phi(i)\right]$$

$$= i\hbar\left(-\sqrt{\frac{3}{8\pi}}\right)\left[\sin\phi\,\cos\theta\,e^{i\phi} + i\,\cos\theta\,\cos\phi\,e^{i}\phi\right]$$

$$= i\hbar\left(-\sqrt{\frac{3}{8\pi}}\right)e^{i\phi} + \cos\theta\left[\sin\phi + i\,\cos\phi\right]$$

$$= i\hbar\left(-\sqrt{\frac{3}{8\pi}}\right)e^{i\phi} + \cos\theta\left[\cos\phi + i\,\sin\phi\right]$$

$$= -\hbar\left(-\sqrt{\frac{3}{8\pi}}\right)e^{i\phi}\,\cos\theta \times e^{-i\phi}$$

$$= -\hbar\,\cos\theta\left(-\sqrt{\frac{3}{8\pi}}\right)$$

So, given function is not a eigenstate of $\hat{L}_x$.

(b) Calculate $\left\langle V(r)\right\rangle = \dfrac{e^2}{4\pi\,\epsilon_0}\left\langle\dfrac{1}{r}\right\rangle$ for the first excited state of the hydrogen

atom with the wave function $\left[\psi_{210} = \dfrac{1}{\sqrt{\pi}}\left\{\dfrac{1}{2a_0}\right\}^{5/2} re^{-1/2a_0}\cos\theta\right]$. (7)

Ans. $\left\langle V\,(r)\right\rangle = \dfrac{-e^2}{4\pi\varepsilon_0}\left\langle\dfrac{1}{r}\right\rangle$

$$\psi_{210} = \dfrac{1}{\sqrt{\pi}}\left\{\dfrac{1}{2a_0}\right\}^{5/2} re^{-r/2a_0}\cos\theta$$

$$\left\langle V\,(r)\right\rangle = \int\dfrac{1}{\pi}\left(\dfrac{1}{2a_0}\right)^{s} r^7 e^{-r/a_0}\cos^2\theta\,\dfrac{1}{r}\,dv$$

$$= \dfrac{1}{\pi}\left(\dfrac{1}{2a_0}\right)^{s}\iiint re^{-r/a_0}\cos^2\theta\left[r^2\sin\phi\,dr d\theta d\phi\right]$$

$$= \frac{1}{\pi} \left(\frac{1}{2a_0} \right)^s \int_0^\pi \int_0^{2\pi} \int_{-\infty}^\infty r^3 \, e^{-r/a_0} \, dr \cos^2 \theta \, d\theta \, \sin \phi \, d\phi$$

$$= \frac{1}{\pi} \times \frac{1}{32a_0 s} \times 2\pi \int r^3 e^{-r/a_0} \, dr$$

$$= \frac{1}{16a_0^s} \int_{-\infty}^\infty r^3 \, e^{-r/a_0} \, dr$$

Solve by parts (same as Q. 1. (g)

$$\langle V(r) \rangle = \frac{-e^2}{4\pi\varepsilon_0} \times \frac{1}{(2)^2 a_0} = \frac{-e^2}{4\pi\varepsilon_0} \times \frac{1}{4a_0}$$

(c) The electron in the hydrogen atom is replaced by a muon of mass $m_\mu = 200 m_e$, where m_e is the mass of the electron. Determine the corresponding changes in the following :

(i) The Larmor frequency and hence the Zeeman splitting for the 2p level in the presence of a magnetic field of 1 Tesla. (Ignore the electron spin)

(ii) The wavelength of the corresponding H$_\alpha$ line. Will it be in the visible region ? (Rydberg constant R = 1.097 × 10^7 m^{-1} for the hydrogen atom) (3 + 4)

Ans. (i) $\qquad\qquad m_\mu = 200 \, m_e$

$$w_L \text{ or } e = \frac{e \, B}{\alpha \, m_e}$$

For muan charge is some, $m_\mu = 200 \, m_e$

So, $\qquad\qquad w_L = \dfrac{e \, B}{2 \times 200 \times m_e}$

$$w_L = \frac{e}{400 \, m_e}$$

$2P \rightarrow \quad l = 1 \qquad \Rightarrow \quad (2l+1) = 3$

So, this will split into three components

$$m_l = -1, 0, +1$$

(ii) $\qquad\qquad \lambda = \dfrac{c}{v} = \dfrac{2\pi c}{2\pi v} = \dfrac{2\pi c}{w}$

$$\lambda = \frac{2 \times 3.14 \times 3 \times 10^8}{1.6 \times 10^{-19}} \times 400 \times 9.1 \times 10^{-31}$$

$$= \frac{685.776 \times 10^{-21}}{1.6 \times 10^{-19}}$$

$$= 428.61 \times 10^{-2}$$

$$= 4.2861 \text{ m}$$

No, + S not belong to visible region.

Q. 5. (a) Consider a particle trapped inside a one dimensional finite square well. Solve time independent Schrodinger equation for the system and obtain the bound state eigenfunctions. Discuss how the energy levels are obtained graphically. (7)
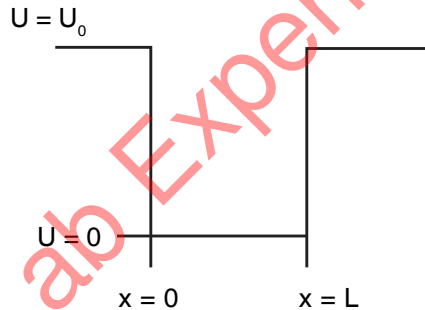
Ans. Consider the following piecewise continuous, finite potential energy :

$$U = U_0 \qquad\qquad x < 0 \qquad\qquad (1)$$
$$U = 0 \qquad\qquad 0 \leq x \leq L \qquad\qquad (2)$$
$$U = U_0 \qquad\qquad L < x \qquad\qquad (3)$$

We want to solve Schroedinger's Equation for this potential to get the wavefunctions and allowed energies for $E < U_0$. I will refer to the three regions as regions 0, 1, and 2 with associated wavefunctions ψ_0, ψ_1, ψ_2.

The time-invariant, non-relativistic Schroedinger's equation is

$$\frac{-h^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi \qquad\qquad (4)$$

that can be rearranged to give

$$\frac{d^2\psi}{dx^2} = \frac{2m}{h^2} (U - E)\psi \qquad\qquad (5)$$

It is convenient to define two new variables (both positive), one for regious 0 and 2, and one for region 1—they are wavenumbers :

$$k_0^2 = \frac{2m}{h^2}(U_0 - E) \qquad\qquad (6)$$

$$k_1^2 = \frac{2m}{h^2} E \tag{7}$$

and Schroedinger's equation becomes

$$\frac{d^2\psi_{0,2}}{dx^2} = k_0^2\psi_{0,2} \qquad x < 0 \text{ or } L < x \tag{8}$$

$$\frac{d^2\psi_1}{dx^2} = -k_1^2\psi_1 \qquad 0 < x < L \tag{9}$$

In regions 0 and 2 the general solution is a linear combination of exponentials with the same form, but with different constant, namely

$$\psi_0 = A \exp(-k_0 x) + B \exp(+k_0 x) \qquad x < 0 \tag{10}$$
$$\psi_2 = F \exp(-k_0 x) + G \exp(+k_0 x) \qquad L < x \tag{11}$$

In region I we have the same general solution that we had for the infinite square well,

$$\psi_1 = C \sin(k_1 x) + D \cos(k_1 x) \qquad 0 < x < L \tag{12}$$

Equations (10) to (12) have 7 unknowns A, B, C, D, E, F and the energy E that is implicitly contained in the variables k_0, k_1. Therefore we need to get 7 equations to be able to solve for the unknowns.

We will first use the requirement that the wavefunction remain finite everywhere. Consider ψ_2 as $x \rightarrow \infty$. For this to remain finite we must require $G-0$. Similarly, as $x \rightarrow \infty$, we require $A = 0$. Our solution become

$$\psi_0 = B \exp(+k_0 x) \qquad x < 0 \tag{13}$$
$$\psi_2 = F \exp(-k_0 x) \qquad L < x \tag{14}$$

The next step is to require that the wavefunction and its first derivative be continuous everywhere, and in our case we look at the boundaries, $x = 0$ and $x = L$.

$$\psi_0(0) = \psi_1(0)$$
$$B = D \tag{15}$$

Hence $\qquad\qquad\qquad \psi_0 = D \exp(+k_0 x).$

Take derivatives of the wavefunctions,

$$\frac{d\psi_0}{dx} = k_0 D \exp(k_0 x) \tag{16}$$

$$\frac{d\psi_1}{dx} = k_1 C \cos(k_1 x) - k_1 D \sin(k_1 x) \tag{17}$$

$$\frac{d\psi_2}{dx} = -k_0 F \exp(-k_0 x) \tag{18}$$

and at $x = 0$ we get

$$\frac{\psi_0}{dx}(0) = \frac{d\psi_1}{dx}(0)$$

$$k_0 D = k_1 C \tag{19}$$

So

$$\psi_1 = \frac{k_0}{k_1} D \sin(k_1 x) + D \cos(k_1 x) \tag{20}$$

$$\frac{d\psi_1}{dx} = k_0 D \cos(k_1 x) - k_1 D \sin(k_1 x) \tag{21}$$

There remain 3 unknows, D, F, and E. Finding them is a bit messier! Consider the boundary conditions at $x = L$,

$$\psi_1(L) = \psi_2(L)$$

$$\frac{k_0}{k_1} D \sin(k_1 L) + \cos(k_1 L) = F \exp(-k_0 L) \tag{22}$$

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

$$k_0 D \cos(k_1 L) - k_1 D \sin(k_1 L) = k_0 F \exp(-k_0 L) \tag{23}$$

We are not going much farther, but if we divided Equation (22) by equation (23), we can see that the constants D and F cancel leaving us with one rather ugly equation to solve for energy E (remember this is implicitly included in the value of k_1 and k_0.) The solution must be done numerically, and is left for other course. At the end of this document the next steps are shown.

How can we get the remaining constant? There is one remaining condition, normalization, that for this problem is

$$\int_{-\infty}^{0} \psi_0^2 \, dx + \int_{0}^{L} \psi_1^2 \, dx + \int_{L}^{\infty} \psi_2^2 \, dx = 1 \tag{24}$$

Even without solving the entire problem we can make some conclusions about the wave-function and the allowed energy levels. Recall that for an infinite square well potential of width L the allowed energies are quantized and

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

with n being any positive integer. Outside the well the wavefunction is 0. We are certain that the particle is somewhere inside the box, so $\Delta x^{\infty} - L$.

With the finite well, the wavefunction is not zero outside the well, $\Delta x^{\text{finite}} > L$, hence from the uncertainty principle, $\Delta px^{\text{finite}} < \Delta px^{\infty}$. This suggests that the average value of momentum is less for the finite well, and therefore that the kinetic energy inside the well is less for the finite well than for the infinite well. Indeed this is borne out with detailed analysis. In addition, the number of allowed energy levels

is finite, and there is a possibility that a well may be sufficiently narrow or sufficiently shallow that no energy levels are allowed.

Also note that the non-zero wavefunction in regions 0 and 2 mean that there is a non-zero probability of finding the particle in a region that is classically forbidden, a region where the total energy is less than the potential energy so that the kinetic energy is negative. We will have more to say about this later when we discuss quantum mechanical tunneling.

(b) (i) Derive the relationship between magnetic dipole moment and orbital angular momentum of an electron revolving around a nucleus. **(3)**

(ii) Explain space quantization. Calculate the possible orientation of the total angular momentum vector J corresponding to $j = 3/2$ with respect to a magnetic field along the z-axis. **(4)**

Ans. Imagine a particle with mass M and charge q moving in a circle of radius R with speed v. Treating the motion of this particle classically, with speed much less than the speed of light, the orbital angular momentum of the particle is L = MvR. The time for the particle to make one revolution is T = 2πR/v, so the circular current represented by this moving charge is $i = q/T = qv/(2πR)$. The magnetic moment generated by this circular current is the current times the area of the circle, or $m = iA = i\pi R^2$. The ratio of the magnetic moment to the angular momentum of the particle

$$\gamma = \frac{m}{L} = \frac{q}{2M}$$

is called the gyromagnetic ratio.

(c) (i) What is Larmor Precession ? Derive the expression for Lannor frequency. **(4)**

(ii) A beam electron enters a uniform magnetic field of flux density 1.2 tesla. Calculate the energy difference between electrons whose spins are parallel and antiparallel to the field. **(3)**

Ans. (i) Find the solution to this question in the text book.

(ii) $\quad \Delta E = E(ms = 1/2) - E(ms = -1/2)$

$$= mB\,Bg = \frac{g\,B\,e\,h}{4\pi m}$$

$$= 1.2$$

$$\Delta E = \frac{1.2 \times 1.6 \times 10^{-19} \times 6.6 \times 10^{-34}}{4 \times 3.14 \times 9.1 \times 10^{-31}}\,g$$

$$= \frac{12.672}{114.296} \times 10^{-22}\,g$$

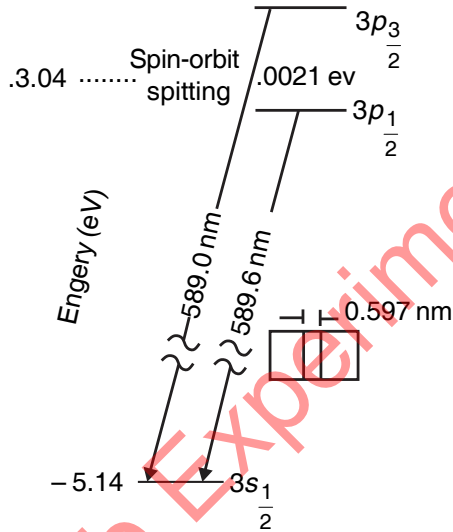$$= 1.1 \times 10^{-23}g.$$

Q. 6. (*a*) (*i*) Explain Normal Zeeman Effect. **(2)**

(*ii*) **Write the term diagram for the splitting of the yellow line of sodium $(1s^2, 2s^2, 2p^6)3s^1$ into two components D1 and D2.** **(2)**

(*iii*) **In a Stern-Gerlach experiment, a beam of hydrogen atom with velocity 3×10^3 m/s, passes through an inhomogeneous magnetic field of length 50 cm and having gradient of 200 T/m perpendicular to the direction of the incident beam. Find out the transverse deflection of the atoms at the point where the beam leaves the field. (Bohr magneton 9.24×10^{-24} J/T, M = 1.67×10^{-27} kg).** **(3)**

Ans. (*i*) Find its solution in this text book.

(*ii*)

(*iii*)

$$V = 3 \times 10^3 \text{ m/s}, \qquad l = 50 \text{ cm}$$
$$\mu_B = 9.24 \times 10^{-24}, \qquad M = 1.67 \times 10^{-27} \text{ kg}$$

$$\frac{dB}{dz} = 200 \text{ T/m}$$

$$F_z = \mu \cos\theta \, \frac{dB}{dz}$$

$$F_z = \mu z \frac{dB}{dz}$$

$$\mu_z = -g_s \frac{e}{2m} S = -g_s \frac{e}{2m} m_s \hbar$$

So,
$$F_z = -g_s \frac{e}{2m} m_s \hbar \frac{dB}{dz}$$

$$= \frac{1.6 \times 10^{-19} \times 6.6 \times 10^{-34}}{4 \times 3.14 \times 9.1 \times 10^{-31}} \times 200 = 1.85 \times 10^{-21}$$

$$D = \frac{1}{2} a J^2$$

$$= \frac{1}{2} \left(\frac{F_z}{m_H} \right) \left(\frac{L}{V} \right)^2$$

$$= \frac{1}{2} \left(\frac{1.85 \times 10^{-21}}{1.67 \times 10^{-27}} \right) \left(\frac{0.5}{3 \times 10^3} \right)^2$$

$$= 0.54 \times 10^6 \times \frac{0.25}{9 \times 10^6}$$

$$= 0.01511 \text{ m} = 1.5 \text{ cm}$$

Total = 2D = 2 × 1.5 = 3 cm

(*b*) (*i*) **Write down the normal electronic configuration of Carbon atom (Z = 6) and obtain the spectral terms arising from equivalent electrons.** (4)
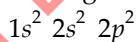
(*ii*) **The quantum number of two optical electrons in a two valence electron atom are**

$$n_1 = 6, \quad 1_1 = 3, \quad s_1 = 1/2$$
$$n_2 = 5, \quad 1_2 = 3, \quad s_2 = 1/2$$

assuming *j-j* coupling, find the possible values of J. (3)

Ans. (*i*) Electronic configuration of Carbon atom (Z = 6)

$$1s^2 \; 2s^2 \; 2p^2$$

So, Angular momentum is determined by two 2*p* electron two electrons hair spin 1/2 so, after coupling

Total spin $\Rightarrow$ S = 0, S = 1

Two individual coupling of *l* = 1, yields

L = 0, 1 or 2

But from principle total wavefunction has to be antisymmetric. So, spin and orbital parts have opposite symmetrics.

$$S = 0 \; \rightarrow \; \text{Antisymmetric}, \quad S = 1 \rightarrow = \text{Symmetric}$$
$$L = 1 \; \rightarrow \; \text{Antisymmetric}, \quad L = 2, 0 \rightarrow \text{Symmetric}$$
$$\text{States} = {}^1S0, \; {}^3P0, \; {}^3P1 \; \text{ or } {}^1D2.$$

The one which has lowest energy will be ground state of carbon.

According to Hund's rule, $S = 1$, $L = 1$

So, $J = 0, 1, 2$ [L – S to L + S)

Since $2p$ shell is less than half filled

$$J = 0$$

So, $3P0 \rightarrow$ Lowest energy $\rightarrow$ spectral term.

(**ii**) $n_1 = 6$, $l_1 = 3$, $s_1 = 1/2$

$n_2 = 5$, $l_2 = 1$, $s_2 = 1/2$

$$J_1 = l_1 + s_1 = 3 + \frac{1}{2} = \frac{7}{2}$$

$$J_2 = l_2 + s_2 = 1 + \frac{1}{2} = \frac{3}{2}$$

$$J = \left|J_1 - J_2\right| ....\left|J_1 + J_2\right|$$

$$= \left|\frac{7}{2} - \frac{3}{2}\right| ....\left|\frac{7}{2} + \frac{3}{2}\right|$$

$$= 2, ... 5$$

$J = 2, 3, 4, 5 \rightarrow$ Possible value of J.

(**c**) (**i**) **What is spin orbit coupling. Calculates the change in the energy level due to this.** **(5)**

(**ii**) **Write the term symbol for the ground state of the hydrogen atom in the LS coupling scheme.** **(2)**

Ans. (**i**) **Spin Orbit Coupling :** When we consider the splitting of structural lines due to an interaction between the magnetic moments due to spin and the orbit motion of the electron, the effect is called spin orbit coupling.

• Consider hydrogen atom with atomic namber z, moving in a arcular orbit of radius with speed varound nucleus.

$$I = \frac{ze}{\dfrac{2\pi r}{v}} = \frac{zev}{2\pi r}$$

$$\text{Magnetic field} = B = \frac{\mu_0 I}{2r} = \frac{\mu_0 zev}{4\pi r^2}$$

$$\overrightarrow{B}_{(\text{Vector})} = \frac{\mu_0 ze}{4\pi m r^2} (\overrightarrow{r} \times \overrightarrow{p}) \qquad\qquad [P = mv]$$

$$\vec{B} = \frac{ze}{4\pi\varepsilon_0 mc^2 r^3} \vec{L} \qquad \begin{bmatrix} \vec{L} = \vec{r} \times \vec{p} \\ \& \ \mu_0 = \frac{1}{\varepsilon_0 c^2} \end{bmatrix}$$

μ_s = magnetic moment due to spin then

$$H_{spin} - orbit = \frac{-1}{2}\vec{\mu}_s \cdot \vec{B}$$

Put $\qquad\qquad \mu_s = \frac{-ge}{2m}\vec{S}$

$$H_{spin} - orbit = \frac{-1}{2}\left(\frac{-g\,e\,\vec{S}}{2m}\right) \cdot \vec{B}$$

$$H_{spin} - orbit = \frac{-z\,e^2}{8\pi\varepsilon_0\,m^2 c^2 r^3}\vec{L} \cdot \vec{S}$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$J^2 = \vec{J} \cdot \vec{J} = L^2 + S^2\ 2\vec{L} \cdot \vec{S}$$

$$\vec{L} \cdot \vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$$

$$E_{spin} - orbit = <H_{spin} - orbit)$$

$$= \frac{z\,e^2}{16\pi\varepsilon_0\,m^2 c^2}\left\langle \frac{J^2 - L^2 - S^2}{r^3} \right\rangle$$

where, $\left\langle \dfrac{J^2 - L^2 - S^2}{r^3} \right\rangle = \left[\displaystyle\int \psi^*_{nij}\left(\frac{J^2 - L^2 - S^2}{2}\right)^{\psi_{nis}} dv\right]$

Eigen value of J^2, L^2, and S^2 are $J\,(J + U\,h^2$, $(L\,(L + 1)h^2$ and $S\,(S + 1)\,h^2$

$$S = \frac{1}{2}, \ So, \ S(S + 1)^2\hbar^2 = \frac{3}{4}\hbar^2$$

So, $$E_{spin} - orbit = \frac{z\,e^2\,\hbar^2}{16\pi\varepsilon_0 m^2\,c^2 r^3}\left[J(J+1) - l(l+1) - \frac{3}{4}\right]\left\langle\frac{1}{r^3}\right\rangle$$

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{z^3}{a_0^3 n^3 l\left(l+\frac{1}{2}\right)(l+1)}$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

$$E_{spin} - orbit = \frac{mc^2\,z^4\,\alpha^4}{2n^3\,(l+1)\,(2l+1)} \qquad \text{For } J = l + \frac{1}{2}$$

$$= \frac{mc^2 z^4 \alpha^4}{2n^3\,l\,(2l+1)} \qquad \text{For } J = l - \frac{1}{2}$$

(*ii*) Term symbol for hydorgen (H2) in LS cauplying scheme :

$$2P_{3/2} \ \& \ 2P_{1/2} \qquad\qquad l = 1, S = 1/2$$

$$J = \frac{3}{2}, \frac{1}{2} \qquad\qquad J = l + S, l - S$$

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